Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:31 AM UTC

PDB ID	:	6PNJ / pdb_00006pnj
EMDB ID	:	EMD-20397
Title	:	Structure of Photosystem I Acclimated to Far-red Light
Authors	:	Gisriel, C.J.; Shen, G.; Kurashov, V.; Ho, M.; Zhang, S.; Williams, D.; Golbeck, J.H.; Fromme, P.; Bryant, D.A.
Deposited on	:	2019-07-02
Resolution	:	3.19 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

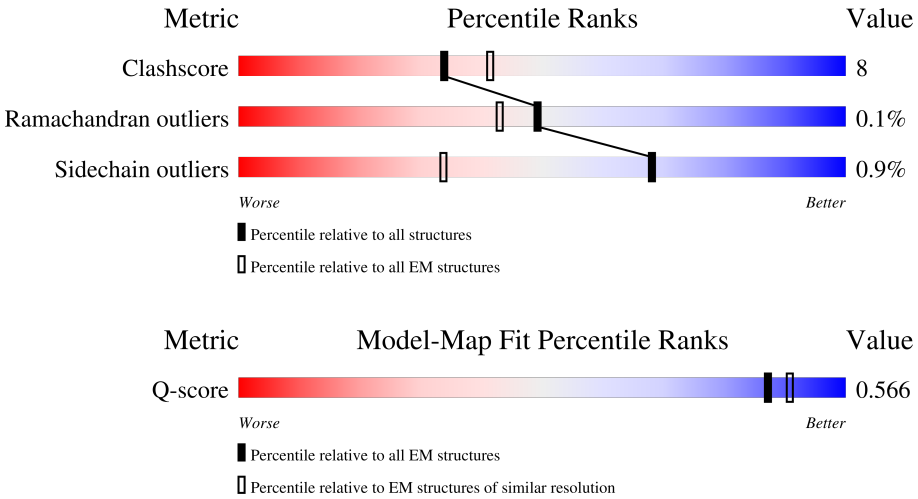
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.19 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14455 (2.69 - 3.69)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7% 79% 15% 5%
1	G	788	7% 79% 16% 5%
1	a	788	7% 79% 16% 5%
2	B	741	5% 83% 17%

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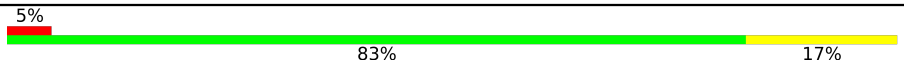
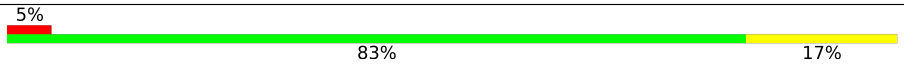
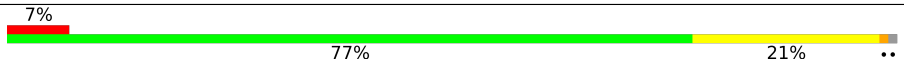
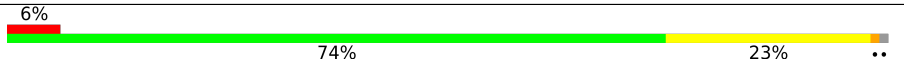
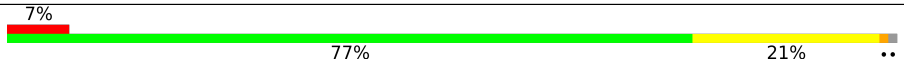
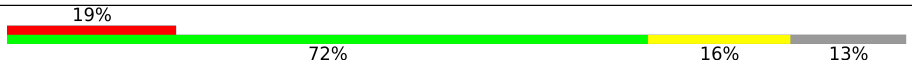
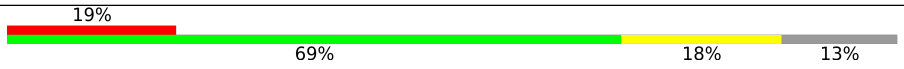
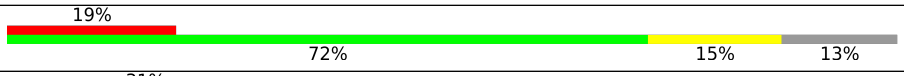
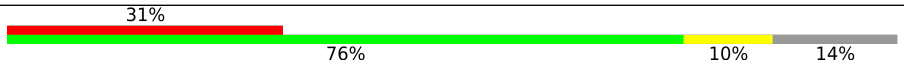
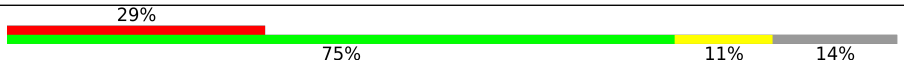
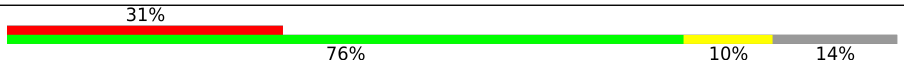
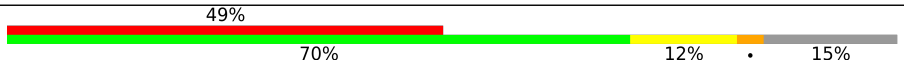
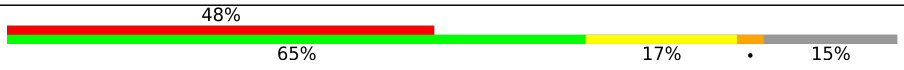
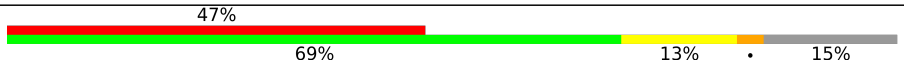
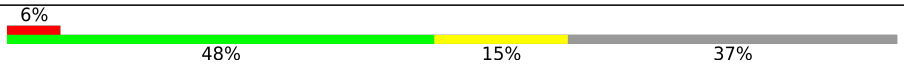
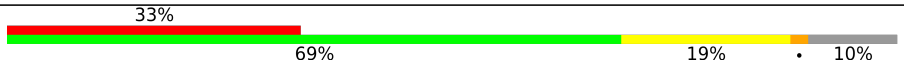
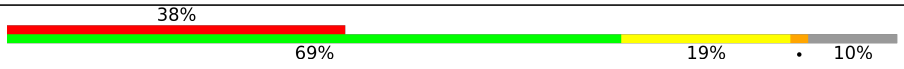
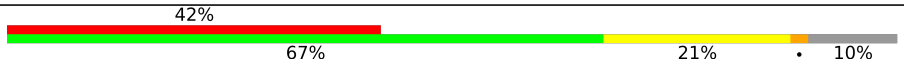
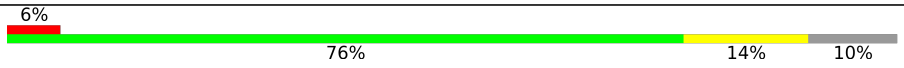
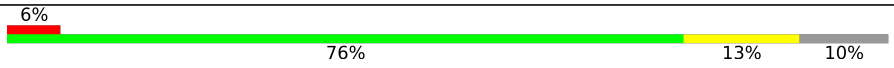
Mol	Chain	Length	Quality of chain
2	H	741	
2	b	741	
3	C	81	
3	N	81	
3	c	81	
4	D	159	
4	O	159	
4	d	159	
5	E	72	
5	P	72	
5	e	72	
6	F	159	
6	Q	159	
6	f	159	
7	I	67	
7	R	67	
7	i	67	
8	J	48	
8	S	48	
8	j	48	
9	K	39	
9	T	39	
9	k	39	
10	L	174	
10	U	174	

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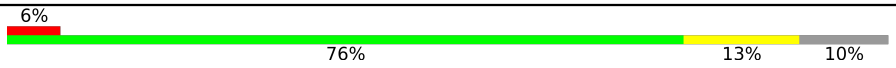
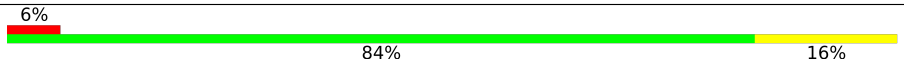
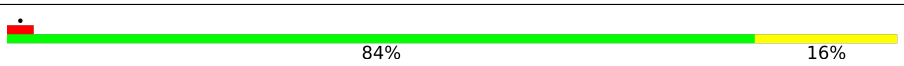
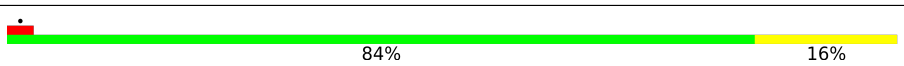
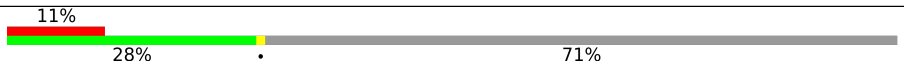
Mol	Chain	Length	Quality of chain
10	l	174	
11	M	31	
11	V	31	
11	m	31	
12	W	101	
12	X	101	
12	x	101	

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	1122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	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	1207	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	1238	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	1012	X	-	-	-
14	CLA	H	1021	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	1207	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
14	CLA	H	1236	X	-	-	-
14	CLA	H	1238	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	1122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	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	1207	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	1238	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	-	-	-
15	F6C	A	1120	X	-	-	-
15	F6C	A	1121	X	-	-	-
15	F6C	B	1230	X	-	-	-
15	F6C	B	1237	X	-	-	-
15	F6C	G	1120	X	-	-	-
15	F6C	G	1121	X	-	-	-
15	F6C	H	1230	X	-	-	-
15	F6C	H	1237	X	-	-	-
15	F6C	a	1120	X	-	-	-
15	F6C	a	1121	X	-	-	-
15	F6C	b	1230	X	-	-	-
15	F6C	b	1237	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 71511 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	747	Total	C	N	O	S	0	0
			5906	3877	1008	988	33		
1	G	747	Total	C	N	O	S	0	0
			5906	3877	1008	988	33		
1	a	747	Total	C	N	O	S	0	0
			5906	3877	1008	988	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	738	Total	C	N	O	S	0	0
			5909	3894	996	1001	18		
2	H	738	Total	C	N	O	S	0	0
			5909	3894	996	1001	18		
2	b	738	Total	C	N	O	S	0	0
			5909	3894	996	1001	18		

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	MET	-	initiating methionine	UNP A0A2N6MR25
R	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	J	43	Total	C	N	O	0	0
			344	238	51	55		
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		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	34	Total	C	N	O	S	0	0
			201	130	36	34	1		
9	T	34	Total	C	N	O	S	0	0
			201	130	36	34	1		
9	k	34	Total	C	N	O	S	0	0
			201	130	36	34	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	156	Total	C	N	O	S	0	0
			1172	760	198	209	5		
10	U	156	Total	C	N	O	S	0	0
			1172	760	198	209	5		
10	l	156	Total	C	N	O	S	0	0
			1172	760	198	209	5		

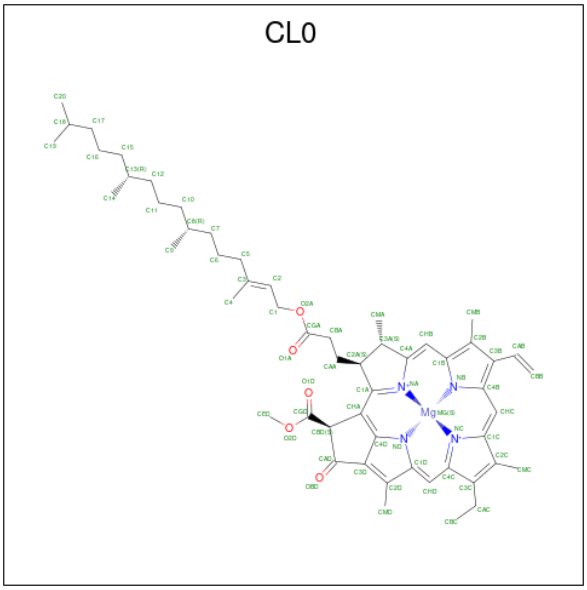
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 12 is a protein called Photosystem one PsaX.

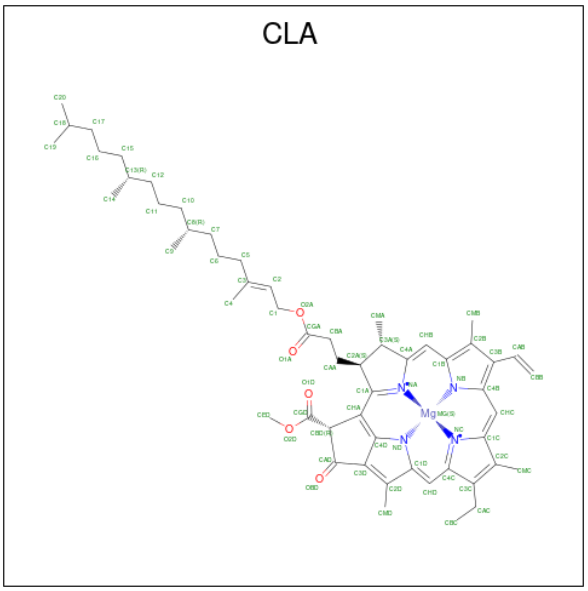
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total 246	C 172	N 36	O 38	0	0
12	X	29	Total 246	C 172	N 36	O 38	0	0
12	x	29	Total 246	C 172	N 36	O 38	0	0

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



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

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



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

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

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

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

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

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

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

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

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

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

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

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

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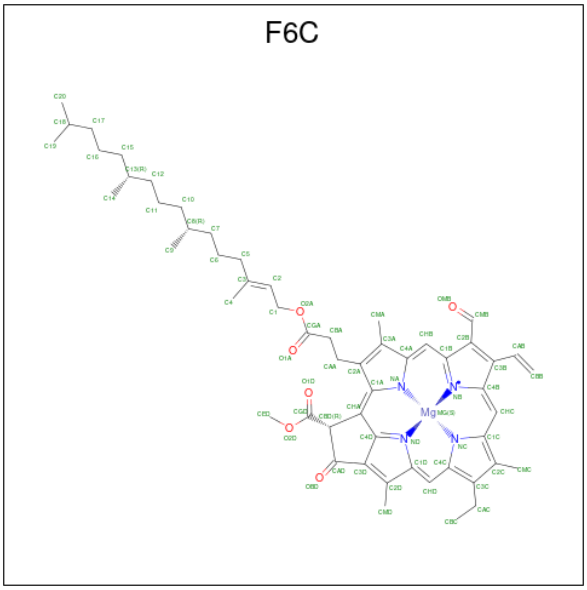
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	x	1	Total	C	Mg	N	O	0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

- Molecule 15 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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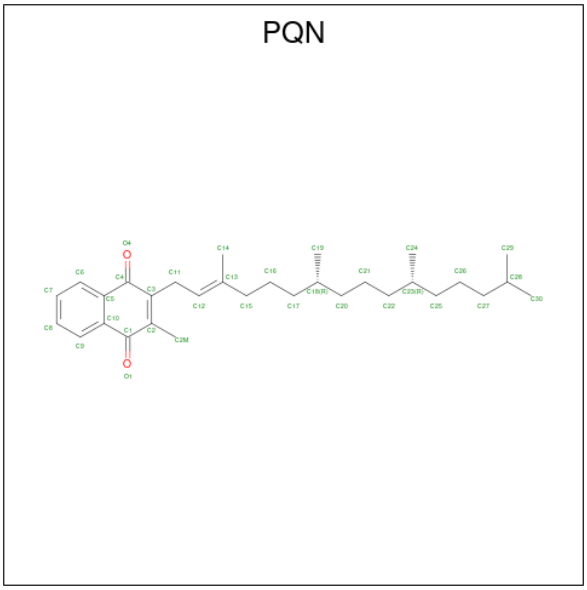
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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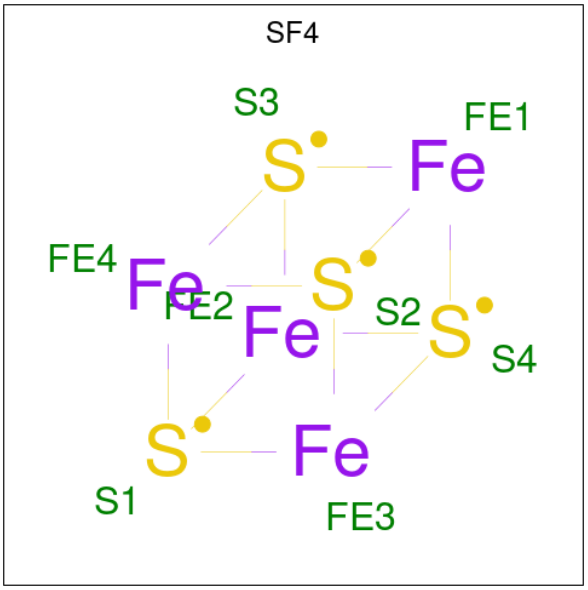
Mol	Chain	Residues	Atoms	AltConf
16	H	1	Total C O 33 31 2	0
16	a	1	Total C O 33 31 2	0
16	b	1	Total C O 33 31 2	0

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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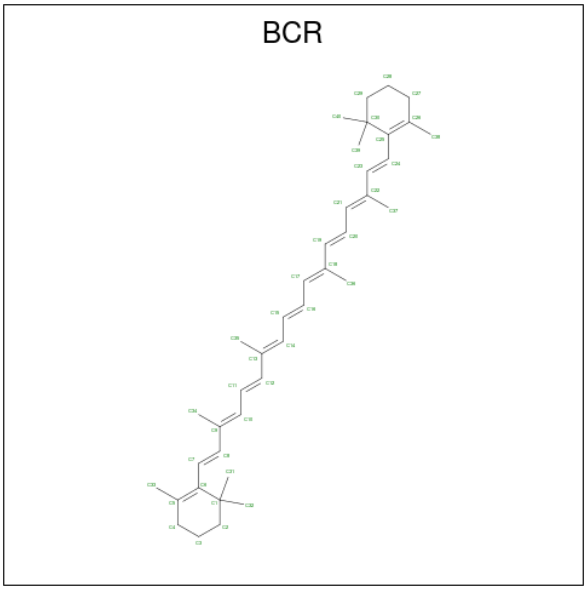
Mol	Chain	Residues	Atoms	AltConf
17	c	1	Total Fe S 8 4 4	0

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms	AltConf
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	B	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	G	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0
18	H	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	H	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	M	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	R	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

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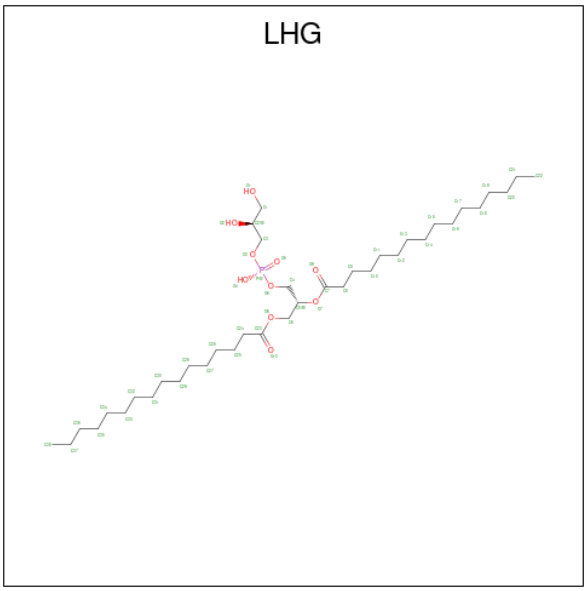
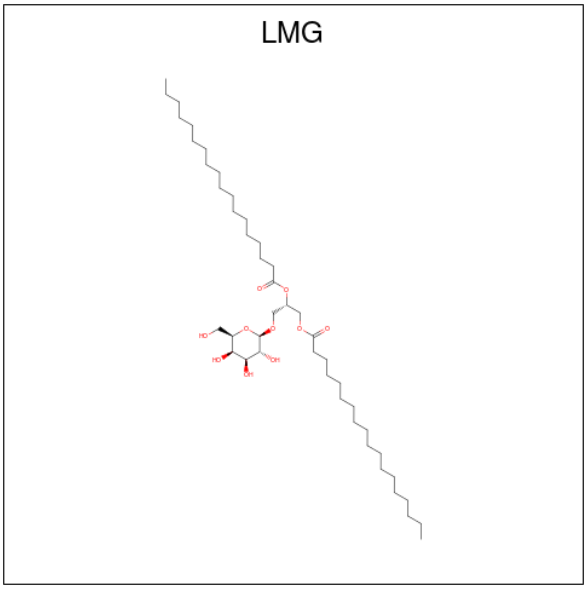
Mol	Chain	Residues	Atoms	AltConf
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	m	1	Total C 40 40	0

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



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

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			46	36	10	
20	B	1	Total	C	O	0
			46	36	10	
20	G	1	Total	C	O	0
			46	36	10	
20	H	1	Total	C	O	0
			46	36	10	
20	I	1	Total	C	O	0
			37	27	10	

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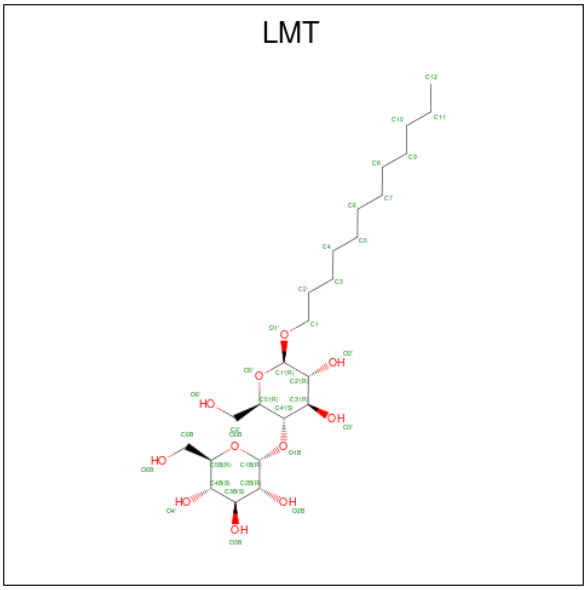
Mol	Chain	Residues	Atoms	AltConf
20	L	1	Total C O 50 40 10	0
20	R	1	Total C O 37 27 10	0
20	U	1	Total C O 50 40 10	0
20	a	1	Total C O 46 36 10	0
20	b	1	Total C O 46 36 10	0
20	i	1	Total C O 37 27 10	0
20	l	1	Total C O 50 40 10	0

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C O 31 20 11	0
21	A	1	Total C O 28 17 11	0
21	G	1	Total C O 31 20 11	0
21	G	1	Total C O 28 17 11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C O 31 20 11	0
21	a	1	Total C O 28 17 11	0

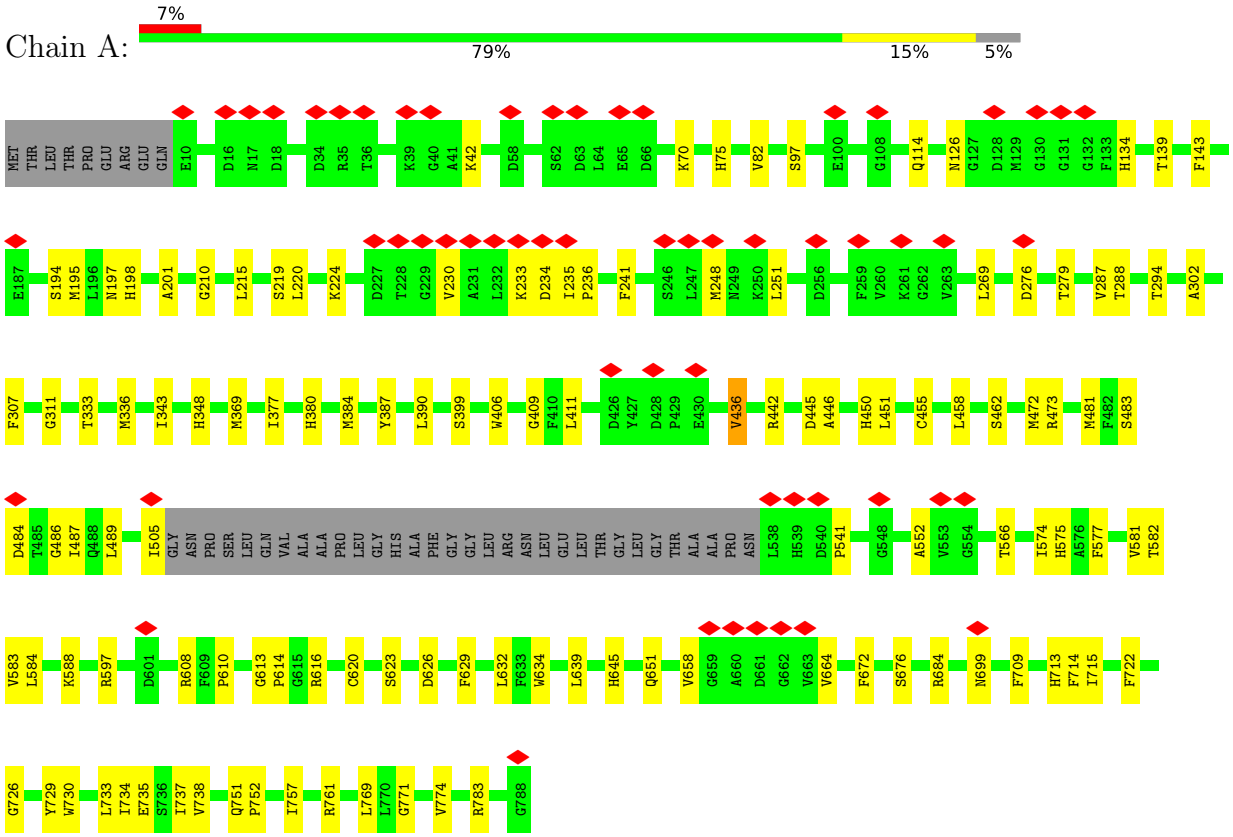
- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

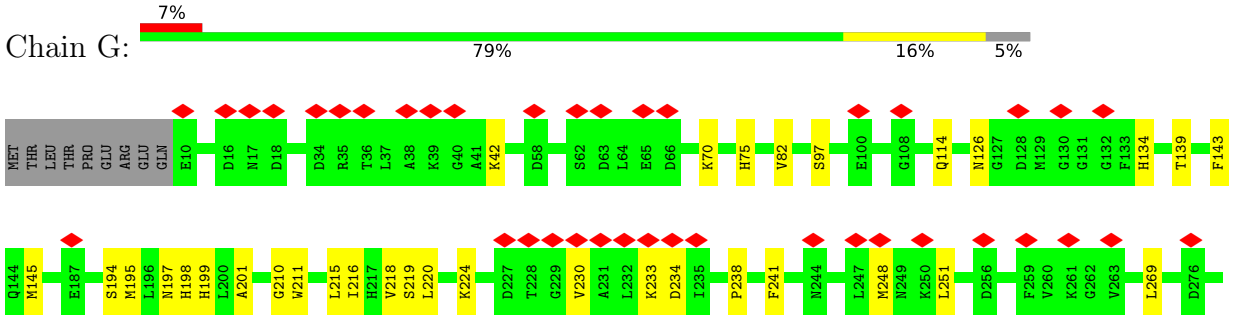
3 Residue-property plots (i)

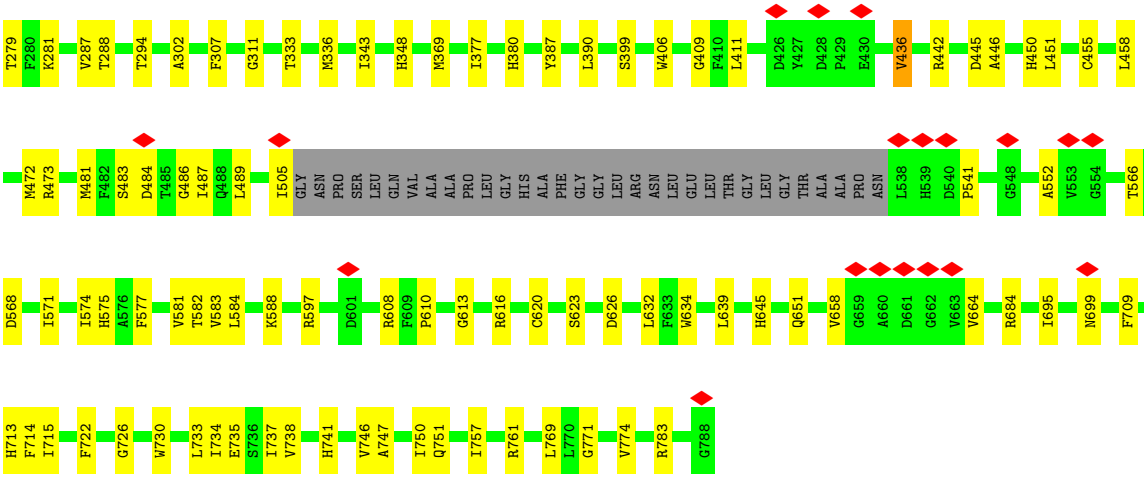
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



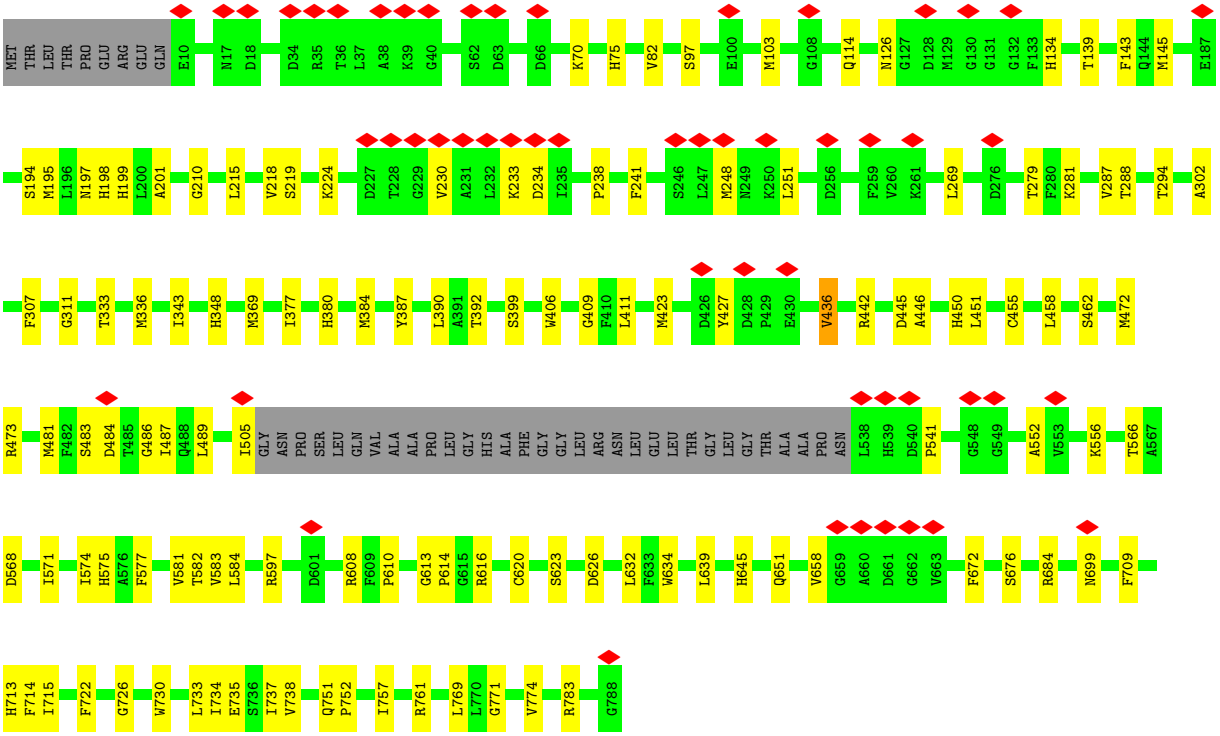
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





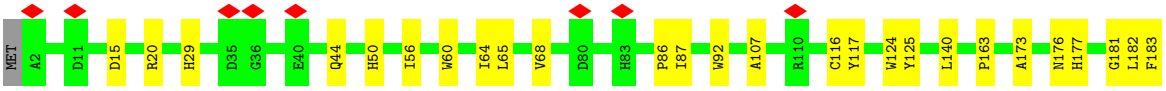
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

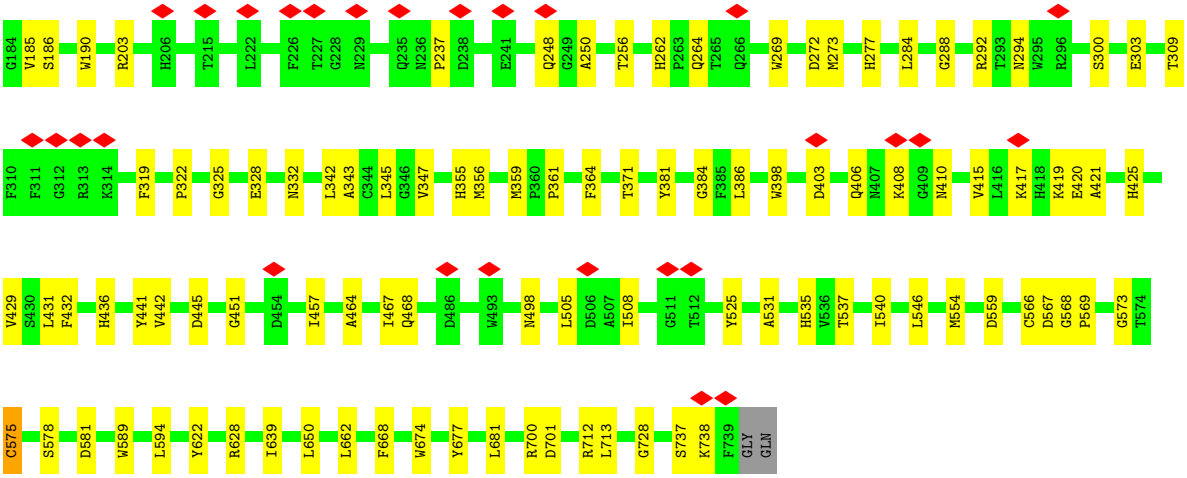
Chain a:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

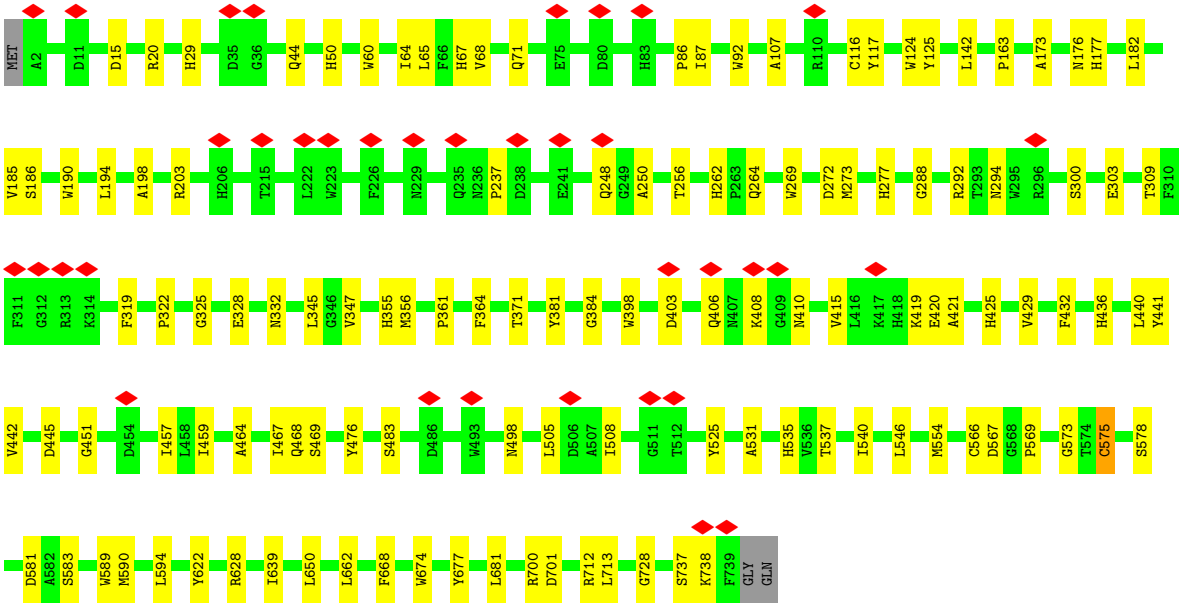
Chain B:





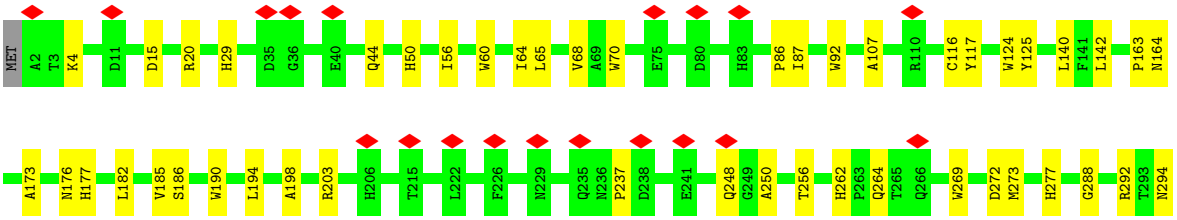
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

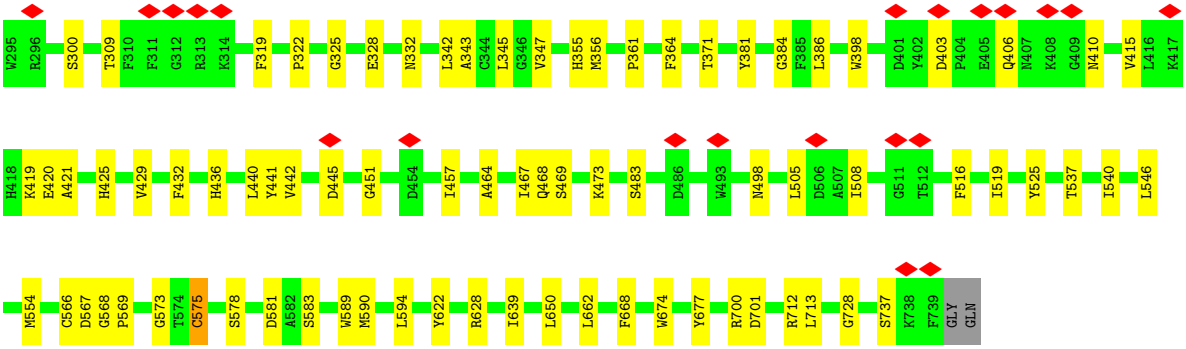
Chain H:



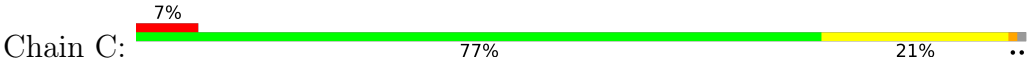
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

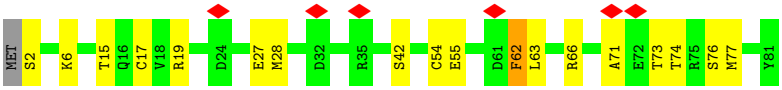
Chain b:



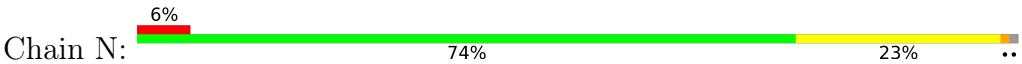


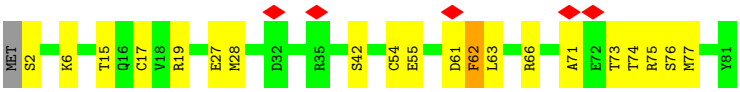
• Molecule 3: Photosystem I iron-sulfur center



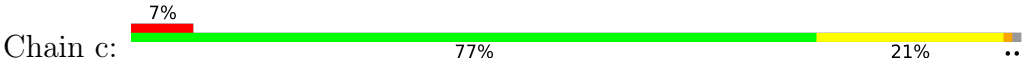


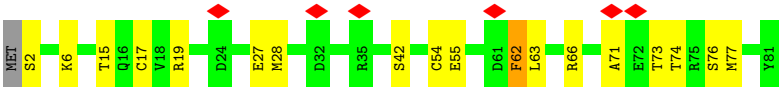
• Molecule 3: Photosystem I iron-sulfur center



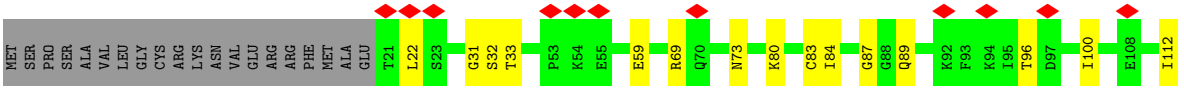


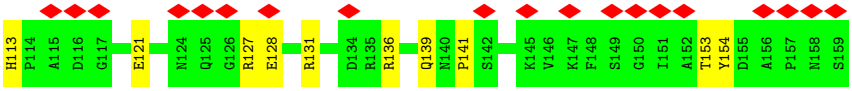
• Molecule 3: Photosystem I iron-sulfur center



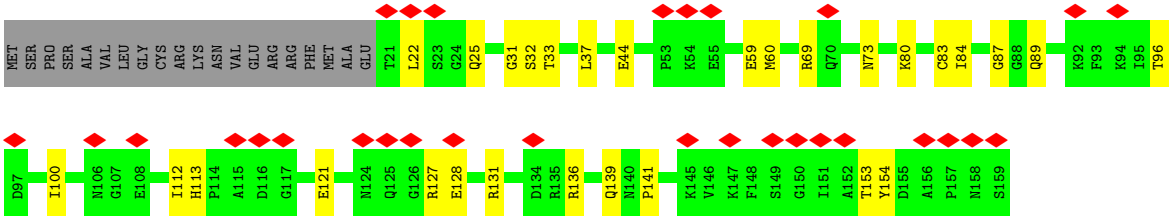


• Molecule 4: Photosystem I protein PsaD



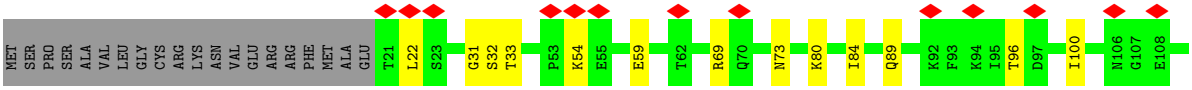


• Molecule 4: Photosystem I protein PsaD



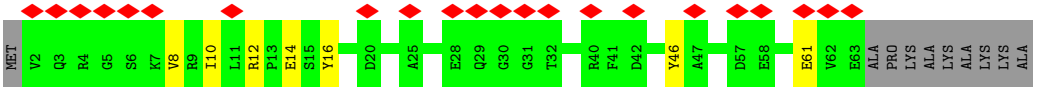
• Molecule 4: Photosystem I protein PsaD

Chain d:



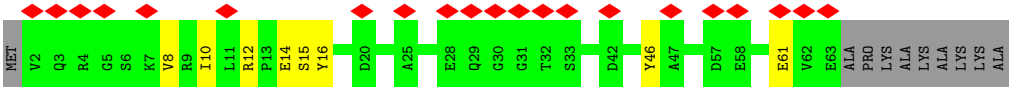
• Molecule 5: Photosystem I reaction center subunit IV

Chain E:



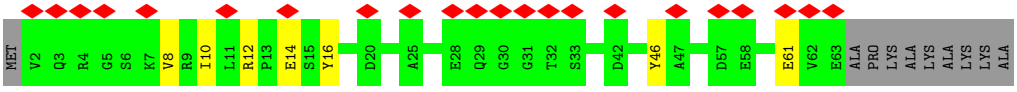
• Molecule 5: Photosystem I reaction center subunit IV

Chain P:



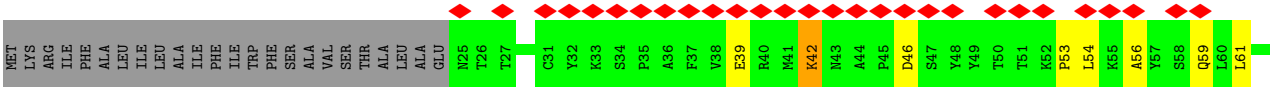
• Molecule 5: Photosystem I reaction center subunit IV

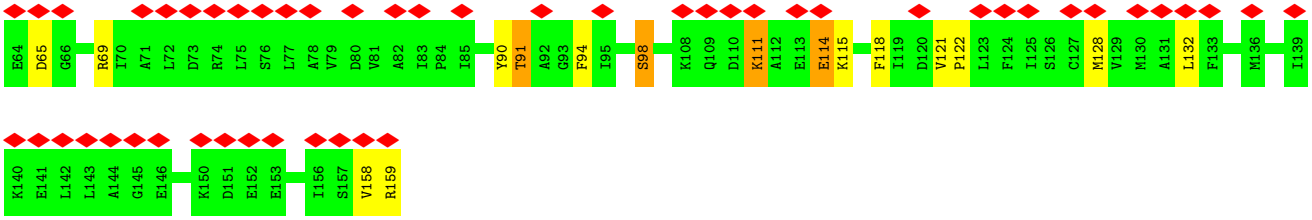
Chain e:



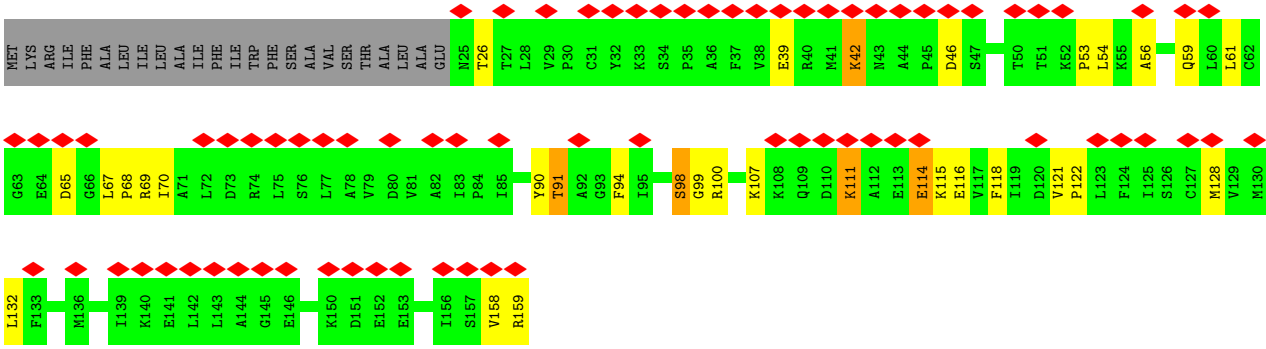
• Molecule 6: Photosystem I reaction center protein PsaF subunit III

Chain F:

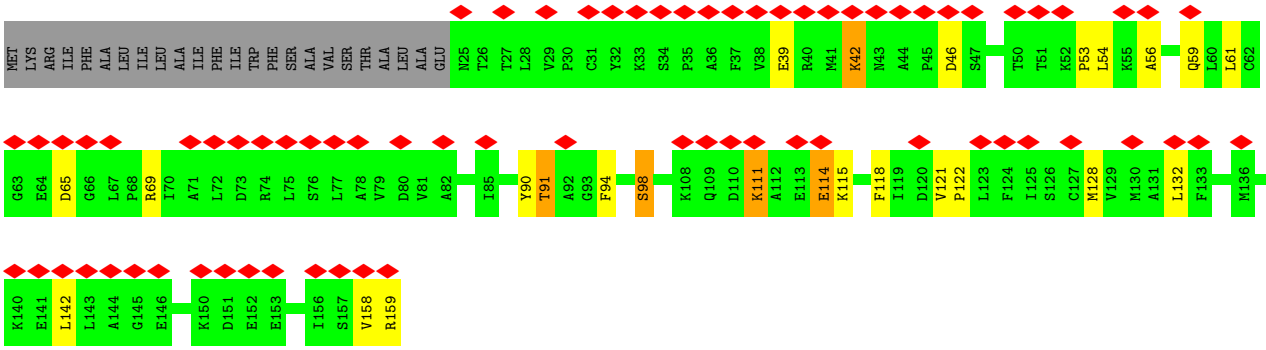




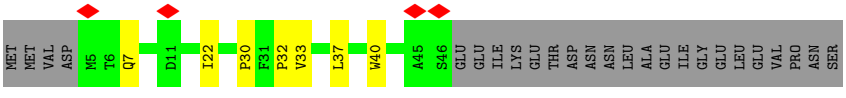
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



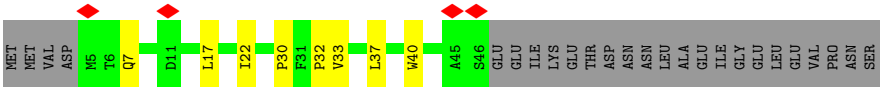
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



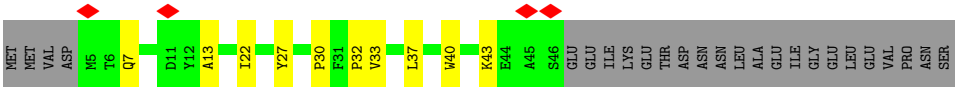
• Molecule 7: photosystem I subunit VIII



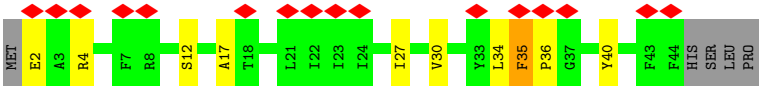
• Molecule 7: photosystem I subunit VIII



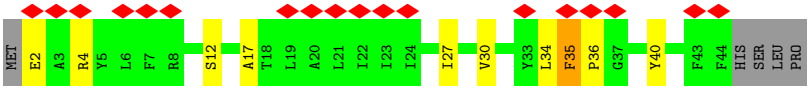
• Molecule 7: photosystem I subunit VIII



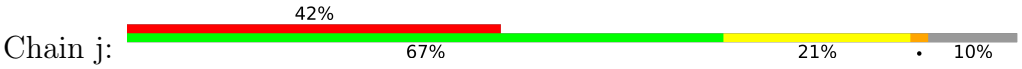
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ

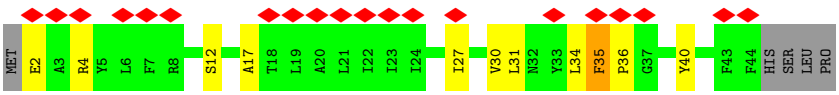


• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ

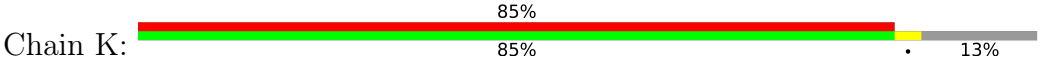


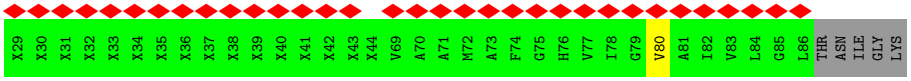
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



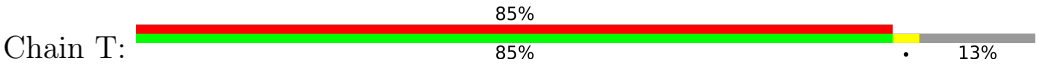


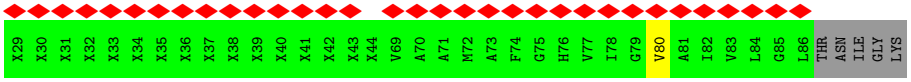
• Molecule 9: photosystem I reaction center subunit PsaK





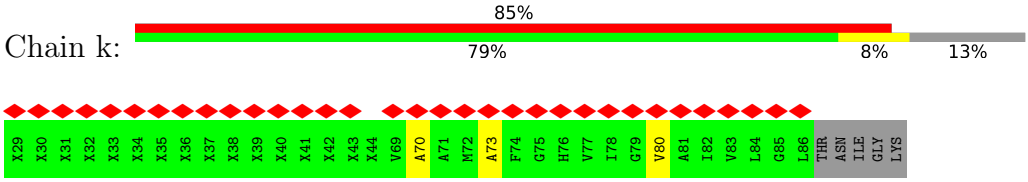
• Molecule 9: photosystem I reaction center subunit PsaK





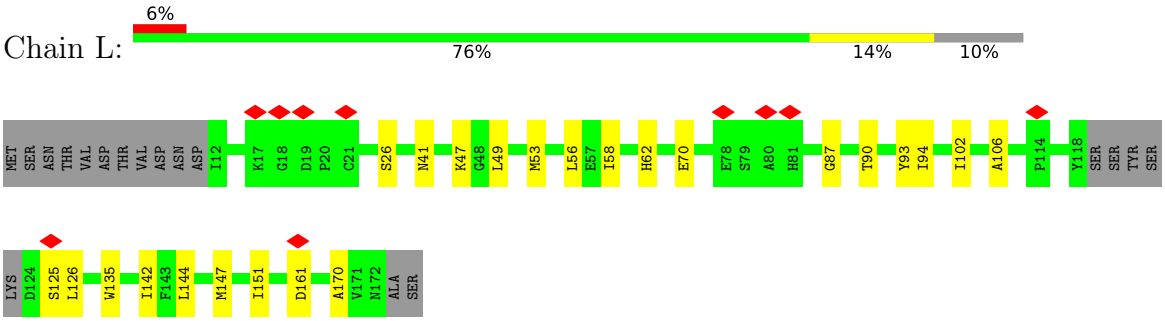
• Molecule 9: photosystem I reaction center subunit PsaK

Chain k:



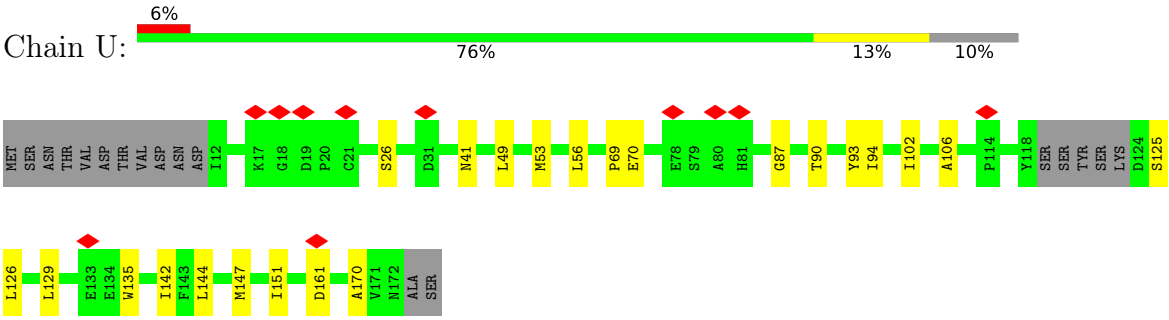
• Molecule 10: Photosystem I reaction center protein subunit XI

Chain L:



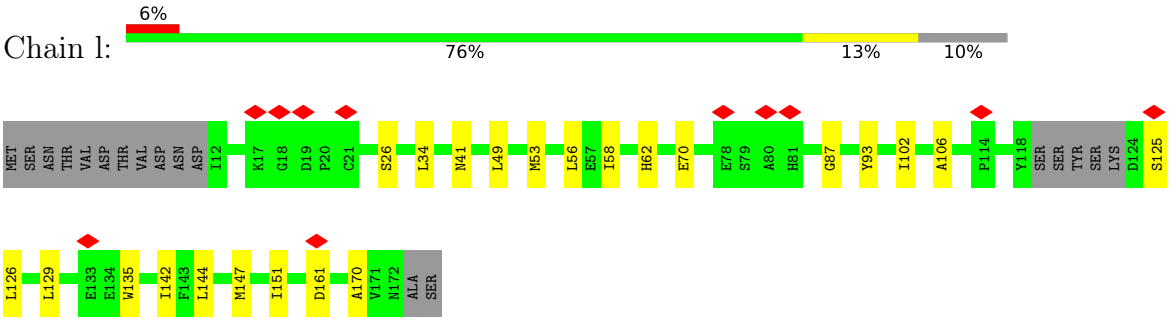
• Molecule 10: Photosystem I reaction center protein subunit XI

Chain U:



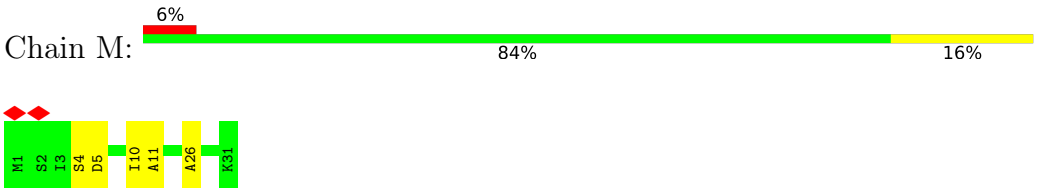
• Molecule 10: Photosystem I reaction center protein subunit XI

Chain l:



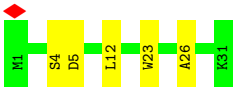
• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



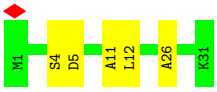
• Molecule 11: Photosystem I reaction center subunit XII

Chain V:



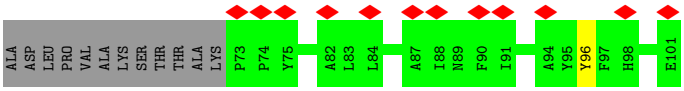
• Molecule 11: Photosystem I reaction center subunit XII

Chain m:



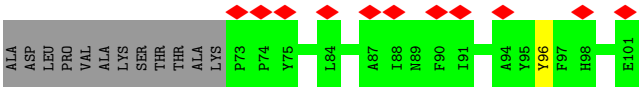
• Molecule 12: Photosystem one PsaX

Chain W:



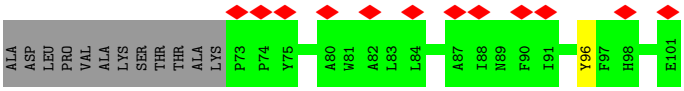
• Molecule 12: Photosystem one PsaX

Chain X:



• Molecule 12: Photosystem one PsaX

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	178666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5252	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	0.251	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0293	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: CA, CLA, LHG, CL0, F6C, BCR, LMT, PQN, SF4, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/6112	0.50	0/8325
1	G	0.43	0/6112	0.50	0/8325
1	a	0.43	0/6112	0.50	0/8325
2	B	0.44	0/6131	0.51	0/8380
2	H	0.44	0/6131	0.51	0/8380
2	b	0.44	0/6131	0.51	0/8380
3	C	0.39	0/611	0.68	2/828 (0.2%)
3	N	0.39	0/611	0.69	2/828 (0.2%)
3	c	0.39	0/611	0.68	2/828 (0.2%)
4	D	0.30	0/1116	0.52	0/1505
4	O	0.30	0/1116	0.51	0/1505
4	d	0.30	0/1116	0.52	0/1505
5	E	0.25	0/506	0.50	0/686
5	P	0.25	0/506	0.50	0/686
5	e	0.25	0/506	0.50	0/686
6	F	0.26	0/1084	0.63	1/1470 (0.1%)
6	Q	0.26	0/1084	0.63	1/1470 (0.1%)
6	f	0.26	0/1084	0.63	1/1470 (0.1%)
7	I	0.41	0/365	0.64	0/502
7	R	0.41	0/365	0.63	0/502
7	i	0.41	0/365	0.63	0/502
8	J	0.30	0/353	0.74	0/482
8	S	0.30	0/353	0.75	0/482
8	j	0.30	0/353	0.74	0/482
9	K	0.21	0/122	0.46	0/165
9	T	0.21	0/122	0.46	0/165
9	k	0.21	0/122	0.46	0/165
10	L	0.41	0/1198	0.63	2/1624 (0.1%)
10	U	0.42	0/1198	0.62	2/1624 (0.1%)
10	l	0.42	0/1198	0.63	2/1624 (0.1%)
11	M	0.32	0/250	0.51	0/340
11	V	0.32	0/250	0.51	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	m	0.32	0/250	0.51	0/340
12	W	0.20	0/256	0.55	0/350
12	X	0.21	0/256	0.55	0/350
12	x	0.21	0/256	0.55	0/350
All	All	0.40	0/54312	0.54	15/73971 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	a	0	1
6	F	0	1
6	Q	0	1
6	f	0	1
8	J	0	1
8	S	0	1
8	j	0	1
All	All	0	9

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	26	SER	CA-C-N	6.40	139.15	120.97
10	U	26	SER	C-N-CA	6.40	139.15	120.97
10	l	26	SER	CA-C-N	6.38	139.10	120.97
10	l	26	SER	C-N-CA	6.38	139.10	120.97
10	L	26	SER	CA-C-N	6.38	139.09	120.97
10	L	26	SER	C-N-CA	6.38	139.09	120.97
6	f	114	GLU	CA-CB-CG	6.21	126.51	114.10
6	F	114	GLU	CA-CB-CG	6.19	126.48	114.10
6	Q	114	GLU	CA-CB-CG	6.17	126.45	114.10
3	c	62	PHE	CA-C-N	5.43	131.91	121.54
3	c	62	PHE	C-N-CA	5.43	131.91	121.54
3	N	62	PHE	CA-C-N	5.43	131.90	121.54
3	N	62	PHE	C-N-CA	5.43	131.90	121.54
3	C	62	PHE	CA-C-N	5.42	131.89	121.54
3	C	62	PHE	C-N-CA	5.42	131.89	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	THR	Peptide
6	F	46	ASP	Peptide
1	G	333	THR	Peptide
8	J	35	PHE	Peptide
6	Q	46	ASP	Peptide
8	S	35	PHE	Peptide
1	a	333	THR	Peptide
6	f	46	ASP	Peptide
8	j	35	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5906	0	5753	91	0
1	G	5906	0	5753	92	0
1	a	5906	0	5753	91	0
2	B	5909	0	5668	96	0
2	H	5909	0	5668	95	0
2	b	5909	0	5668	99	0
3	C	601	0	585	15	0
3	N	601	0	585	18	0
3	c	601	0	585	16	0
4	D	1092	0	1098	14	0
4	O	1092	0	1098	18	0
4	d	1092	0	1098	14	0
5	E	497	0	482	5	0
5	P	497	0	482	6	0
5	e	497	0	482	5	0
6	F	1060	0	1091	15	0
6	Q	1060	0	1091	22	0
6	f	1060	0	1091	16	0
7	I	350	0	354	5	0
7	R	350	0	354	6	0
7	i	350	0	354	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	344	0	360	7	0
8	S	344	0	360	7	0
8	j	344	0	360	9	0
9	K	201	0	152	1	0
9	T	201	0	152	1	0
9	k	201	0	152	3	0
10	L	1172	0	1191	18	0
10	U	1172	0	1191	19	0
10	l	1172	0	1191	16	0
11	M	245	0	259	4	0
11	V	245	0	259	4	0
11	m	245	0	259	4	0
12	W	246	0	246	1	0
12	X	246	0	246	1	0
12	x	246	0	246	1	0
13	A	65	0	72	1	0
13	G	65	0	72	2	0
13	a	65	0	72	1	0
14	A	2140	0	1975	61	0
14	B	2280	0	2206	95	0
14	G	2140	0	1975	65	0
14	H	2280	0	2206	94	0
14	K	45	0	33	0	0
14	L	185	0	189	7	0
14	T	45	0	33	0	0
14	U	185	0	189	8	0
14	W	45	0	32	2	0
14	X	45	0	32	1	0
14	a	2140	0	1975	66	0
14	b	2280	0	2206	93	0
14	k	45	0	33	0	0
14	l	185	0	189	6	0
14	x	45	0	32	1	0
15	A	92	0	0	0	0
15	B	107	0	0	4	0
15	G	92	0	0	0	0
15	H	107	0	0	3	0
15	a	92	0	0	0	0
15	b	107	0	0	6	0
16	A	33	0	46	6	0
16	B	33	0	46	4	0
16	G	33	0	46	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	H	33	0	46	4	0
16	a	33	0	46	6	0
16	b	33	0	46	4	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
17	G	8	0	0	0	0
17	N	16	0	0	0	0
17	a	8	0	0	0	0
17	c	16	0	0	0	0
18	A	240	0	293	17	0
18	B	400	0	487	27	0
18	G	240	0	293	16	0
18	H	400	0	487	26	0
18	I	80	0	97	8	0
18	L	80	0	98	6	0
18	M	40	0	48	3	0
18	R	80	0	97	9	0
18	U	80	0	98	6	0
18	V	40	0	48	4	0
18	a	240	0	292	18	0
18	b	400	0	487	26	0
18	i	80	0	97	5	0
18	l	80	0	98	6	0
18	m	40	0	48	2	0
19	A	42	0	54	1	0
19	B	44	0	61	0	0
19	G	42	0	54	1	0
19	H	44	0	61	1	0
19	a	42	0	54	1	0
19	b	44	0	61	0	0
20	A	46	0	65	0	0
20	B	46	0	62	3	0
20	G	46	0	65	1	0
20	H	46	0	62	3	0
20	I	37	0	44	2	0
20	L	50	0	70	2	0
20	R	37	0	44	5	0
20	U	50	0	70	3	0
20	a	46	0	65	1	0
20	b	46	0	62	3	0
20	i	37	0	44	2	0
20	l	50	0	70	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	59	0	58	0	0
21	G	59	0	57	1	0
21	a	59	0	57	0	0
22	L	1	0	0	0	0
22	U	1	0	0	0	0
22	l	1	0	0	0	0
All	All	71511	0	69822	1161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:b:1230:F6C:OMB	8:j:40:TYR:OH	1.85	0.92
3:N:2:SER:N	3:N:76:SER:HG	1.80	0.80
3:C:2:SER:N	3:C:76:SER:HG	1.79	0.79
14:b:1223:CLA:H2	18:b:4010:BCR:H14C	1.65	0.78
14:B:1223:CLA:H2	18:B:4010:BCR:H14C	1.66	0.77
14:H:1223:CLA:H2	18:H:4010:BCR:H14C	1.66	0.77
1:a:406:TRP:CD1	14:a:1126:CLA:HAB	2.21	0.76
1:A:406:TRP:CD1	14:A:1126:CLA:HAB	2.20	0.76
1:G:406:TRP:CD1	14:G:1126:CLA:HAB	2.20	0.76
3:c:2:SER:N	3:c:76:SER:HG	1.83	0.74
15:b:1230:F6C:O1A	8:j:31:LEU:HD11	1.90	0.71
2:H:29:HIS:HD2	14:H:1202:CLA:HAB	1.56	0.71
16:B:2002:PQN:H301	20:B:5002:LMG:H191	1.73	0.70
2:b:29:HIS:HD2	14:b:1202:CLA:HAB	1.56	0.70
16:H:2002:PQN:H301	20:H:5002:LMG:H191	1.73	0.70
2:H:442:VAL:HG23	15:H:1230:F6C:CMC	2.21	0.70
14:H:1209:CLA:HBB2	14:H:1217:CLA:H92	1.74	0.69
1:A:336:MET:HE2	1:A:343:ILE:HD11	1.74	0.69
14:H:1214:CLA:HBA2	14:H:1223:CLA:HBB2	1.75	0.69
2:B:29:HIS:HD2	14:B:1202:CLA:HAB	1.56	0.69
14:B:1214:CLA:HBA2	14:B:1223:CLA:HBB2	1.75	0.69
16:b:2002:PQN:H301	20:b:5002:LMG:H191	1.73	0.69
2:b:442:VAL:HG23	15:b:1230:F6C:CMC	2.23	0.69
4:D:69:ARG:H	4:D:73:ASN:HD21	1.41	0.68
4:O:69:ARG:H	4:O:73:ASN:HD21	1.41	0.68
14:B:1209:CLA:HBB2	14:B:1217:CLA:H92	1.73	0.68
1:a:336:MET:HE2	1:a:343:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:1214:CLA:HBA2	14:b:1223:CLA:HBB2	1.75	0.68
2:B:442:VAL:HG23	15:B:1230:F6C:CMC	2.23	0.68
14:b:1209:CLA:HBB2	14:b:1217:CLA:H92	1.73	0.68
1:G:336:MET:HE2	1:G:343:ILE:HD11	1.74	0.68
1:A:409:GLY:HA3	1:A:639:LEU:HD11	1.76	0.67
4:d:69:ARG:H	4:d:73:ASN:HD21	1.41	0.67
1:a:409:GLY:HA3	1:a:639:LEU:HD11	1.76	0.67
4:O:136:ARG:H	4:O:139:GLN:HE21	1.44	0.66
4:d:136:ARG:H	4:d:139:GLN:HE21	1.44	0.66
1:G:409:GLY:HA3	1:G:639:LEU:HD11	1.76	0.65
7:I:7:GLN:HG3	10:U:170:ALA:HB2	1.78	0.65
4:D:136:ARG:H	4:D:139:GLN:HE21	1.44	0.65
1:A:473:ARG:HE	1:A:481:MET:HE1	1.62	0.64
1:a:473:ARG:HE	1:a:481:MET:HE1	1.62	0.64
1:a:114:GLN:NE2	14:a:1107:CLA:OBD	2.31	0.63
1:G:114:GLN:NE2	14:G:1107:CLA:OBD	2.31	0.63
1:A:114:GLN:NE2	14:A:1107:CLA:OBD	2.31	0.63
1:G:473:ARG:HE	1:G:481:MET:HE1	1.62	0.62
1:G:651:GLN:HE22	1:G:783:ARG:HE	1.48	0.62
1:a:651:GLN:HE22	1:a:783:ARG:HE	1.48	0.62
8:S:27:ILE:HA	8:S:30:VAL:HG12	1.82	0.62
2:b:322:PRO:HB2	2:b:410:ASN:HA	1.82	0.62
2:H:468:GLN:NE2	14:H:1234:CLA:OBD	2.33	0.62
2:H:322:PRO:HB2	2:H:410:ASN:HA	1.82	0.61
8:j:27:ILE:HA	8:j:30:VAL:HG12	1.82	0.61
1:A:70:LYS:HZ1	14:A:1109:CLA:HED2	1.65	0.61
2:H:442:VAL:HA	2:H:445:ASP:HB2	1.82	0.61
2:B:442:VAL:HA	2:B:445:ASP:HB2	1.82	0.61
14:A:1127:CLA:H61	18:A:4003:BCR:H23C	1.82	0.61
2:B:468:GLN:NE2	14:B:1234:CLA:OBD	2.33	0.61
1:A:651:GLN:HE22	1:A:783:ARG:HE	1.48	0.61
2:b:70:TRP:NE1	7:i:13:ALA:O	2.25	0.61
2:B:322:PRO:HB2	2:B:410:ASN:HA	1.82	0.60
14:G:1124:CLA:H52	14:G:1133:CLA:HAB	1.83	0.60
1:a:626:ASP:OD2	1:a:761:ARG:NH1	2.34	0.60
1:A:626:ASP:OD2	1:A:761:ARG:NH1	2.34	0.60
14:a:1127:CLA:H61	18:a:4003:BCR:H23C	1.82	0.60
14:A:1124:CLA:H52	14:A:1133:CLA:HAB	1.84	0.60
1:G:626:ASP:OD2	1:G:761:ARG:NH1	2.34	0.60
14:G:1127:CLA:H61	18:G:4003:BCR:H23C	1.82	0.60
6:F:53:PRO:HD3	8:J:35:PHE:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:LEU:HD21	9:T:80:VAL:HG22	1.83	0.60
1:G:70:LYS:HZ1	14:G:1109:CLA:HED2	1.66	0.59
2:b:468:GLN:NE2	14:b:1234:CLA:OBD	2.33	0.59
2:b:442:VAL:HA	2:b:445:ASP:HB2	1.82	0.59
8:J:27:ILE:HA	8:J:30:VAL:HG12	1.82	0.59
10:L:170:ALA:HB2	7:i:7:GLN:HG3	1.83	0.59
20:L:5007:LMG:H322	20:i:5006:LMG:HC61	1.84	0.59
14:a:1124:CLA:H52	14:a:1133:CLA:HAB	1.83	0.59
14:H:1023:CLA:H142	18:R:4018:BCR:H271	1.84	0.59
16:a:2001:PQN:H292	8:j:17:ALA:HB1	1.84	0.59
2:b:537:THR:HG21	14:b:1222:CLA:HBC3	1.85	0.59
3:C:15:THR:HG22	3:C:28:MET:HG3	1.83	0.59
14:b:1023:CLA:H142	18:i:4018:BCR:H271	1.84	0.59
3:N:15:THR:HG22	3:N:28:MET:HG3	1.83	0.59
3:c:15:THR:HG22	3:c:28:MET:HG3	1.84	0.58
1:A:307:PHE:HE1	14:A:1119:CLA:HAB	1.68	0.58
1:a:632:LEU:HB3	1:a:769:LEU:HD11	1.85	0.58
1:A:632:LEU:HB3	1:A:769:LEU:HD11	1.85	0.58
1:a:307:PHE:HE1	14:a:1119:CLA:HAB	1.68	0.58
14:B:1023:CLA:H142	18:I:4018:BCR:H271	1.84	0.58
7:R:7:GLN:HG3	10:l:170:ALA:HB2	1.85	0.58
2:B:537:THR:HG21	14:B:1222:CLA:HBC3	1.85	0.58
1:G:197:ASN:ND2	1:G:311:GLY:O	2.35	0.58
14:G:1119:CLA:H2	14:G:1123:CLA:HBB1	1.86	0.57
14:A:1119:CLA:H2	14:A:1123:CLA:HBB1	1.86	0.57
1:G:632:LEU:HB3	1:G:769:LEU:HD11	1.85	0.57
1:G:380:HIS:ND1	14:G:1116:CLA:OBD	2.38	0.57
2:H:537:THR:HG21	14:H:1222:CLA:HBC3	1.85	0.57
15:H:1230:F6C:OMB	8:S:40:TYR:OH	2.11	0.57
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.87	0.57
1:A:446:ALA:O	1:A:450:HIS:ND1	2.32	0.57
1:G:751:GLN:NE2	5:P:16:TYR:OH	2.38	0.57
1:A:632:LEU:HD21	14:A:1128:CLA:HBC1	1.87	0.57
1:G:307:PHE:HE1	14:G:1119:CLA:HAB	1.68	0.57
1:a:70:LYS:HZ1	14:a:1109:CLA:HED2	1.70	0.57
1:a:445:ASP:OD2	1:a:597:ARG:NH1	2.37	0.57
1:A:608:ARG:NH1	19:A:5001:LHG:O10	2.38	0.57
2:b:578:SER:OG	2:b:581:ASP:OD2	2.23	0.57
1:G:632:LEU:HD21	14:G:1128:CLA:HBC1	1.87	0.56
1:A:380:HIS:ND1	14:A:1116:CLA:OBD	2.38	0.56
1:A:126:ASN:HB3	1:A:134:HIS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ASN:HB3	1:G:134:HIS:HB3	1.87	0.56
10:L:41:ASN:HB3	14:L:1501:CLA:HAC1	1.87	0.56
2:b:15:ASP:HB3	2:b:20:ARG:HB2	1.87	0.56
1:a:751:GLN:NE2	5:e:16:TYR:OH	2.39	0.56
2:H:15:ASP:HB3	2:H:20:ARG:HB2	1.87	0.56
1:a:126:ASN:HB3	1:a:134:HIS:HB3	1.87	0.56
1:a:608:ARG:NH1	19:a:5001:LHG:O10	2.38	0.56
2:b:182:LEU:O	2:b:186:SER:OG	2.22	0.56
1:A:445:ASP:OD2	1:A:597:ARG:NH1	2.37	0.56
20:I:5006:LMG:HC61	20:U:5007:LMG:H322	1.88	0.56
14:a:1119:CLA:H2	14:a:1123:CLA:HBB1	1.86	0.56
2:B:269:TRP:HB2	2:B:272:ASP:HB2	1.88	0.56
1:G:608:ARG:NH1	19:G:5001:LHG:O10	2.38	0.56
2:H:355:HIS:ND1	14:H:1214:CLA:OBD	2.38	0.56
2:H:429:VAL:HG13	14:H:1235:CLA:HBB1	1.88	0.56
2:B:578:SER:OG	2:B:581:ASP:OD2	2.23	0.56
3:c:42:SER:O	4:d:131:ARG:NH2	2.39	0.56
1:A:241:PHE:HB3	1:A:248:MET:HE2	1.88	0.55
2:B:429:VAL:HG13	14:B:1235:CLA:HBB1	1.88	0.55
3:N:42:SER:O	4:O:131:ARG:NH2	2.39	0.55
4:O:100:ILE:HB	4:O:113:HIS:HB3	1.88	0.55
1:a:380:HIS:ND1	14:a:1116:CLA:OBD	2.38	0.55
14:H:1238:CLA:HAB	16:H:2002:PQN:H141	1.88	0.55
1:A:751:GLN:NE2	5:E:16:TYR:OH	2.39	0.55
1:G:241:PHE:HB3	1:G:248:MET:HE2	1.88	0.55
2:b:429:VAL:HG13	14:b:1235:CLA:HBB1	1.88	0.55
10:l:41:ASN:HB3	14:l:1501:CLA:HAC1	1.87	0.55
2:B:415:VAL:HG11	18:B:4009:BCR:H381	1.88	0.55
10:U:147:MET:HB3	18:U:4022:BCR:H393	1.89	0.55
10:l:147:MET:HB3	18:l:4022:BCR:H393	1.89	0.55
3:C:42:SER:O	4:D:131:ARG:NH2	2.39	0.55
10:U:41:ASN:HB3	14:U:1501:CLA:HAC1	1.87	0.55
1:a:241:PHE:HB3	1:a:248:MET:HE2	1.88	0.55
1:A:411:LEU:HD21	14:A:1104:CLA:H142	1.89	0.55
2:B:182:LEU:O	2:B:186:SER:OG	2.22	0.55
2:H:182:LEU:O	2:H:186:SER:OG	2.22	0.55
2:H:578:SER:OG	2:H:581:ASP:OD2	2.23	0.55
1:A:197:ASN:ND2	1:A:311:GLY:O	2.35	0.55
2:H:457:ILE:O	2:H:525:TYR:OH	2.25	0.55
14:a:1012:CLA:H2	2:b:662:LEU:HD22	1.89	0.55
2:H:68:VAL:HG21	2:H:124:TRP:HZ3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:TRP:HB2	2:H:272:ASP:HB2	1.88	0.55
1:a:632:LEU:HD21	14:a:1128:CLA:HBC1	1.87	0.55
2:b:68:VAL:HG21	2:b:124:TRP:HZ3	1.72	0.55
2:b:415:VAL:HG11	18:b:4009:BCR:H381	1.88	0.55
14:b:1238:CLA:HAB	16:b:2002:PQN:H141	1.88	0.55
3:c:55:GLU:OE2	3:c:66:ARG:NH1	2.40	0.55
4:D:100:ILE:HB	4:D:113:HIS:HB3	1.89	0.55
2:H:415:VAL:HG11	18:H:4009:BCR:H381	1.88	0.55
7:I:32:PRO:HG3	14:U:1501:CLA:H12	1.88	0.55
14:a:1126:CLA:H142	14:b:1022:CLA:H112	1.89	0.55
14:A:1126:CLA:H142	14:B:1022:CLA:H112	1.89	0.54
2:B:68:VAL:HG21	2:B:124:TRP:HZ3	1.72	0.54
6:Q:94:PHE:O	6:Q:98:SER:OG	2.24	0.54
1:G:445:ASP:OD2	1:G:597:ARG:NH1	2.37	0.54
10:L:147:MET:HB3	18:L:4022:BCR:H393	1.89	0.54
1:a:406:TRP:HD1	14:a:1126:CLA:HAB	1.71	0.54
4:d:100:ILE:HB	4:d:113:HIS:HB3	1.88	0.54
14:G:1012:CLA:H2	2:H:662:LEU:HD22	1.89	0.54
14:H:1212:CLA:HHB	18:H:4006:BCR:HC8	1.90	0.54
2:b:269:TRP:HB2	2:b:272:ASP:HB2	1.88	0.54
1:A:406:TRP:HD1	14:A:1126:CLA:HAB	1.71	0.54
2:B:498:ASN:ND2	14:B:1232:CLA:O1D	2.41	0.54
2:b:50:HIS:HE1	14:b:1202:CLA:H122	1.73	0.54
14:A:1012:CLA:H2	2:B:662:LEU:HD22	1.89	0.54
2:B:319:PHE:CD1	14:B:1219:CLA:HAB	2.43	0.54
2:B:355:HIS:ND1	14:B:1214:CLA:OBD	2.38	0.54
2:H:50:HIS:HE1	14:H:1202:CLA:H122	1.73	0.54
2:b:498:ASN:ND2	14:b:1232:CLA:O1D	2.41	0.54
6:F:94:PHE:O	6:F:98:SER:OG	2.24	0.54
2:H:319:PHE:CD1	14:H:1219:CLA:HAB	2.43	0.54
1:a:197:ASN:ND2	1:a:311:GLY:O	2.35	0.54
1:A:623:SER:OG	1:A:626:ASP:OD1	2.26	0.54
14:B:1238:CLA:HAB	16:B:2002:PQN:H141	1.88	0.54
3:C:55:GLU:OE2	3:C:66:ARG:NH1	2.40	0.54
1:G:411:LEU:HD21	14:G:1104:CLA:H142	1.89	0.54
2:b:86:PRO:HB2	2:b:116:CYS:HB3	1.90	0.54
2:B:662:LEU:HG	14:B:1239:CLA:HAB	1.91	0.53
2:H:262:HIS:HD2	2:H:264:GLN:H	1.56	0.53
2:H:701:ASP:N	2:H:701:ASP:OD1	2.41	0.53
3:N:55:GLU:OE2	3:N:66:ARG:NH1	2.40	0.53
2:H:498:ASN:ND2	14:H:1232:CLA:O1D	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:662:LEU:HG	14:H:1239:CLA:HAB	1.91	0.53
2:b:319:PHE:CD1	14:b:1219:CLA:HAB	2.43	0.53
14:b:1212:CLA:HHB	18:b:4006:BCR:HC8	1.90	0.53
10:l:102:ILE:HB	10:l:135:TRP:HE1	1.73	0.53
14:G:1126:CLA:H142	14:H:1012:CLA:H112	1.89	0.53
2:H:420:GLU:HG3	6:Q:159:ARG:HH11	1.74	0.53
1:a:623:SER:OG	1:a:626:ASP:OD1	2.26	0.53
6:f:94:PHE:O	6:f:98:SER:OG	2.24	0.53
2:B:173:ALA:O	2:B:177:HIS:ND1	2.36	0.53
2:B:86:PRO:HB2	2:B:116:CYS:HB3	1.90	0.53
1:G:582:THR:HG21	14:G:1124:CLA:HAC2	1.91	0.53
2:b:457:ILE:O	2:b:525:TYR:OH	2.25	0.53
2:b:701:ASP:OD1	2:b:701:ASP:N	2.41	0.53
3:c:17:CYS:HB2	3:c:54:CYS:HB2	1.91	0.53
6:F:91:THR:HA	6:F:94:PHE:HB3	1.91	0.53
1:G:623:SER:OG	1:G:626:ASP:OD1	2.26	0.53
2:B:262:HIS:HD2	2:B:264:GLN:H	1.56	0.53
6:Q:91:THR:HA	6:Q:94:PHE:HB3	1.91	0.53
2:b:292:ARG:HD3	2:b:300:SER:HB2	1.91	0.53
14:b:1225:CLA:H202	18:b:4005:BCR:H352	1.91	0.53
14:B:1212:CLA:HHB	18:B:4006:BCR:HC8	1.90	0.52
1:G:406:TRP:HD1	14:G:1126:CLA:HAB	1.71	0.52
2:H:86:PRO:HB2	2:H:116:CYS:HB3	1.90	0.52
7:R:32:PRO:HG3	14:l:1501:CLA:H12	1.91	0.52
1:a:411:LEU:HD21	14:a:1104:CLA:H142	1.89	0.52
2:b:662:LEU:HG	14:b:1239:CLA:HAB	1.91	0.52
15:b:1230:F6C:CGA	8:j:31:LEU:HD11	2.39	0.52
6:f:91:THR:HA	6:f:94:PHE:HB3	1.91	0.52
1:A:455:CYS:HB3	1:A:581:VAL:HG22	1.92	0.52
2:B:50:HIS:HE1	14:B:1202:CLA:H122	1.73	0.52
10:U:102:ILE:HB	10:U:135:TRP:HE1	1.73	0.52
10:l:151:ILE:HG13	18:l:4022:BCR:H291	1.92	0.52
1:A:377:ILE:HD13	14:A:1127:CLA:HHD	1.92	0.52
14:B:1227:CLA:HMC2	18:B:4009:BCR:H281	1.91	0.52
2:H:668:PHE:HB2	14:H:1023:CLA:HMC2	1.91	0.52
2:B:292:ARG:HD3	2:B:300:SER:HB2	1.91	0.52
14:B:1225:CLA:H202	18:B:4005:BCR:H352	1.91	0.52
14:a:1124:CLA:HAB	18:a:4008:BCR:H311	1.91	0.52
2:B:650:LEU:HD11	2:B:737:SER:HB3	1.92	0.52
14:B:1204:CLA:HBB1	14:B:1204:CLA:H112	1.91	0.52
14:b:1227:CLA:HMC2	18:b:4009:BCR:H281	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:582:THR:HG21	14:a:1124:CLA:HAC2	1.91	0.52
2:B:701:ASP:OD1	2:B:701:ASP:N	2.41	0.52
2:H:292:ARG:HD3	2:H:300:SER:HB2	1.91	0.52
10:L:151:ILE:HG13	18:L:4022:BCR:H291	1.92	0.52
3:N:17:CYS:HB2	3:N:54:CYS:HB2	1.91	0.52
2:b:173:ALA:O	2:b:177:HIS:ND1	2.36	0.52
2:b:262:HIS:HD2	2:b:264:GLN:H	1.56	0.52
2:b:381:TYR:CD2	14:b:1224:CLA:HAB	2.45	0.52
2:B:668:PHE:HB2	14:B:1023:CLA:HMC2	1.91	0.52
18:B:4009:BCR:H383	18:B:4010:BCR:H272	1.92	0.52
18:B:4009:BCR:H402	18:B:4010:BCR:H383	1.92	0.52
3:C:17:CYS:HB2	3:C:54:CYS:HB2	1.91	0.52
1:G:446:ALA:O	1:G:450:HIS:ND1	2.32	0.52
18:H:4009:BCR:H383	18:H:4010:BCR:H272	1.92	0.52
2:B:56:ILE:HD11	18:M:4021:BCR:HC7	1.90	0.52
2:B:381:TYR:CD2	14:B:1224:CLA:HAB	2.44	0.52
1:G:634:TRP:HH2	14:G:1012:CLA:HAB	1.75	0.52
1:a:455:CYS:HB3	1:a:581:VAL:HG22	1.91	0.52
2:b:92:TRP:HB3	7:i:22:ILE:HG13	1.92	0.52
14:B:1023:CLA:H201	14:B:1239:CLA:H61	1.93	0.51
14:G:1124:CLA:HAB	18:G:4008:BCR:H311	1.91	0.51
2:H:273:MET:O	2:H:277:HIS:ND1	2.43	0.51
14:b:1021:CLA:H71	14:b:1022:CLA:HED2	1.92	0.51
14:b:1229:CLA:CAB	15:b:1230:F6C:CMB	2.88	0.51
2:H:650:LEU:HD11	2:H:737:SER:HB3	1.92	0.51
10:L:102:ILE:HB	10:L:135:TRP:HE1	1.73	0.51
1:A:634:TRP:CH2	14:A:1012:CLA:HAB	2.45	0.51
14:B:1021:CLA:H71	14:B:1022:CLA:HED2	1.93	0.51
14:H:1012:CLA:HED2	14:H:1021:CLA:H71	1.92	0.51
14:H:1204:CLA:H112	14:H:1204:CLA:HBB1	1.91	0.51
2:b:56:ILE:HD11	18:m:4021:BCR:HC7	1.90	0.51
2:b:176:ASN:ND2	2:b:288:GLY:O	2.43	0.51
14:A:1124:CLA:HAB	18:A:4008:BCR:H311	1.91	0.51
14:H:1225:CLA:H202	18:H:4005:BCR:H352	1.91	0.51
2:b:668:PHE:HB2	14:b:1023:CLA:HMC2	1.91	0.51
14:b:1204:CLA:HBB1	14:b:1204:CLA:H112	1.91	0.51
2:B:347:VAL:HG13	14:B:1222:CLA:HED1	1.93	0.51
14:B:1239:CLA:H193	18:I:4018:BCR:H372	1.93	0.51
1:G:377:ILE:HD13	14:G:1127:CLA:HHD	1.91	0.51
2:H:176:ASN:ND2	2:H:288:GLY:O	2.44	0.51
14:H:1023:CLA:H201	14:H:1239:CLA:H61	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:634:TRP:CH2	14:a:1012:CLA:HAB	2.45	0.51
1:a:634:TRP:HH2	14:a:1012:CLA:HAB	1.75	0.51
14:b:1023:CLA:H201	14:b:1239:CLA:H61	1.92	0.51
6:F:111:LYS:HD2	6:F:115:LYS:HE3	1.93	0.51
1:G:455:CYS:HB3	1:G:581:VAL:HG22	1.92	0.51
14:G:1125:CLA:H172	14:G:1133:CLA:H93	1.92	0.51
2:H:381:TYR:CD2	14:H:1224:CLA:HAB	2.44	0.51
14:H:1227:CLA:HMC2	18:H:4009:BCR:H281	1.91	0.51
1:a:446:ALA:O	1:a:450:HIS:ND1	2.32	0.51
1:A:582:THR:HG21	14:A:1124:CLA:HAC2	1.91	0.51
1:A:699:ASN:HD22	2:B:451:GLY:HA2	1.75	0.51
2:H:347:VAL:HG13	14:H:1222:CLA:HED1	1.93	0.51
2:b:273:MET:O	2:b:277:HIS:ND1	2.43	0.51
2:b:650:LEU:HD11	2:b:737:SER:HB3	1.92	0.51
1:G:699:ASN:HD22	2:H:451:GLY:HA2	1.74	0.51
2:H:713:LEU:HD13	20:H:5002:LMG:H322	1.93	0.51
1:a:210:GLY:C	14:a:1112:CLA:HAB	2.36	0.51
18:b:4009:BCR:H383	18:b:4010:BCR:H272	1.92	0.51
1:A:230:VAL:HB	1:A:234:ASP:HB3	1.93	0.51
1:A:634:TRP:HH2	14:A:1012:CLA:HAB	1.75	0.51
14:A:1125:CLA:H172	14:A:1133:CLA:H93	1.92	0.51
14:B:1210:CLA:H141	14:B:1216:CLA:HBB2	1.93	0.51
1:G:75:HIS:ND1	14:G:1111:CLA:OBD	2.42	0.51
1:G:634:TRP:CH2	14:G:1012:CLA:HAB	2.45	0.51
14:H:1203:CLA:H151	14:H:1225:CLA:HBB2	1.92	0.51
10:U:151:ILE:HG13	18:U:4022:BCR:H291	1.92	0.51
2:b:117:TYR:HA	2:b:371:THR:HG22	1.93	0.51
2:B:176:ASN:ND2	2:B:288:GLY:O	2.43	0.50
1:G:287:VAL:HG13	1:G:288:THR:HG23	1.94	0.50
6:Q:111:LYS:HD2	6:Q:115:LYS:HE3	1.93	0.50
1:a:699:ASN:HD22	2:b:451:GLY:HA2	1.75	0.50
3:c:2:SER:N	3:c:76:SER:OG	2.44	0.50
1:A:733:LEU:HD21	14:A:1013:CLA:HED2	1.94	0.50
2:B:117:TYR:HA	2:B:371:THR:HG22	1.93	0.50
1:G:210:GLY:C	14:G:1112:CLA:HAB	2.36	0.50
18:H:4009:BCR:H402	18:H:4010:BCR:H383	1.92	0.50
1:a:287:VAL:HG13	1:a:288:THR:HG23	1.94	0.50
14:b:1224:CLA:H202	18:i:4018:BCR:H311	1.93	0.50
1:G:224:LYS:HG2	1:G:251:LEU:HD22	1.93	0.50
1:a:377:ILE:HD13	14:a:1127:CLA:HHD	1.91	0.50
2:b:347:VAL:HG13	14:b:1222:CLA:HED1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:1239:CLA:H193	18:R:4018:BCR:H372	1.93	0.50
18:a:4001:BCR:H353	9:k:73:ALA:HB1	1.93	0.50
2:b:713:LEU:HD13	20:b:5002:LMG:H322	1.93	0.50
16:A:2001:PQN:H292	8:J:17:ALA:HB1	1.92	0.50
1:G:230:VAL:HB	1:G:234:ASP:HB3	1.93	0.50
2:H:117:TYR:HA	2:H:371:THR:HG22	1.93	0.50
14:H:1204:CLA:H61	18:R:4018:BCR:HC32	1.93	0.50
14:H:1207:CLA:HMC2	18:R:4018:BCR:H19C	1.94	0.50
1:a:75:HIS:ND1	14:a:1111:CLA:OBD	2.42	0.50
14:b:1203:CLA:H151	14:b:1225:CLA:HBB2	1.92	0.50
14:b:1210:CLA:H141	14:b:1216:CLA:HBB2	1.93	0.50
6:f:53:PRO:HD3	8:j:35:PHE:HB2	1.94	0.50
14:H:1210:CLA:H141	14:H:1216:CLA:HBB2	1.93	0.50
1:A:75:HIS:ND1	14:A:1111:CLA:OBD	2.42	0.50
1:A:210:GLY:C	14:A:1112:CLA:HAB	2.36	0.50
1:A:287:VAL:HG13	1:A:288:THR:HG23	1.94	0.50
14:B:1203:CLA:H151	14:B:1225:CLA:HBB2	1.92	0.50
4:O:80:LYS:HE3	4:O:112:ILE:HD12	1.94	0.50
14:a:1012:CLA:H151	14:b:1207:CLA:HMC2	1.93	0.50
14:a:1125:CLA:H172	14:a:1133:CLA:H93	1.92	0.50
4:d:80:LYS:HE3	4:d:112:ILE:HD12	1.94	0.50
1:A:224:LYS:HG2	1:A:251:LEU:HD22	1.93	0.50
2:B:457:ILE:O	2:B:525:TYR:OH	2.25	0.50
3:C:2:SER:N	3:C:76:SER:OG	2.44	0.50
2:H:476:TYR:HB3	6:Q:26:THR:HG23	1.93	0.50
10:L:106:ALA:HB2	10:L:135:TRP:CD1	2.47	0.50
6:Q:118:PHE:HA	8:S:12:SER:HA	1.94	0.50
2:b:355:HIS:ND1	14:b:1214:CLA:OBD	2.38	0.50
2:b:566:CYS:SG	2:b:567:ASP:N	2.85	0.50
1:A:276:ASP:OD1	1:A:276:ASP:N	2.42	0.50
2:B:273:MET:O	2:B:277:HIS:ND1	2.43	0.50
16:G:2001:PQN:H292	8:S:17:ALA:HB1	1.93	0.50
10:l:106:ALA:HB2	10:l:135:TRP:CD1	2.47	0.50
2:B:713:LEU:HD13	20:B:5002:LMG:H322	1.93	0.49
14:B:1022:CLA:H191	18:B:4012:BCR:H363	1.94	0.49
20:R:5006:LMG:HC61	20:l:5007:LMG:H322	1.94	0.49
14:H:1229:CLA:CAB	15:H:1230:F6C:CMB	2.89	0.49
1:a:733:LEU:HD21	14:a:1013:CLA:HED2	1.94	0.49
1:G:733:LEU:HD21	14:G:1013:CLA:HED2	1.94	0.49
14:H:1012:CLA:H191	18:H:4012:BCR:H363	1.94	0.49
2:b:432:PHE:O	2:b:436:HIS:ND1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:b:4009:BCR:H402	18:b:4010:BCR:H383	1.92	0.49
1:A:201:ALA:HB2	1:A:311:GLY:HA3	1.94	0.49
1:A:269:LEU:HD21	9:K:80:VAL:HG22	1.93	0.49
1:A:726:GLY:HA3	2:B:575:CYS:HB2	1.94	0.49
14:B:1204:CLA:H61	18:I:4018:BCR:HC32	1.93	0.49
2:H:505:LEU:HA	2:H:508:ILE:HG22	1.95	0.49
14:H:1210:CLA:H203	14:H:1215:CLA:HBB2	1.95	0.49
10:L:70:GLU:HB3	10:L:87:GLY:HA2	1.94	0.49
10:U:70:GLU:HB3	10:U:87:GLY:HA2	1.94	0.49
1:a:224:LYS:HG2	1:a:251:LEU:HD22	1.93	0.49
18:a:4011:BCR:H393	18:b:4012:BCR:H321	1.94	0.49
14:B:1207:CLA:HMC2	18:I:4018:BCR:H19C	1.94	0.49
1:G:726:GLY:HA3	2:H:575:CYS:HB2	1.93	0.49
1:a:230:VAL:HB	1:a:234:ASP:HB3	1.93	0.49
2:B:140:LEU:HD21	11:M:11:ALA:HA	1.95	0.49
3:N:2:SER:OG	3:N:71:ALA:O	2.30	0.49
14:b:1022:CLA:H191	18:b:4012:BCR:H363	1.94	0.49
14:b:1210:CLA:H203	14:b:1215:CLA:HBB2	1.95	0.49
2:B:403:ASP:OD2	2:B:403:ASP:N	2.46	0.49
14:a:1013:CLA:HMD3	2:b:540:ILE:HG12	1.95	0.49
6:f:111:LYS:HD2	6:f:115:LYS:HE3	1.93	0.49
18:A:4011:BCR:H393	18:B:4012:BCR:H321	1.94	0.49
2:B:505:LEU:HA	2:B:508:ILE:HG22	1.95	0.49
2:B:566:CYS:SG	2:B:567:ASP:N	2.85	0.49
3:C:2:SER:OG	3:C:71:ALA:O	2.30	0.49
10:U:106:ALA:HB2	10:U:135:TRP:CD1	2.47	0.49
1:a:574:ILE:HD12	13:a:1011:CL0:H61	1.95	0.49
14:a:1116:CLA:HBA2	14:a:1116:CLA:H3A	1.67	0.49
1:A:505:ILE:HG21	1:A:541:PRO:HA	1.95	0.49
14:B:1210:CLA:H203	14:B:1215:CLA:HBB2	1.95	0.49
3:C:6:LYS:NZ	4:D:154:TYR:O	2.46	0.49
1:G:201:ALA:HB2	1:G:311:GLY:HA3	1.94	0.49
14:b:1204:CLA:HMB3	14:b:1205:CLA:HHB	1.95	0.49
14:b:1205:CLA:H43	14:b:1224:CLA:H11	1.95	0.49
2:B:421:ALA:O	2:B:425:HIS:ND1	2.46	0.49
14:G:1013:CLA:HMD3	2:H:540:ILE:HG12	1.95	0.49
2:H:421:ALA:O	2:H:425:HIS:ND1	2.46	0.49
14:H:1210:CLA:H102	14:H:1215:CLA:H92	1.95	0.49
16:H:2002:PQN:H141	16:H:2002:PQN:H161	1.61	0.49
2:b:403:ASP:OD2	2:b:403:ASP:N	2.46	0.49
14:A:1013:CLA:HMD3	2:B:540:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:ILE:HD12	13:A:1011:CL0:H61	1.94	0.48
14:B:1204:CLA:HMB3	14:B:1205:CLA:HHB	1.95	0.48
14:H:1205:CLA:H43	14:H:1224:CLA:H11	1.95	0.48
1:a:726:GLY:HA3	2:b:575:CYS:HB2	1.94	0.48
14:b:1022:CLA:H41	14:b:1022:CLA:H61	1.57	0.48
3:N:15:THR:OG1	3:N:19:ARG:NH1	2.47	0.48
1:a:201:ALA:HB2	1:a:311:GLY:HA3	1.94	0.48
14:B:1210:CLA:H102	14:B:1215:CLA:H92	1.95	0.48
20:R:5006:LMG:H361	18:V:4021:BCR:H392	1.95	0.48
2:b:421:ALA:O	2:b:425:HIS:ND1	2.46	0.48
2:b:505:LEU:HA	2:b:508:ILE:HG22	1.95	0.48
18:G:4011:BCR:H393	18:H:4012:BCR:H321	1.94	0.48
2:H:432:PHE:O	2:H:436:HIS:ND1	2.39	0.48
14:a:1111:CLA:H102	18:a:4003:BCR:H353	1.95	0.48
2:b:176:ASN:HB3	14:b:1217:CLA:HMD2	1.95	0.48
14:A:1140:CLA:HAC1	16:A:2001:PQN:H161	1.96	0.48
14:B:1238:CLA:HAB	16:B:2002:PQN:H161	1.95	0.48
14:L:1501:CLA:H12	7:i:32:PRO:HG3	1.95	0.48
6:Q:91:THR:O	6:Q:91:THR:OG1	2.29	0.48
1:G:574:ILE:HD12	13:G:1011:CL0:H61	1.94	0.48
2:H:566:CYS:SG	2:H:567:ASP:N	2.85	0.48
3:N:62:PHE:CD2	5:P:14:GLU:HB2	2.49	0.48
3:c:6:LYS:NZ	4:d:154:TYR:O	2.46	0.48
10:l:70:GLU:HB3	10:l:87:GLY:HA2	1.94	0.48
6:F:91:THR:O	6:F:91:THR:OG1	2.29	0.48
2:H:441:TYR:O	2:H:445:ASP:N	2.46	0.48
18:A:4007:BCR:H351	18:A:4007:BCR:H15C	1.63	0.48
2:B:176:ASN:HB3	14:B:1217:CLA:HMD2	1.95	0.48
14:G:1111:CLA:H102	18:G:4003:BCR:H353	1.95	0.48
8:J:2:GLU:HG2	8:J:4:ARG:H	1.79	0.48
5:P:10:ILE:HG22	5:P:12:ARG:H	1.79	0.48
14:a:1103:CLA:H42	18:a:4003:BCR:H272	1.95	0.48
14:b:1201:CLA:H62	14:b:1201:CLA:H41	1.64	0.48
14:b:1206:CLA:HBA2	14:b:1206:CLA:H3A	1.53	0.48
18:b:4009:BCR:H351	18:b:4009:BCR:H15C	1.58	0.48
3:c:2:SER:OG	3:c:71:ALA:O	2.30	0.48
14:B:1223:CLA:H71	14:B:1223:CLA:H111	1.75	0.48
4:D:80:LYS:HE3	4:D:112:ILE:HD12	1.94	0.48
2:H:176:ASN:HB3	14:H:1217:CLA:HMD2	1.95	0.48
8:S:2:GLU:HG2	8:S:4:ARG:H	1.79	0.48
15:B:1230:F6C:OMB	8:J:40:TYR:OH	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:THR:OG1	3:C:19:ARG:NH1	2.47	0.47
5:E:10:ILE:HG22	5:E:12:ARG:H	1.79	0.47
14:G:1130:CLA:H41	14:G:1130:CLA:H61	1.70	0.47
2:b:325:GLY:O	2:b:406:GLN:NE2	2.47	0.47
2:H:325:GLY:O	2:H:406:GLN:NE2	2.47	0.47
1:a:97:SER:HB2	1:a:143:PHE:HZ	1.79	0.47
14:b:1210:CLA:H102	14:b:1215:CLA:H92	1.95	0.47
6:f:90:TYR:OH	6:f:132:LEU:O	2.32	0.47
8:j:2:GLU:HG2	8:j:4:ARG:H	1.79	0.47
2:B:432:PHE:O	2:B:436:HIS:ND1	2.39	0.47
14:B:1205:CLA:H43	14:B:1224:CLA:H11	1.95	0.47
1:G:505:ILE:HG21	1:G:541:PRO:HA	1.95	0.47
18:L:4022:BCR:H14C	14:U:1503:CLA:H193	1.97	0.47
1:a:709:PHE:O	1:a:713:HIS:ND1	2.42	0.47
18:a:4001:BCR:H343	9:k:70:ALA:HB1	1.96	0.47
2:H:403:ASP:OD2	2:H:403:ASP:N	2.46	0.47
14:H:1202:CLA:HBA1	14:H:1202:CLA:H3A	1.78	0.47
3:N:6:LYS:NZ	4:O:154:TYR:O	2.47	0.47
1:a:505:ILE:HG21	1:a:541:PRO:HA	1.95	0.47
14:H:1204:CLA:HMB3	14:H:1205:CLA:HHB	1.95	0.47
1:a:458:LEU:O	1:a:462:SER:OG	2.26	0.47
3:c:15:THR:OG1	3:c:19:ARG:NH1	2.47	0.47
14:A:1111:CLA:H102	18:A:4003:BCR:H353	1.95	0.47
2:B:325:GLY:O	2:B:406:GLN:NE2	2.47	0.47
14:B:1217:CLA:H3A	14:B:1217:CLA:HBA2	1.66	0.47
2:H:29:HIS:CD2	14:H:1202:CLA:HAB	2.45	0.47
2:H:345:LEU:HD22	14:H:1202:CLA:HED1	1.97	0.47
2:H:361:PRO:HG3	14:H:1215:CLA:HBA1	1.97	0.47
14:H:1203:CLA:H61	14:H:1203:CLA:H41	1.54	0.47
2:B:441:TYR:O	2:B:445:ASP:N	2.46	0.47
1:G:97:SER:HB2	1:G:143:PHE:HZ	1.79	0.47
7:I:30:PRO:HA	7:I:33:VAL:HB	1.96	0.47
6:Q:53:PRO:HD3	8:S:35:PHE:HB2	1.96	0.47
14:U:1501:CLA:H143	14:U:1503:CLA:H192	1.97	0.47
11:V:23:TRP:CH2	10:l:34:LEU:HB2	2.50	0.47
14:b:1238:CLA:HAB	16:b:2002:PQN:H161	1.95	0.47
14:A:1103:CLA:H42	18:A:4003:BCR:H272	1.96	0.47
18:B:4010:BCR:H24C	18:B:4010:BCR:H371	1.67	0.47
14:H:1229:CLA:H62	14:H:1229:CLA:H41	1.72	0.47
2:b:345:LEU:HD22	14:b:1202:CLA:HED1	1.97	0.47
18:l:4022:BCR:H15C	18:l:4022:BCR:H351	1.64	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:4001:BCR:H15C	18:A:4001:BCR:H351	1.73	0.47
2:B:44:GLN:NE2	2:B:163:PRO:O	2.47	0.47
2:B:420:GLU:HG3	6:F:159:ARG:HH11	1.80	0.47
2:B:581:ASP:OD1	2:B:712:ARG:NH1	2.48	0.47
18:G:4011:BCR:H14C	14:H:1012:CLA:H161	1.97	0.47
3:N:2:SER:N	3:N:76:SER:OG	2.44	0.47
14:b:1217:CLA:H3A	14:b:1217:CLA:HBA2	1.65	0.47
2:H:173:ALA:O	2:H:177:HIS:ND1	2.36	0.47
14:H:1206:CLA:H3A	14:H:1206:CLA:HBA2	1.53	0.47
7:R:30:PRO:HA	7:R:33:VAL:HB	1.96	0.47
6:F:121:VAL:HG23	6:F:122:PRO:HD3	1.97	0.46
14:G:1103:CLA:H42	18:G:4003:BCR:H272	1.95	0.46
1:a:194:SER:O	1:a:198:HIS:ND1	2.40	0.46
1:a:369:MET:HE3	14:a:1119:CLA:H93	1.97	0.46
7:i:30:PRO:HA	7:i:33:VAL:HB	1.96	0.46
14:l:1501:CLA:H143	14:l:1503:CLA:H192	1.97	0.46
14:B:1234:CLA:H52	14:B:1234:CLA:H11	1.70	0.46
14:B:1238:CLA:HBD	14:B:1238:CLA:HBA1	1.98	0.46
18:B:4005:BCR:H351	18:B:4005:BCR:H15C	1.70	0.46
2:b:419:LYS:HB2	2:b:546:LEU:HD13	1.97	0.46
2:b:420:GLU:HG3	6:f:159:ARG:HH11	1.80	0.46
5:e:10:ILE:HG22	5:e:12:ARG:H	1.79	0.46
2:B:677:TYR:OH	14:B:1023:CLA:OBD	2.33	0.46
14:G:1140:CLA:HAC1	16:G:2001:PQN:H161	1.96	0.46
14:H:1211:CLA:H142	14:H:1211:CLA:H112	1.80	0.46
1:G:552:ALA:HB1	1:G:658:VAL:HG21	1.98	0.46
18:G:4002:BCR:H351	18:G:4002:BCR:H15C	1.68	0.46
2:H:384:GLY:HA3	2:H:594:LEU:HD11	1.97	0.46
14:L:1501:CLA:H143	14:L:1503:CLA:H192	1.97	0.46
14:b:1205:CLA:H2	14:b:1205:CLA:H61	1.72	0.46
14:H:1238:CLA:HAB	16:H:2002:PQN:H161	1.95	0.46
14:a:1140:CLA:HAC1	16:a:2001:PQN:H161	1.96	0.46
2:b:581:ASP:OD1	2:b:712:ARG:NH1	2.48	0.46
14:b:1211:CLA:H12	14:b:1211:CLA:H51	1.74	0.46
14:G:1106:CLA:HBB1	18:H:4012:BCR:H19C	1.98	0.46
19:H:5004:LHG:H361	14:W:1701:CLA:HBC1	1.98	0.46
18:U:4022:BCR:H24C	18:U:4022:BCR:H371	1.70	0.46
1:a:552:ALA:HB1	1:a:658:VAL:HG21	1.98	0.46
18:a:4011:BCR:H14C	14:b:1022:CLA:H161	1.97	0.46
2:b:384:GLY:HA3	2:b:594:LEU:HD11	1.97	0.46
18:G:4003:BCR:H351	18:G:4003:BCR:H15C	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:203:ARG:HD3	2:H:250:ALA:HB1	1.98	0.46
14:H:1211:CLA:HMA3	18:H:4006:BCR:H292	1.98	0.46
10:U:125:SER:OG	10:U:126:LEU:N	2.49	0.46
14:a:1133:CLA:H62	14:a:1133:CLA:H92	1.80	0.46
2:B:345:LEU:HD22	14:B:1202:CLA:HED1	1.97	0.46
2:B:441:TYR:HD2	14:B:1021:CLA:H203	1.81	0.46
14:B:1211:CLA:H142	14:B:1211:CLA:H112	1.80	0.46
2:H:441:TYR:HD2	14:H:1021:CLA:H203	1.81	0.46
2:H:583:SER:O	2:H:583:SER:OG	2.33	0.46
6:Q:90:TYR:OH	6:Q:132:LEU:O	2.31	0.46
18:R:4018:BCR:H24C	18:R:4018:BCR:H371	1.74	0.46
14:a:1127:CLA:H12	18:a:4003:BCR:H403	1.98	0.46
14:a:1140:CLA:H41	14:a:1140:CLA:H62	1.74	0.46
2:b:361:PRO:HG3	14:b:1215:CLA:HBA1	1.97	0.46
18:A:4003:BCR:H15C	18:A:4003:BCR:H351	1.58	0.46
1:A:97:SER:HB2	1:A:143:PHE:HZ	1.79	0.46
1:A:552:ALA:HB1	1:A:658:VAL:HG21	1.98	0.46
2:B:419:LYS:HB2	2:B:546:LEU:HD13	1.97	0.46
1:a:774:VAL:HG11	18:a:4011:BCR:H352	1.98	0.46
2:b:203:ARG:HD3	2:b:250:ALA:HB1	1.98	0.46
14:b:1203:CLA:H112	14:b:1203:CLA:H152	1.66	0.46
10:l:125:SER:OG	10:l:126:LEU:N	2.49	0.46
18:A:4011:BCR:H14C	14:B:1022:CLA:H161	1.97	0.45
2:B:361:PRO:HG3	14:B:1215:CLA:HBA1	1.97	0.45
2:B:622:TYR:OH	2:B:628:ARG:NH2	2.49	0.45
14:B:1022:CLA:H61	14:B:1022:CLA:H41	1.58	0.45
1:G:139:THR:O	1:G:399:SER:OG	2.35	0.45
1:G:369:MET:HE3	14:G:1119:CLA:H93	1.97	0.45
14:H:1203:CLA:H152	14:H:1203:CLA:H112	1.66	0.45
14:H:1225:CLA:HBA2	14:H:1225:CLA:H3A	1.55	0.45
6:Q:121:VAL:HG23	6:Q:122:PRO:HD3	1.97	0.45
2:b:441:TYR:O	2:b:445:ASP:N	2.46	0.45
10:l:142:ILE:HD13	18:l:4019:BCR:H292	1.98	0.45
1:A:369:MET:HE3	14:A:1119:CLA:H93	1.97	0.45
1:A:774:VAL:HG11	18:A:4011:BCR:H352	1.98	0.45
14:A:1136:CLA:H62	14:A:1136:CLA:H41	1.61	0.45
6:F:61:LEU:O	6:F:69:ARG:N	2.49	0.45
1:G:451:LEU:HG	1:G:584:LEU:HB2	1.98	0.45
18:L:4022:BCR:H351	18:L:4022:BCR:H15C	1.64	0.45
1:a:215:LEU:HA	1:a:219:SER:HB2	1.99	0.45
14:b:1203:CLA:H41	14:b:1203:CLA:H61	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:O	1:A:399:SER:OG	2.35	0.45
1:A:451:LEU:HG	1:A:584:LEU:HB2	1.98	0.45
2:B:384:GLY:HA3	2:B:594:LEU:HD11	1.97	0.45
2:H:65:LEU:HD11	18:H:4006:BCR:H281	1.99	0.45
10:L:142:ILE:HD13	18:L:4019:BCR:H292	1.98	0.45
14:a:1133:CLA:HBA2	14:a:1133:CLA:H3A	1.64	0.45
14:b:1211:CLA:HMA3	18:b:4006:BCR:H292	1.98	0.45
1:A:620:CYS:SG	2:B:674:TRP:HB3	2.57	0.45
14:B:1220:CLA:H2	14:B:1220:CLA:H61	1.68	0.45
6:F:56:ALA:O	6:F:59:GLN:NE2	2.50	0.45
14:G:1127:CLA:H12	18:G:4003:BCR:H403	1.98	0.45
14:H:1023:CLA:H111	14:H:1023:CLA:H143	1.85	0.45
14:H:1220:CLA:H2	14:H:1220:CLA:H61	1.68	0.45
2:b:65:LEU:HD11	18:b:4006:BCR:H281	1.99	0.45
2:b:140:LEU:HD21	11:m:11:ALA:HA	1.99	0.45
14:b:1208:CLA:H12	14:b:1208:CLA:H52	1.73	0.45
14:A:1013:CLA:C1D	2:B:589:TRP:HE1	2.30	0.45
3:C:19:ARG:HG2	4:D:121:GLU:HG2	1.98	0.45
1:G:215:LEU:HA	1:G:219:SER:HB2	1.99	0.45
14:G:1013:CLA:C1D	2:H:589:TRP:HE1	2.30	0.45
14:G:1125:CLA:H152	14:G:1125:CLA:H112	1.50	0.45
14:G:1133:CLA:H3A	14:G:1133:CLA:HBA2	1.64	0.45
2:H:419:LYS:HB2	2:H:546:LEU:HD13	1.97	0.45
2:H:581:ASP:OD1	2:H:712:ARG:NH1	2.48	0.45
14:H:1231:CLA:H52	14:H:1231:CLA:H12	1.72	0.45
14:H:1238:CLA:H41	14:H:1238:CLA:H61	1.71	0.45
6:Q:61:LEU:O	6:Q:69:ARG:N	2.50	0.45
10:U:144:LEU:HD21	10:l:56:LEU:HD11	1.98	0.45
1:a:451:LEU:HG	1:a:584:LEU:HB2	1.99	0.45
14:b:1223:CLA:H71	14:b:1223:CLA:H111	1.75	0.45
6:f:56:ALA:O	6:f:59:GLN:NE2	2.50	0.45
1:A:215:LEU:HA	1:A:219:SER:HB2	1.99	0.45
14:B:1211:CLA:HMA3	18:B:4006:BCR:H292	1.98	0.45
14:B:1229:CLA:CAB	15:B:1230:F6C:CMB	2.95	0.45
18:B:4017:BCR:H15C	18:B:4017:BCR:H351	1.60	0.45
1:G:684:ARG:HA	2:H:639:ILE:HD12	1.99	0.45
1:G:737:ILE:O	1:G:741:HIS:ND1	2.41	0.45
14:a:1013:CLA:C1D	2:b:589:TRP:HE1	2.30	0.45
2:b:356:MET:HE2	2:b:356:MET:HB3	1.71	0.45
14:b:1208:CLA:H201	14:b:1211:CLA:H191	1.98	0.45
6:f:42:LYS:HA	6:f:42:LYS:HD2	1.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:4006:BCR:H351	18:B:4006:BCR:H15C	1.64	0.45
6:Q:39:GLU:HA	6:Q:42:LYS:HB2	1.99	0.45
14:a:1130:CLA:H41	14:a:1130:CLA:H61	1.70	0.45
18:b:4017:BCR:H351	18:b:4017:BCR:H15C	1.60	0.45
18:l:4022:BCR:H24C	18:l:4022:BCR:H371	1.70	0.45
1:A:735:GLU:OE2	5:E:46:TYR:OH	2.27	0.45
14:A:1116:CLA:HBA2	14:A:1116:CLA:H3A	1.67	0.45
14:A:1127:CLA:H12	18:A:4003:BCR:H403	1.98	0.45
16:A:2001:PQN:H192	16:A:2001:PQN:H162	1.80	0.45
2:B:554:MET:SD	3:C:66:ARG:NH2	2.89	0.45
6:F:90:TYR:OH	6:F:132:LEU:O	2.31	0.45
14:H:1208:CLA:H201	14:H:1211:CLA:H191	1.98	0.45
3:N:61:ASP:OD2	5:P:15:SER:OG	2.28	0.45
6:Q:42:LYS:HD2	6:Q:42:LYS:HA	1.58	0.45
6:f:61:LEU:O	6:f:69:ARG:N	2.49	0.45
6:f:121:VAL:HG23	6:f:122:PRO:HD3	1.97	0.45
14:H:1234:CLA:H11	14:H:1234:CLA:H52	1.70	0.45
14:H:1238:CLA:HBA1	14:H:1238:CLA:HBD	1.98	0.45
6:Q:56:ALA:O	6:Q:59:GLN:NE2	2.50	0.45
1:a:684:ARG:HA	2:b:639:ILE:HD12	1.98	0.45
14:a:1104:CLA:H112	14:a:1104:CLA:H71	1.87	0.45
16:a:2001:PQN:H211	16:a:2001:PQN:H191	1.79	0.45
2:b:469:SER:O	2:b:483:SER:OG	2.31	0.45
2:b:554:MET:SD	3:c:66:ARG:NH2	2.89	0.45
14:b:1238:CLA:H92	14:b:1238:CLA:H62	1.82	0.45
14:A:1106:CLA:HBB1	18:B:4012:BCR:H19C	1.99	0.45
14:A:1125:CLA:H112	14:A:1125:CLA:H152	1.50	0.45
14:H:1216:CLA:HMB2	14:H:1221:CLA:HMA3	1.99	0.45
1:a:139:THR:O	1:a:399:SER:OG	2.35	0.45
14:b:1238:CLA:HBD	14:b:1238:CLA:HBA1	1.98	0.45
14:l:1503:CLA:H142	14:l:1503:CLA:H111	1.86	0.45
1:A:684:ARG:HA	2:B:639:ILE:HD12	1.99	0.44
14:B:1226:CLA:H112	14:B:1226:CLA:H142	1.82	0.44
14:B:1229:CLA:H62	14:B:1229:CLA:H41	1.72	0.44
1:G:774:VAL:HG11	18:G:4011:BCR:H352	1.98	0.44
14:G:1124:CLA:HBA2	14:G:1124:CLA:H3A	1.63	0.44
2:H:319:PHE:HD1	14:H:1219:CLA:HAB	1.82	0.44
18:a:4001:BCR:H351	18:a:4001:BCR:H15C	1.73	0.44
2:b:622:TYR:OH	2:b:628:ARG:NH2	2.49	0.44
1:A:722:PHE:HA	16:A:2001:PQN:H9	2.00	0.44
14:B:1238:CLA:H92	14:B:1238:CLA:H62	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:GLN:NE2	2:H:163:PRO:O	2.47	0.44
1:a:489:LEU:HB2	1:a:566:THR:HG23	1.99	0.44
14:a:1126:CLA:H41	14:a:1126:CLA:H62	1.81	0.44
6:f:91:THR:O	6:f:91:THR:OG1	2.28	0.44
2:B:203:ARG:HD3	2:B:250:ALA:HB1	1.98	0.44
14:B:1023:CLA:H143	14:B:1023:CLA:H111	1.85	0.44
14:B:1205:CLA:H2	14:B:1205:CLA:H61	1.72	0.44
14:B:1206:CLA:H3A	14:B:1206:CLA:HBA2	1.53	0.44
14:B:1208:CLA:H201	14:B:1211:CLA:H191	1.98	0.44
1:G:620:CYS:SG	2:H:674:TRP:HB3	2.57	0.44
18:H:4009:BCR:H24C	18:H:4009:BCR:H371	1.73	0.44
7:R:17:LEU:HD21	11:V:12:LEU:HD11	1.98	0.44
10:U:142:ILE:HD13	18:U:4019:BCR:H292	1.98	0.44
1:a:307:PHE:CE1	14:a:1119:CLA:HAB	2.51	0.44
14:a:1117:CLA:HBA2	14:a:1117:CLA:H3A	1.74	0.44
3:c:19:ARG:HG2	4:d:121:GLU:HG2	1.98	0.44
6:f:118:PHE:HA	8:j:12:SER:HA	1.99	0.44
2:B:190:TRP:NE1	14:B:1215:CLA:O1D	2.48	0.44
1:G:722:PHE:HA	16:G:2001:PQN:H9	2.00	0.44
2:H:92:TRP:HB3	7:R:22:ILE:HG13	1.99	0.44
2:H:622:TYR:OH	2:H:628:ARG:NH2	2.49	0.44
18:i:4020:BCR:H351	18:i:4020:BCR:H15C	1.80	0.44
1:A:279:THR:OG1	1:A:294:THR:OG1	2.29	0.44
2:B:92:TRP:HB3	7:I:22:ILE:HG13	1.99	0.44
4:D:83:CYS:O	4:D:87:GLY:N	2.47	0.44
1:G:489:LEU:HB2	1:G:566:THR:HG23	1.99	0.44
14:G:1116:CLA:HBA2	14:G:1116:CLA:H3A	1.67	0.44
14:G:1136:CLA:H41	14:G:1136:CLA:H62	1.61	0.44
2:H:328:GLU:O	2:H:332:ASN:ND2	2.51	0.44
18:L:4019:BCR:H15C	18:L:4019:BCR:H351	1.83	0.44
1:a:269:LEU:HD21	9:k:80:VAL:HG22	1.98	0.44
1:a:369:MET:HG3	14:a:1123:CLA:HHB	1.99	0.44
1:a:620:CYS:SG	2:b:674:TRP:HB3	2.57	0.44
14:a:1125:CLA:H112	14:a:1125:CLA:H152	1.50	0.44
1:A:709:PHE:O	1:A:713:HIS:ND1	2.43	0.44
2:H:294:ASN:OD1	2:H:294:ASN:N	2.50	0.44
14:a:1106:CLA:HBB1	18:b:4012:BCR:H19C	1.99	0.44
2:b:29:HIS:CD2	14:b:1202:CLA:HAB	2.45	0.44
14:b:1202:CLA:HBA1	14:b:1202:CLA:H3A	1.79	0.44
14:b:1222:CLA:HBA2	14:b:1222:CLA:H3A	1.83	0.44
1:A:369:MET:HG3	14:A:1123:CLA:HHB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:4011:BCR:H281	18:B:4012:BCR:H321	1.99	0.44
16:B:2002:PQN:H141	16:B:2002:PQN:H161	1.61	0.44
18:B:4014:BCR:H351	18:B:4014:BCR:H15C	1.77	0.44
6:F:42:LYS:HD2	6:F:42:LYS:HA	1.58	0.44
18:H:4017:BCR:H351	18:H:4017:BCR:H15C	1.60	0.44
11:V:4:SER:OG	11:V:5:ASP:N	2.50	0.44
1:a:672:PHE:O	1:a:676:SER:OG	2.31	0.44
1:a:722:PHE:HA	16:a:2001:PQN:H9	2.00	0.44
2:b:441:TYR:HD2	14:b:1021:CLA:H203	1.81	0.44
14:b:1234:CLA:H52	14:b:1234:CLA:H11	1.70	0.44
16:b:2002:PQN:H141	16:b:2002:PQN:H161	1.61	0.44
1:A:384:MET:HB2	1:A:384:MET:HE3	1.78	0.44
1:A:610:PRO:HB3	1:A:757:ILE:HB	2.00	0.44
2:B:294:ASN:OD1	2:B:294:ASN:N	2.50	0.44
2:B:441:TYR:CD2	14:B:1021:CLA:H203	2.53	0.44
14:B:1208:CLA:H52	14:B:1208:CLA:H12	1.73	0.44
14:H:1224:CLA:H92	14:H:1224:CLA:H62	1.81	0.44
18:I:4020:BCR:H332	10:L:90:THR:HA	2.00	0.44
2:b:441:TYR:CD2	14:b:1021:CLA:H203	2.53	0.44
18:b:4010:BCR:H371	18:b:4010:BCR:H24C	1.67	0.44
4:d:54:LYS:HE3	4:d:54:LYS:HB2	1.83	0.44
14:B:1210:CLA:H112	14:B:1210:CLA:H142	1.78	0.44
18:B:4009:BCR:H371	18:B:4009:BCR:H24C	1.73	0.44
1:G:42:LYS:HD3	1:G:42:LYS:HA	1.87	0.44
1:G:451:LEU:HD21	1:G:583:VAL:HG12	1.99	0.44
1:G:616:ARG:HA	3:N:77:MET:HA	2.00	0.44
18:G:4007:BCR:H351	18:G:4007:BCR:H15C	1.62	0.44
2:H:590:MET:HE3	2:H:590:MET:HB3	1.86	0.44
2:H:738:LYS:HD2	2:H:738:LYS:HA	1.86	0.44
11:M:4:SER:OG	11:M:5:ASP:N	2.50	0.44
18:U:4022:BCR:H14C	14:l:1503:CLA:H193	2.00	0.44
1:a:103:MET:HE3	1:a:103:MET:HB3	1.93	0.44
1:a:145:MET:HE2	1:a:145:MET:HB3	1.93	0.44
18:b:4004:BCR:H15C	18:b:4004:BCR:H351	1.72	0.44
18:b:4005:BCR:H15C	18:b:4005:BCR:H351	1.70	0.44
4:d:32:SER:OG	4:d:33:THR:N	2.51	0.44
2:B:356:MET:HE2	2:B:356:MET:HB3	1.71	0.43
14:B:1226:CLA:HBC2	20:B:5002:LMG:H331	2.00	0.43
18:B:4005:BCR:H24C	18:B:4005:BCR:H371	1.77	0.43
6:F:39:GLU:HA	6:F:42:LYS:HB2	1.99	0.43
2:H:464:ALA:HA	2:H:467:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:83:CYS:O	4:O:87:GLY:N	2.47	0.43
14:b:1229:CLA:H62	14:b:1229:CLA:H41	1.72	0.43
18:b:4014:BCR:H15C	18:b:4014:BCR:H351	1.77	0.43
6:f:39:GLU:HA	6:f:42:LYS:HB2	1.99	0.43
1:A:451:LEU:HD21	1:A:583:VAL:HG12	1.99	0.43
14:B:1231:CLA:H52	14:B:1231:CLA:H12	1.72	0.43
14:G:1140:CLA:H41	14:G:1140:CLA:H62	1.74	0.43
2:H:728:GLY:HA3	14:H:1224:CLA:H43	2.00	0.43
14:H:1012:CLA:H41	14:H:1012:CLA:H61	1.57	0.43
10:L:56:LEU:HD11	10:l:144:LEU:HD21	2.00	0.43
14:b:1238:CLA:H41	14:b:1238:CLA:H61	1.71	0.43
14:B:1216:CLA:HMB2	14:B:1221:CLA:HMA3	1.99	0.43
3:c:62:PHE:CD2	5:e:14:GLU:HB2	2.54	0.43
4:d:141:PRO:O	4:d:153:THR:OG1	2.36	0.43
1:A:489:LEU:HB2	1:A:566:THR:HG23	1.99	0.43
2:B:328:GLU:O	2:B:332:ASN:ND2	2.51	0.43
2:B:728:GLY:HA3	14:B:1224:CLA:H43	2.00	0.43
14:B:1219:CLA:HBC3	18:B:4009:BCR:H323	2.00	0.43
18:G:4011:BCR:H281	18:H:4012:BCR:H321	2.00	0.43
2:H:441:TYR:CD2	14:H:1021:CLA:H203	2.53	0.43
14:H:1208:CLA:H52	14:H:1208:CLA:H12	1.73	0.43
14:H:1238:CLA:H92	14:H:1238:CLA:H62	1.82	0.43
4:O:80:LYS:HE2	4:O:84:ILE:HD11	2.01	0.43
8:S:34:LEU:HD23	8:S:34:LEU:HA	1.87	0.43
2:b:319:PHE:HD1	14:b:1219:CLA:HAB	1.82	0.43
2:b:700:ARG:HB2	14:b:1238:CLA:HED3	2.01	0.43
14:b:1216:CLA:HMB2	14:b:1221:CLA:HMA3	1.99	0.43
10:l:129:LEU:HD23	10:l:129:LEU:HA	1.92	0.43
1:A:672:PHE:O	1:A:676:SER:OG	2.32	0.43
16:A:2001:PQN:H191	16:A:2001:PQN:H211	1.80	0.43
1:G:387:TYR:HB2	1:G:390:LEU:HB2	2.01	0.43
1:a:442:ARG:NH1	4:d:31:GLY:O	2.50	0.43
14:a:1131:CLA:HMA3	18:i:4018:BCR:H292	2.00	0.43
18:a:4011:BCR:H281	18:b:4012:BCR:H321	1.99	0.43
2:b:44:GLN:NE2	2:b:163:PRO:O	2.47	0.43
2:b:328:GLU:O	2:b:332:ASN:ND2	2.51	0.43
14:B:1204:CLA:HHB	14:B:1205:CLA:HMB2	2.01	0.43
14:H:1204:CLA:HHB	14:H:1205:CLA:HMB2	2.01	0.43
14:H:1205:CLA:H2	14:H:1205:CLA:H61	1.72	0.43
7:I:37:LEU:HD12	7:I:40:TRP:HE1	1.83	0.43
3:N:19:ARG:HG2	4:O:121:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:392:THR:O	1:a:556:LYS:NZ	2.46	0.43
14:a:1136:CLA:H3A	14:a:1136:CLA:HBA2	1.80	0.43
3:c:66:ARG:HA	3:c:66:ARG:HD2	1.85	0.43
1:A:715:ILE:HB	1:A:771:GLY:HA3	2.01	0.43
14:A:1140:CLA:H62	14:A:1140:CLA:H41	1.74	0.43
14:B:1221:CLA:H92	14:B:1221:CLA:H61	1.83	0.43
6:F:65:ASP:OD2	6:F:69:ARG:NH1	2.52	0.43
14:G:1106:CLA:H3A	14:G:1106:CLA:HBA2	1.53	0.43
2:H:64:ILE:HG23	14:H:1205:CLA:HED2	2.01	0.43
14:H:1223:CLA:H92	14:H:1223:CLA:H62	1.85	0.43
1:a:451:LEU:HD21	1:a:583:VAL:HG12	1.99	0.43
1:a:610:PRO:HB3	1:a:757:ILE:HB	2.00	0.43
20:a:5005:LMG:H322	20:a:5005:LMG:H291	1.79	0.43
2:b:64:ILE:HG23	14:b:1205:CLA:HED2	2.01	0.43
14:b:1222:CLA:H91	14:b:1222:CLA:H111	1.80	0.43
14:b:1226:CLA:HBC2	20:b:5002:LMG:H331	2.00	0.43
2:B:65:LEU:HD11	18:B:4006:BCR:H281	1.99	0.43
2:B:531:ALA:O	2:B:535:HIS:ND1	2.33	0.43
14:B:1213:CLA:H92	14:B:1213:CLA:H61	1.88	0.43
2:H:408:LYS:HA	2:H:408:LYS:HD2	1.85	0.43
10:L:125:SER:OG	10:L:126:LEU:N	2.49	0.43
10:L:144:LEU:HD21	10:U:56:LEU:HD11	2.01	0.43
18:R:4020:BCR:H15C	18:R:4020:BCR:H351	1.80	0.43
1:a:70:LYS:NZ	14:a:1109:CLA:OBD	2.44	0.43
14:a:1126:CLA:H62	14:a:1126:CLA:H92	1.87	0.43
2:b:125:TYR:HE2	2:b:364:PHE:HE2	1.66	0.43
2:b:190:TRP:NE1	14:b:1215:CLA:O1D	2.48	0.43
14:b:1219:CLA:HBC3	18:b:4009:BCR:H323	2.00	0.43
2:B:738:LYS:HD2	2:B:738:LYS:HA	1.86	0.43
14:B:1203:CLA:H41	14:B:1203:CLA:H61	1.54	0.43
1:G:715:ILE:HB	1:G:771:GLY:HA3	2.01	0.43
20:G:5005:LMG:H291	20:G:5005:LMG:H322	1.79	0.43
18:H:4005:BCR:H351	18:H:4005:BCR:H15C	1.70	0.43
18:I:4018:BCR:H24C	18:I:4018:BCR:H371	1.74	0.43
4:O:37:LEU:HD23	4:O:37:LEU:HA	1.91	0.43
2:b:583:SER:O	2:b:583:SER:OG	2.33	0.43
14:b:1202:CLA:HED3	14:b:1226:CLA:HBB2	2.01	0.43
14:b:1204:CLA:HHB	14:b:1205:CLA:HMB2	2.01	0.43
3:c:27:GLU:OE1	4:d:127:ARG:NH1	2.52	0.43
1:A:194:SER:O	1:A:198:HIS:ND1	2.40	0.43
1:G:734:ILE:HG22	1:G:738:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:750:ILE:HG12	6:Q:116:GLU:OE1	2.19	0.43
14:G:1117:CLA:HBA2	14:G:1117:CLA:H3A	1.74	0.43
18:H:4010:BCR:H24C	18:H:4010:BCR:H371	1.67	0.43
11:M:26:ALA:HB2	18:M:4021:BCR:HC41	2.01	0.43
7:R:37:LEU:HD12	7:R:40:TRP:HE1	1.83	0.43
14:a:1110:CLA:HAB	14:a:1118:CLA:C4C	2.49	0.43
14:a:1131:CLA:H143	14:a:1131:CLA:H111	1.86	0.43
2:b:473:LYS:NZ	2:b:516:PHE:O	2.49	0.43
14:b:1224:CLA:H62	14:b:1224:CLA:H92	1.81	0.43
14:b:1235:CLA:H92	14:b:1236:CLA:HAC2	2.01	0.43
14:A:1132:CLA:H92	14:A:1132:CLA:H61	1.79	0.42
14:B:1202:CLA:HED3	14:B:1226:CLA:HBB2	2.01	0.42
1:G:442:ARG:NH1	4:O:31:GLY:O	2.50	0.42
1:G:610:PRO:HB3	1:G:757:ILE:HB	2.00	0.42
1:G:737:ILE:HD13	14:G:1138:CLA:HMD2	2.01	0.42
14:G:1012:CLA:H92	14:G:1012:CLA:H62	1.86	0.42
2:H:125:TYR:HE2	2:H:364:PHE:HE2	1.66	0.42
14:H:1202:CLA:H91	14:H:1202:CLA:H112	1.87	0.42
1:a:195:MET:HE1	14:a:1123:CLA:H101	2.01	0.42
1:a:384:MET:HB2	1:a:384:MET:HE3	1.78	0.42
2:b:164:ASN:OD1	2:b:164:ASN:N	2.49	0.42
18:A:4008:BCR:H371	18:A:4008:BCR:H24C	1.84	0.42
14:B:1203:CLA:H161	14:B:1203:CLA:H193	1.82	0.42
4:D:32:SER:OG	4:D:33:THR:N	2.51	0.42
14:H:1226:CLA:H203	14:H:1226:CLA:H161	1.88	0.42
3:N:75:ARG:NH2	4:O:44:GLU:OE2	2.41	0.42
18:R:4020:BCR:H332	10:U:90:THR:HA	2.00	0.42
10:U:49:LEU:HD22	10:U:53:MET:HB3	2.01	0.42
14:a:1130:CLA:H52	14:l:1502:CLA:H12	2.01	0.42
1:A:387:TYR:HB2	1:A:390:LEU:HB2	2.01	0.42
1:A:472:MET:HB2	1:A:481:MET:HB3	2.02	0.42
14:A:1130:CLA:H52	14:L:1502:CLA:H12	2.01	0.42
1:G:369:MET:HG3	14:G:1123:CLA:HHB	1.99	0.42
2:H:356:MET:HE2	2:H:356:MET:HB3	1.71	0.42
2:H:700:ARG:HB2	14:H:1238:CLA:HED3	2.01	0.42
14:H:1226:CLA:HBC2	20:H:5002:LMG:H331	2.00	0.42
3:N:27:GLU:OE1	4:O:127:ARG:NH1	2.52	0.42
3:N:66:ARG:HD2	3:N:66:ARG:HA	1.85	0.42
14:U:1501:CLA:H91	14:U:1501:CLA:H112	1.88	0.42
2:b:87:ILE:HD11	2:b:107:ALA:HB3	2.01	0.42
1:A:442:ARG:NH1	4:D:31:GLY:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:1203:CLA:H152	14:B:1203:CLA:H112	1.66	0.42
14:G:1103:CLA:H112	18:G:4003:BCR:H372	2.01	0.42
2:H:87:ILE:HD11	2:H:107:ALA:HB3	2.01	0.42
18:M:4021:BCR:H371	18:M:4021:BCR:H24C	1.79	0.42
12:W:96:TYR:CG	14:W:1701:CLA:HED1	2.55	0.42
1:a:387:TYR:HB2	1:a:390:LEU:HB2	2.01	0.42
1:a:472:MET:HB2	1:a:481:MET:HB3	2.02	0.42
18:a:4007:BCR:H15C	18:a:4007:BCR:H351	1.62	0.42
14:b:1225:CLA:H3A	14:b:1225:CLA:HBA2	1.55	0.42
14:b:1226:CLA:H142	14:b:1226:CLA:H112	1.82	0.42
14:A:1131:CLA:HAB	14:A:1132:CLA:HHB	2.02	0.42
15:B:1230:F6C:C4C	18:B:4012:BCR:H332	2.49	0.42
1:G:709:PHE:O	1:G:713:HIS:ND1	2.43	0.42
16:G:2001:PQN:H243	16:G:2001:PQN:H261	1.86	0.42
2:H:185:VAL:HG13	18:H:4005:BCR:HC31	2.02	0.42
14:H:1202:CLA:HED3	14:H:1226:CLA:HBB2	2.00	0.42
14:H:1219:CLA:HBC3	18:H:4009:BCR:H323	2.00	0.42
2:b:398:TRP:HE1	18:b:4010:BCR:H271	1.84	0.42
4:d:80:LYS:HE2	4:d:84:ILE:HD11	2.01	0.42
11:m:4:SER:OG	11:m:5:ASP:N	2.50	0.42
1:A:616:ARG:HA	3:C:77:MET:HA	2.01	0.42
14:A:1110:CLA:HAB	14:A:1118:CLA:C4C	2.49	0.42
14:A:1124:CLA:H3A	14:A:1124:CLA:HBA2	1.63	0.42
14:A:1133:CLA:H3A	14:A:1133:CLA:HBA2	1.64	0.42
2:B:64:ILE:HG23	14:B:1205:CLA:HED2	2.01	0.42
14:B:1224:CLA:H92	14:B:1224:CLA:H62	1.81	0.42
1:G:145:MET:HE2	1:G:145:MET:HB3	1.93	0.42
1:G:458:LEU:HB3	1:G:577:PHE:HB2	2.02	0.42
2:H:60:TRP:HB2	14:H:1205:CLA:H192	2.01	0.42
2:H:190:TRP:NE1	14:H:1215:CLA:O1D	2.48	0.42
14:H:1204:CLA:H141	14:H:1204:CLA:H161	1.87	0.42
14:H:1217:CLA:H3A	14:H:1217:CLA:HBA2	1.66	0.42
14:L:1503:CLA:H141	14:L:1503:CLA:H162	1.85	0.42
4:O:32:SER:OG	4:O:33:THR:N	2.51	0.42
18:U:4022:BCR:H351	18:U:4022:BCR:H15C	1.64	0.42
1:a:735:GLU:OE2	5:e:46:TYR:OH	2.27	0.42
2:b:590:MET:HE3	2:b:590:MET:HB3	1.86	0.42
2:b:677:TYR:OH	14:b:1023:CLA:OBD	2.33	0.42
1:A:613:GLY:HA2	2:B:569:PRO:HD3	2.02	0.42
14:A:1103:CLA:H61	14:A:1103:CLA:H41	1.94	0.42
2:B:125:TYR:HE2	2:B:364:PHE:HE2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:TRP:HE1	18:B:4010:BCR:H271	1.84	0.42
3:C:27:GLU:OE1	4:D:127:ARG:NH1	2.52	0.42
3:C:62:PHE:CD2	5:E:14:GLU:HB2	2.54	0.42
5:E:8:VAL:HA	5:E:61:GLU:HA	2.02	0.42
1:G:279:THR:OG1	1:G:294:THR:OG1	2.29	0.42
14:G:1110:CLA:HAB	14:G:1118:CLA:C4C	2.49	0.42
2:H:554:MET:SD	3:N:66:ARG:NH2	2.89	0.42
1:a:734:ILE:HG22	1:a:738:VAL:HG23	2.01	0.42
2:b:185:VAL:HG13	18:b:4005:BCR:HC31	2.02	0.42
2:b:294:ASN:OD1	2:b:294:ASN:N	2.50	0.42
5:e:8:VAL:HA	5:e:61:GLU:HA	2.02	0.42
6:f:65:ASP:OD2	6:f:69:ARG:NH1	2.52	0.42
12:x:96:TYR:CG	14:x:1701:CLA:HED1	2.55	0.42
14:A:1130:CLA:H41	14:A:1130:CLA:H61	1.70	0.42
4:D:80:LYS:HE2	4:D:84:ILE:HD11	2.01	0.42
1:G:82:VAL:HG11	14:G:1103:CLA:H41	2.02	0.42
1:G:472:MET:HB2	1:G:481:MET:HB3	2.02	0.42
1:G:487:ILE:HD11	14:G:1132:CLA:HED1	2.02	0.42
1:G:746:VAL:HG23	6:Q:100:ARG:HA	2.02	0.42
14:G:1131:CLA:HAB	14:G:1132:CLA:HHB	2.02	0.42
2:H:237:PRO:HB3	2:H:256:THR:HG21	2.02	0.42
2:H:677:TYR:OH	14:H:1023:CLA:OBD	2.33	0.42
18:V:4021:BCR:H24C	18:V:4021:BCR:H371	1.79	0.42
12:X:96:TYR:CG	14:X:1701:CLA:HED1	2.55	0.42
14:a:1124:CLA:HBA2	14:a:1124:CLA:H3A	1.63	0.42
14:a:1131:CLA:HAB	14:a:1132:CLA:HHB	2.02	0.42
16:a:2001:PQN:H162	16:a:2001:PQN:H192	1.80	0.42
18:a:4002:BCR:H351	18:a:4002:BCR:H15C	1.68	0.42
14:b:1214:CLA:H62	14:b:1214:CLA:H41	1.87	0.42
7:i:37:LEU:HD12	7:i:40:TRP:HE1	1.83	0.42
1:A:82:VAL:HG11	14:A:1103:CLA:H41	2.02	0.42
14:B:1203:CLA:H112	14:B:1203:CLA:H93	1.85	0.42
14:B:1225:CLA:H3A	14:B:1225:CLA:HBA2	1.55	0.42
1:G:199:HIS:ND1	14:G:1123:CLA:OBD	2.36	0.42
2:H:398:TRP:HE1	18:H:4010:BCR:H271	1.84	0.42
14:H:1205:CLA:H91	14:H:1224:CLA:H203	2.01	0.42
18:H:4009:BCR:H351	18:H:4009:BCR:H15C	1.58	0.42
4:O:60:MET:HE3	4:O:60:MET:HB3	1.88	0.42
20:U:5007:LMG:H311	20:U:5007:LMG:H342	1.80	0.42
7:i:27:TYR:O	10:l:93:TYR:OH	2.32	0.42
1:A:730:TRP:O	1:A:734:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1103:CLA:H112	18:A:4003:BCR:H372	2.02	0.42
2:B:60:TRP:HB2	14:B:1205:CLA:H192	2.01	0.42
2:B:464:ALA:HA	2:B:467:ILE:HG12	2.00	0.42
14:B:1205:CLA:H91	14:B:1224:CLA:H203	2.01	0.42
14:B:1214:CLA:H62	14:B:1214:CLA:H41	1.87	0.42
14:G:1103:CLA:H92	14:G:1103:CLA:H61	1.90	0.42
14:H:1201:CLA:H41	14:H:1201:CLA:H62	1.64	0.42
14:H:1215:CLA:H112	14:H:1215:CLA:H91	1.77	0.42
18:I:4020:BCR:C10	10:L:94:ILE:HD11	2.50	0.42
14:L:1503:CLA:H193	18:l:4022:BCR:H14C	2.01	0.42
6:Q:65:ASP:OD2	6:Q:69:ARG:NH1	2.52	0.42
1:a:82:VAL:HG11	14:a:1103:CLA:H41	2.02	0.42
1:a:751:GLN:HA	1:a:752:PRO:HD3	1.94	0.42
2:b:728:GLY:HA3	14:b:1224:CLA:H43	2.00	0.42
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.91	0.41
14:A:1117:CLA:H3A	14:A:1117:CLA:HBA2	1.74	0.41
2:B:185:VAL:HG13	18:B:4005:BCR:HC31	2.02	0.41
14:B:1215:CLA:H3A	14:B:1215:CLA:HBA2	1.70	0.41
6:F:118:PHE:HA	8:J:12:SER:HA	2.02	0.41
1:G:575:HIS:HE1	1:G:645:HIS:ND1	2.18	0.41
1:G:613:GLY:HA2	2:H:569:PRO:HD3	2.02	0.41
14:H:1211:CLA:H51	14:H:1211:CLA:H12	1.74	0.41
14:H:1235:CLA:H91	14:H:1235:CLA:H112	1.84	0.41
4:O:141:PRO:O	4:O:153:THR:OG1	2.36	0.41
11:V:26:ALA:HB2	18:V:4021:BCR:HC41	2.01	0.41
2:b:237:PRO:HB3	2:b:256:THR:HG21	2.02	0.41
2:b:464:ALA:HA	2:b:467:ILE:HG12	2.00	0.41
10:l:49:LEU:HD22	10:l:53:MET:HB3	2.01	0.41
1:A:195:MET:HE1	14:A:1123:CLA:H101	2.01	0.41
1:A:483:SER:HB2	1:A:486:GLY:H	1.86	0.41
2:B:700:ARG:HB2	14:B:1238:CLA:HED3	2.01	0.41
14:B:1235:CLA:H92	14:B:1236:CLA:HAC2	2.01	0.41
1:G:483:SER:HB2	1:G:486:GLY:H	1.85	0.41
1:A:458:LEU:HB3	1:A:577:PHE:HB2	2.02	0.41
14:A:1122:CLA:HAC1	18:A:4007:BCR:HC8	2.03	0.41
2:B:319:PHE:HA	14:B:1219:CLA:CAB	2.50	0.41
2:B:417:LYS:HE2	2:B:417:LYS:HB2	1.88	0.41
1:G:195:MET:HE1	14:G:1123:CLA:H101	2.01	0.41
14:G:1130:CLA:H52	14:U:1502:CLA:H12	2.01	0.41
2:H:194:LEU:HA	2:H:198:ALA:HB3	2.02	0.41
5:P:8:VAL:HA	5:P:61:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:483:SER:HB2	1:a:486:GLY:H	1.85	0.41
2:b:60:TRP:HB2	14:b:1205:CLA:H192	2.01	0.41
2:b:440:LEU:HD23	2:b:440:LEU:HA	1.87	0.41
14:b:1239:CLA:H203	14:b:1239:CLA:H161	1.91	0.41
8:j:34:LEU:HD23	8:j:34:LEU:HA	1.87	0.41
1:A:729:TYR:OH	14:A:1013:CLA:OBD	2.35	0.41
1:A:734:ILE:HG22	1:A:738:VAL:HG23	2.01	0.41
2:B:237:PRO:HB3	2:B:256:THR:HG21	2.02	0.41
2:H:67:HIS:ND1	2:H:71:GLN:OE1	2.49	0.41
2:H:142:LEU:HD21	18:H:4006:BCR:H23C	2.02	0.41
14:H:1235:CLA:H92	14:H:1236:CLA:HAC2	2.01	0.41
18:R:4020:BCR:C10	10:U:94:ILE:HD11	2.50	0.41
1:a:715:ILE:HB	1:a:771:GLY:HA3	2.01	0.41
1:a:730:TRP:O	1:a:734:ILE:HG12	2.20	0.41
14:a:1115:CLA:H62	14:a:1115:CLA:H41	1.79	0.41
2:b:319:PHE:HA	14:b:1219:CLA:CAB	2.50	0.41
14:b:1205:CLA:H91	14:b:1224:CLA:H203	2.01	0.41
6:f:98:SER:HB3	6:f:128:MET:HA	2.02	0.41
18:i:4018:BCR:H24C	18:i:4018:BCR:H371	1.74	0.41
1:A:70:LYS:NZ	14:A:1109:CLA:OBD	2.44	0.41
1:A:458:LEU:O	1:A:462:SER:OG	2.26	0.41
2:B:319:PHE:HD1	14:B:1219:CLA:HAB	1.82	0.41
14:B:1238:CLA:H141	10:L:94:ILE:HG23	2.03	0.41
16:G:2001:PQN:H162	16:G:2001:PQN:H192	1.80	0.41
2:H:531:ALA:O	2:H:535:HIS:ND1	2.33	0.41
20:L:5007:LMG:H311	20:L:5007:LMG:H342	1.79	0.41
20:R:5006:LMG:H141	20:R:5006:LMG:H112	1.88	0.41
1:a:487:ILE:HD11	14:a:1132:CLA:HED1	2.02	0.41
1:a:757:ILE:HD11	2:b:573:GLY:HA3	2.02	0.41
2:b:142:LEU:HD21	18:b:4006:BCR:H23C	2.02	0.41
14:b:1204:CLA:H141	14:b:1204:CLA:H161	1.87	0.41
14:b:1215:CLA:H61	14:b:1215:CLA:H2	1.70	0.41
14:b:1215:CLA:HBA2	14:b:1215:CLA:H3A	1.70	0.41
15:b:1230:F6C:C4C	18:b:4012:BCR:H332	2.49	0.41
1:A:302:ALA:CB	14:A:1116:CLA:HAB	2.51	0.41
1:A:348:HIS:HB3	1:A:436:VAL:HB	2.03	0.41
18:A:4011:BCR:H15C	18:A:4011:BCR:H351	1.83	0.41
2:B:87:ILE:HD11	2:B:107:ALA:HB3	2.01	0.41
2:B:359:MET:HE3	2:B:359:MET:HB2	1.87	0.41
14:B:1222:CLA:HBA2	14:B:1222:CLA:H3A	1.83	0.41
14:G:1133:CLA:H92	14:G:1133:CLA:H62	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:319:PHE:HA	14:H:1219:CLA:CAB	2.50	0.41
14:H:1208:CLA:HBB1	14:H:1208:CLA:H18	2.03	0.41
1:a:218:VAL:HG13	1:a:238:PRO:HB3	2.02	0.41
1:a:458:LEU:HB3	1:a:577:PHE:HB2	2.02	0.41
1:a:575:HIS:HE1	1:a:645:HIS:ND1	2.18	0.41
1:a:613:GLY:HA2	2:b:569:PRO:HD3	2.02	0.41
14:b:1220:CLA:H2	14:b:1220:CLA:H61	1.68	0.41
4:d:59:GLU:H	4:d:89:GLN:NE2	2.19	0.41
1:A:487:ILE:HD11	14:A:1132:CLA:HED1	2.02	0.41
1:A:714:PHE:CD2	18:A:4011:BCR:H363	2.55	0.41
14:B:1211:CLA:H12	14:B:1211:CLA:H51	1.74	0.41
14:B:1222:CLA:H111	14:B:1222:CLA:H91	1.80	0.41
6:F:98:SER:HB3	6:F:128:MET:HA	2.03	0.41
1:G:216:ILE:HA	1:G:220:LEU:HB2	2.03	0.41
1:G:730:TRP:O	1:G:734:ILE:HG12	2.20	0.41
1:G:757:ILE:HD11	2:H:573:GLY:HA3	2.02	0.41
4:O:59:GLU:H	4:O:89:GLN:NE2	2.19	0.41
6:Q:98:SER:HB3	6:Q:128:MET:HA	2.03	0.41
1:a:348:HIS:HB3	1:a:436:VAL:HB	2.03	0.41
1:a:714:PHE:CD2	18:a:4011:BCR:H363	2.56	0.41
2:b:4:LYS:HD3	7:i:43:LYS:HG2	2.03	0.41
2:b:343:ALA:HB2	18:b:4010:BCR:H372	2.03	0.41
2:B:342:LEU:HD22	2:B:386:LEU:HD22	2.03	0.41
2:B:408:LYS:HA	2:B:408:LYS:HD2	1.85	0.41
14:B:1201:CLA:H41	14:B:1201:CLA:H62	1.64	0.41
18:B:4004:BCR:H351	18:B:4004:BCR:H15C	1.72	0.41
1:G:194:SER:O	1:G:198:HIS:ND1	2.40	0.41
1:G:588:LYS:HE3	2:H:681:LEU:HB2	2.03	0.41
1:G:695:ILE:HD13	1:G:695:ILE:HA	1.95	0.41
2:H:440:LEU:HA	2:H:440:LEU:HD23	1.87	0.41
14:H:1223:CLA:H111	14:H:1223:CLA:H71	1.75	0.41
6:Q:67:LEU:HA	6:Q:68:PRO:HD3	1.95	0.41
1:a:737:ILE:HD13	14:a:1138:CLA:HMD2	2.01	0.41
14:a:1119:CLA:H161	14:a:1119:CLA:H122	1.88	0.41
2:b:342:LEU:HD22	2:b:386:LEU:HD22	2.03	0.41
6:f:142:LEU:HD23	6:f:142:LEU:HA	1.91	0.41
10:l:58:ILE:O	10:l:62:HIS:ND1	2.54	0.41
1:A:235:ILE:HA	1:A:236:PRO:HD3	1.92	0.41
14:A:1013:CLA:HBA2	2:B:431:LEU:HD22	2.03	0.41
14:A:1136:CLA:H3A	14:A:1136:CLA:HBA2	1.80	0.41
14:A:1140:CLA:H93	14:A:1140:CLA:H61	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:PHE:HB3	2:B:284:LEU:HD13	2.03	0.41
14:B:1210:CLA:H202	14:B:1210:CLA:H162	1.89	0.41
14:B:1238:CLA:H8	14:B:1239:CLA:H152	2.03	0.41
4:D:59:GLU:H	4:D:89:GLN:NE2	2.19	0.41
1:G:279:THR:HG21	1:G:281:LYS:HE3	2.03	0.41
1:G:302:ALA:CB	14:G:1116:CLA:HAB	2.51	0.41
1:G:568:ASP:HA	1:G:571:ILE:HG22	2.03	0.41
14:G:1103:CLA:H41	14:G:1103:CLA:H61	1.94	0.41
14:G:1111:CLA:H51	14:G:1111:CLA:H11	1.88	0.41
14:G:1138:CLA:HBB2	6:Q:99:GLY:HA3	2.03	0.41
18:G:4011:BCR:H15C	18:G:4011:BCR:H351	1.83	0.41
2:H:459:ILE:HD13	6:Q:70:ILE:HD12	2.03	0.41
18:H:4004:BCR:H15C	18:H:4004:BCR:H351	1.72	0.41
18:H:4016:BCR:H371	18:H:4016:BCR:H24C	1.84	0.41
20:I:5006:LMG:H111	20:U:5007:LMG:H162	2.03	0.41
10:L:47:LYS:HD3	10:L:47:LYS:HA	1.92	0.41
10:U:129:LEU:HD23	10:U:129:LEU:HA	1.92	0.41
1:a:568:ASP:HA	1:a:571:ILE:HG22	2.03	0.41
1:a:614:PRO:HD3	2:b:568:GLY:HA2	2.03	0.41
1:a:616:ARG:HA	3:c:77:MET:HA	2.01	0.41
14:a:1106:CLA:H3A	14:a:1106:CLA:HBA2	1.54	0.41
14:a:1124:CLA:H12	14:a:1136:CLA:HBA1	2.03	0.41
2:b:50:HIS:ND1	14:b:1210:CLA:OBD	2.49	0.41
14:b:1204:CLA:HBC1	11:m:12:LEU:HA	2.03	0.41
14:b:1210:CLA:H112	14:b:1210:CLA:H142	1.78	0.41
3:c:73:THR:OG1	3:c:74:THR:N	2.54	0.41
11:m:26:ALA:HB2	18:m:4021:BCR:HC41	2.01	0.41
1:A:751:GLN:HA	1:A:752:PRO:HD3	1.94	0.41
2:B:343:ALA:HB2	18:B:4010:BCR:H372	2.03	0.41
18:B:4014:BCR:H371	18:B:4014:BCR:H24C	1.75	0.41
1:G:218:VAL:HG13	1:G:238:PRO:HB3	2.03	0.41
1:G:348:HIS:HB3	1:G:436:VAL:HB	2.03	0.41
1:G:747:ALA:O	6:Q:107:LYS:NZ	2.38	0.41
21:G:6001:LMT:H72	11:M:10:ILE:HD11	2.03	0.41
14:H:1226:CLA:H112	14:H:1226:CLA:H142	1.82	0.41
1:a:302:ALA:CB	14:a:1116:CLA:HAB	2.51	0.41
14:b:1210:CLA:H202	14:b:1210:CLA:H162	1.89	0.41
14:b:1238:CLA:H8	14:b:1239:CLA:H152	2.03	0.41
18:b:4006:BCR:H15C	18:b:4006:BCR:H351	1.64	0.41
20:i:5006:LMG:H141	20:i:5006:LMG:H112	1.88	0.41
1:A:42:LYS:HA	1:A:42:LYS:HD3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:HIS:HE1	1:A:645:HIS:ND1	2.18	0.40
2:B:559:ASP:OD2	2:B:559:ASP:N	2.55	0.40
1:G:211:TRP:NE1	14:G:1117:CLA:O1D	2.53	0.40
13:G:1011:CL0:H50	13:G:1011:CL0:H59	1.67	0.40
14:G:1140:CLA:H102	16:G:2001:PQN:H202	2.03	0.40
14:H:1224:CLA:H11	14:H:1224:CLA:H52	1.87	0.40
14:H:1238:CLA:H141	10:U:94:ILE:HG23	2.02	0.40
18:H:4010:BCR:H393	18:H:4010:BCR:H281	1.92	0.40
8:J:30:VAL:HG22	8:J:34:LEU:HD12	2.03	0.40
14:L:1501:CLA:H91	14:L:1501:CLA:H112	1.88	0.40
3:N:73:THR:OG1	3:N:74:THR:N	2.54	0.40
4:O:25:GLN:H	4:O:25:GLN:HG2	1.74	0.40
14:a:1103:CLA:H112	18:a:4003:BCR:H372	2.01	0.40
2:b:194:LEU:HA	2:b:198:ALA:HB3	2.02	0.40
1:A:658:VAL:HG12	1:A:664:VAL:HG22	2.03	0.40
2:B:181:GLY:HA3	14:B:1210:CLA:HBB1	2.04	0.40
14:B:1215:CLA:H2	14:B:1215:CLA:H61	1.70	0.40
3:C:73:THR:OG1	3:C:74:THR:N	2.54	0.40
1:G:714:PHE:CD2	18:G:4011:BCR:H363	2.55	0.40
14:G:1104:CLA:H112	14:G:1104:CLA:H71	1.87	0.40
14:G:1129:CLA:HMC1	14:G:1137:CLA:HBB1	2.03	0.40
18:H:4005:BCR:H24C	18:H:4005:BCR:H371	1.77	0.40
18:I:4020:BCR:HC41	10:L:93:TYR:CG	2.56	0.40
10:L:49:LEU:HD22	10:L:53:MET:HB3	2.01	0.40
18:R:4020:BCR:HC41	10:U:93:TYR:CG	2.56	0.40
20:R:5006:LMG:H341	18:V:4021:BCR:H391	2.02	0.40
14:A:1117:CLA:H102	14:A:1117:CLA:H193	2.03	0.40
14:A:1126:CLA:H92	14:A:1126:CLA:H62	1.87	0.40
1:G:307:PHE:CE1	14:G:1119:CLA:HAB	2.51	0.40
1:G:735:GLU:OE2	5:P:46:TYR:OH	2.31	0.40
14:G:1122:CLA:HAC1	18:G:4007:BCR:HC8	2.02	0.40
14:H:1214:CLA:HBA1	14:H:1214:CLA:H12	1.87	0.40
10:L:58:ILE:O	10:L:62:HIS:ND1	2.54	0.40
20:R:5006:LMG:H111	20:l:5007:LMG:H162	2.02	0.40
1:a:279:THR:OG1	1:a:294:THR:OG1	2.29	0.40
14:a:1140:CLA:H102	16:a:2001:PQN:H202	2.03	0.40
14:b:1021:CLA:H202	14:b:1021:CLA:H161	1.88	0.40
14:b:1214:CLA:H52	14:b:1214:CLA:H12	1.88	0.40
1:A:588:LYS:HE3	2:B:681:LEU:HB2	2.03	0.40
1:A:626:ASP:HA	1:A:629:PHE:HB3	2.04	0.40
1:A:737:ILE:HD13	14:A:1138:CLA:HMD2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1102:CLA:H12	14:A:1102:CLA:H52	1.83	0.40
16:A:2001:PQN:H243	16:A:2001:PQN:H261	1.86	0.40
2:B:300:SER:HB3	2:B:303:GLU:HG3	2.03	0.40
14:B:1208:CLA:H18	14:B:1208:CLA:HBB1	2.03	0.40
14:G:1117:CLA:H102	14:G:1117:CLA:H193	2.03	0.40
14:U:1501:CLA:HBA1	14:U:1501:CLA:HBD	2.04	0.40
1:a:199:HIS:ND1	14:a:1123:CLA:OBD	2.36	0.40
14:a:1117:CLA:H193	14:a:1117:CLA:H102	2.03	0.40
14:a:1122:CLA:HAC1	18:a:4007:BCR:HC8	2.02	0.40
1:A:307:PHE:CE1	14:A:1119:CLA:HAB	2.51	0.40
1:A:614:PRO:HD3	2:B:568:GLY:HA2	2.03	0.40
1:A:757:ILE:HD11	2:B:573:GLY:HA3	2.02	0.40
14:A:1104:CLA:H193	14:A:1104:CLA:H161	1.92	0.40
4:D:141:PRO:O	4:D:153:THR:OG1	2.36	0.40
1:G:658:VAL:HG12	1:G:664:VAL:HG22	2.04	0.40
14:G:1102:CLA:H52	14:G:1102:CLA:H12	1.83	0.40
14:G:1124:CLA:H12	14:G:1136:CLA:HBA1	2.03	0.40
2:H:300:SER:HB3	2:H:303:GLU:HG3	2.03	0.40
2:H:469:SER:O	2:H:483:SER:OG	2.30	0.40
14:H:1222:CLA:H3A	14:H:1222:CLA:HBA2	1.83	0.40
10:U:41:ASN:HD22	10:U:41:ASN:HA	1.70	0.40
10:U:69:PRO:HB3	14:U:1503:CLA:HBB1	2.04	0.40
1:a:279:THR:HG21	1:a:281:LYS:HE3	2.03	0.40
1:a:423:MET:HA	1:a:427:TYR:HB2	2.04	0.40
14:a:1119:CLA:H193	18:a:4007:BCR:HC41	2.04	0.40
2:b:140:LEU:HD23	2:b:140:LEU:HA	1.90	0.40
2:b:519:ILE:HD13	2:b:519:ILE:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	743/788 (94%)	699 (94%)	44 (6%)	0	100	100
1	G	743/788 (94%)	700 (94%)	43 (6%)	0	100	100
1	a	743/788 (94%)	699 (94%)	44 (6%)	0	100	100
2	B	736/741 (99%)	706 (96%)	30 (4%)	0	100	100
2	H	736/741 (99%)	706 (96%)	30 (4%)	0	100	100
2	b	736/741 (99%)	706 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
3	c	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
4	D	137/159 (86%)	125 (91%)	12 (9%)	0	100	100
4	O	137/159 (86%)	125 (91%)	12 (9%)	0	100	100
4	d	137/159 (86%)	125 (91%)	12 (9%)	0	100	100
5	E	60/72 (83%)	54 (90%)	6 (10%)	0	100	100
5	P	60/72 (83%)	54 (90%)	6 (10%)	0	100	100
5	e	60/72 (83%)	54 (90%)	6 (10%)	0	100	100
6	F	133/159 (84%)	122 (92%)	11 (8%)	0	100	100
6	Q	133/159 (84%)	122 (92%)	11 (8%)	0	100	100
6	f	133/159 (84%)	122 (92%)	11 (8%)	0	100	100
7	I	40/67 (60%)	33 (82%)	7 (18%)	0	100	100
7	R	40/67 (60%)	33 (82%)	7 (18%)	0	100	100
7	i	40/67 (60%)	33 (82%)	7 (18%)	0	100	100
8	J	41/48 (85%)	36 (88%)	4 (10%)	1 (2%)	4	28
8	S	41/48 (85%)	36 (88%)	4 (10%)	1 (2%)	4	28
8	j	41/48 (85%)	36 (88%)	4 (10%)	1 (2%)	4	28
9	K	16/39 (41%)	16 (100%)	0	0	100	100
9	T	16/39 (41%)	16 (100%)	0	0	100	100
9	k	16/39 (41%)	16 (100%)	0	0	100	100
10	L	152/174 (87%)	140 (92%)	12 (8%)	0	100	100
10	U	152/174 (87%)	140 (92%)	12 (8%)	0	100	100
10	l	152/174 (87%)	140 (92%)	12 (8%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	V	29/31 (94%)	27 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	W	27/101 (27%)	25 (93%)	2 (7%)	0	100	100
12	X	27/101 (27%)	25 (93%)	2 (7%)	0	100	100
12	x	27/101 (27%)	25 (93%)	2 (7%)	0	100	100
All	All	6576/7380 (89%)	6166 (94%)	404 (6%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	63	LEU
3	N	63	LEU
3	c	63	LEU
8	J	36	PRO
8	S	36	PRO
8	j	36	PRO

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	611/641 (95%)	608 (100%)	3 (0%)	81	85
1	G	611/641 (95%)	608 (100%)	3 (0%)	81	85
1	a	611/641 (95%)	608 (100%)	3 (0%)	81	85
2	B	595/597 (100%)	592 (100%)	3 (0%)	81	85
2	H	595/597 (100%)	592 (100%)	3 (0%)	81	85
2	b	595/597 (100%)	592 (100%)	3 (0%)	81	85
3	C	68/69 (99%)	68 (100%)	0	100	100
3	N	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	115/132 (87%)	112 (97%)	3 (3%)	40	69
4	O	115/132 (87%)	112 (97%)	3 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	d	115/132 (87%)	112 (97%)	3 (3%)	40 69
5	E	54/60 (90%)	54 (100%)	0	100 100
5	P	54/60 (90%)	54 (100%)	0	100 100
5	e	54/60 (90%)	54 (100%)	0	100 100
6	F	115/134 (86%)	108 (94%)	7 (6%)	17 49
6	Q	115/134 (86%)	108 (94%)	7 (6%)	17 49
6	f	115/134 (86%)	108 (94%)	7 (6%)	17 49
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
8	J	36/42 (86%)	36 (100%)	0	100 100
8	S	36/42 (86%)	36 (100%)	0	100 100
8	j	36/42 (86%)	36 (100%)	0	100 100
9	K	11/15 (73%)	11 (100%)	0	100 100
9	T	11/15 (73%)	11 (100%)	0	100 100
9	k	11/15 (73%)	11 (100%)	0	100 100
10	L	121/138 (88%)	120 (99%)	1 (1%)	73 82
10	U	121/138 (88%)	120 (99%)	1 (1%)	73 82
10	l	121/138 (88%)	120 (99%)	1 (1%)	73 82
11	M	26/26 (100%)	26 (100%)	0	100 100
11	V	26/26 (100%)	26 (100%)	0	100 100
11	m	26/26 (100%)	26 (100%)	0	100 100
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	5439/5994 (91%)	5388 (99%)	51 (1%)	68 81

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LYS
1	A	436	VAL
1	A	484	ASP

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Mol	Chain	Res	Type
2	B	248	GLN
2	B	309	THR
2	B	575	CYS
4	D	22	LEU
4	D	96	THR
4	D	128	GLU
6	F	42	LYS
6	F	54	LEU
6	F	91	THR
6	F	98	SER
6	F	111	LYS
6	F	114	GLU
6	F	158	VAL
1	G	233	LYS
1	G	436	VAL
1	G	484	ASP
2	H	248	GLN
2	H	309	THR
2	H	575	CYS
10	L	161	ASP
4	O	22	LEU
4	O	96	THR
4	O	128	GLU
6	Q	42	LYS
6	Q	54	LEU
6	Q	91	THR
6	Q	98	SER
6	Q	111	LYS
6	Q	114	GLU
6	Q	158	VAL
10	U	161	ASP
1	a	233	LYS
1	a	436	VAL
1	a	484	ASP
2	b	248	GLN
2	b	309	THR
2	b	575	CYS
4	d	22	LEU
4	d	96	THR
4	d	128	GLU
6	f	42	LYS
6	f	54	LEU

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Mol	Chain	Res	Type
6	f	91	THR
6	f	98	SER
6	f	111	LYS
6	f	114	GLU
6	f	158	VAL
10	l	161	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	49	ASN
1	A	78	HIS
1	A	178	HIS
1	A	217	HIS
1	A	249	ASN
1	A	322	HIS
1	A	360	HIS
1	A	362	GLN
1	A	432	ASN
1	A	575	HIS
1	A	604	ASN
1	A	651	GLN
1	A	680	ASN
1	A	699	ASN
1	A	751	GLN
2	B	53	HIS
2	B	89	HIS
2	B	170	ASN
2	B	206	HIS
2	B	262	HIS
2	B	332	ASN
2	B	337	GLN
2	B	380	GLN
2	B	510	ASN
2	B	592	ASN
2	B	605	HIS
2	B	661	HIS
2	B	679	GLN
2	B	691	GLN
4	D	73	ASN
4	D	89	GLN

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Mol	Chain	Res	Type
4	D	139	GLN
5	E	19	GLN
6	F	109	GLN
1	G	17	ASN
1	G	49	ASN
1	G	78	HIS
1	G	178	HIS
1	G	180	HIS
1	G	217	HIS
1	G	249	ASN
1	G	322	HIS
1	G	348	HIS
1	G	360	HIS
1	G	362	GLN
1	G	432	ASN
1	G	575	HIS
1	G	651	GLN
1	G	680	ASN
1	G	699	ASN
1	G	751	GLN
2	H	53	HIS
2	H	89	HIS
2	H	170	ASN
2	H	206	HIS
2	H	262	HIS
2	H	332	ASN
2	H	337	GLN
2	H	380	GLN
2	H	406	GLN
2	H	510	ASN
2	H	592	ASN
2	H	605	HIS
2	H	679	GLN
2	H	691	GLN
8	J	32	ASN
8	J	39	GLN
10	L	40	ASN
10	L	41	ASN
10	L	84	ASN
11	M	7	GLN
4	O	73	ASN
4	O	89	GLN

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Mol	Chain	Res	Type
4	O	139	GLN
6	Q	109	GLN
10	U	40	ASN
10	U	41	ASN
10	U	84	ASN
11	V	7	GLN
12	W	89	ASN
1	a	17	ASN
1	a	49	ASN
1	a	78	HIS
1	a	178	HIS
1	a	180	HIS
1	a	217	HIS
1	a	249	ASN
1	a	322	HIS
1	a	360	HIS
1	a	362	GLN
1	a	432	ASN
1	a	575	HIS
1	a	651	GLN
1	a	680	ASN
1	a	699	ASN
1	a	751	GLN
2	b	53	HIS
2	b	170	ASN
2	b	206	HIS
2	b	262	HIS
2	b	332	ASN
2	b	380	GLN
2	b	484	ASN
2	b	510	ASN
2	b	592	ASN
2	b	605	HIS
2	b	679	GLN
2	b	689	HIS
2	b	691	GLN
4	d	73	ASN
4	d	89	GLN
4	d	139	GLN
5	e	19	GLN
6	f	109	GLN
10	l	40	ASN

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Mol	Chain	Res	Type
10	l	41	ASN
10	l	84	ASN
10	l	139	ASN
11	m	7	GLN

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 oligosaccharides 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	$\#\|Z\| > 2$
20	LMG	R	5006	-	37,37,55	1.16	3 (8%)	45,45,63	1.22	4 (8%)
18	BCR	G	4007	-	41,41,41	2.76	7 (17%)	56,56,56	6.81	24 (42%)
18	BCR	B	4017	-	41,41,41	2.76	6 (14%)	56,56,56	6.76	18 (32%)
14	CLA	H	1224	-	69,73,73	2.21	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	G	1118	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	29 (41%)
14	CLA	B	1021	-	69,73,73	2.19	21 (30%)	82,113,113	2.55	30 (36%)
21	LMT	A	6001	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	4 (9%)
14	CLA	B	1231	-	59,63,73	2.42	20 (33%)	70,101,113	2.65	26 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	1119	-	69,73,73	2.22	20 (28%)	82,113,113	2.35	28 (34%)
17	SF4	c	3002	-	0,12,12	-	-	-		
14	CLA	b	1206	-	49,53,73	2.49	19 (38%)	58,89,113	2.61	23 (39%)
14	CLA	G	1104	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	25 (30%)
14	CLA	B	1211	-	69,73,73	2.21	20 (28%)	82,113,113	2.40	26 (31%)
14	CLA	B	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.77	23 (39%)
14	CLA	H	1234	-	59,63,73	2.33	20 (33%)	70,101,113	2.66	26 (37%)
13	CL0	A	1011	-	58,73,73	3.15	21 (36%)	60,113,113	3.12	24 (40%)
14	CLA	G	1131	-	64,68,73	2.27	21 (32%)	76,107,113	2.59	25 (32%)
18	BCR	B	4010	-	41,41,41	2.75	6 (14%)	56,56,56	6.74	21 (37%)
14	CLA	A	1138	-	64,68,73	2.30	21 (32%)	76,107,113	2.61	30 (39%)
14	CLA	B	1221	-	64,68,73	2.27	20 (31%)	76,107,113	2.50	27 (35%)
17	SF4	a	3001	-	0,12,12	-	-	-		
14	CLA	G	1114	-	49,53,73	2.55	21 (42%)	58,89,113	2.74	24 (41%)
14	CLA	A	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	26 (34%)
14	CLA	A	1115	-	59,63,73	2.39	21 (35%)	70,101,113	2.71	26 (37%)
18	BCR	U	4019	-	41,41,41	2.68	6 (14%)	56,56,56	6.69	24 (42%)
20	LMG	L	5007	-	50,50,55	1.44	7 (14%)	58,58,63	1.10	2 (3%)
18	BCR	b	4012	-	41,41,41	2.59	6 (14%)	56,56,56	6.78	27 (48%)
14	CLA	G	1138	-	64,68,73	2.29	22 (34%)	76,107,113	2.61	30 (39%)
14	CLA	b	1211	-	69,73,73	2.21	20 (28%)	82,113,113	2.39	26 (31%)
14	CLA	b	1210	-	69,73,73	2.22	21 (30%)	82,113,113	2.56	32 (39%)
17	SF4	C	3002	-	0,12,12	-	-	-		
16	PQN	b	2002	-	34,34,34	1.52	2 (5%)	43,45,45	1.18	1 (2%)
18	BCR	B	4006	-	41,41,41	2.65	6 (14%)	56,56,56	6.70	23 (41%)
15	F6C	B	1230	-	52,54,74	3.08	27 (51%)	59,90,114	3.56	32 (54%)
18	BCR	b	4005	-	41,41,41	2.67	7 (17%)	56,56,56	6.77	28 (50%)
14	CLA	A	1135	-	54,58,73	2.53	21 (38%)	64,95,113	2.84	29 (45%)
14	CLA	T	1401	-	49,53,73	2.55	22 (44%)	58,89,113	2.77	21 (36%)
17	SF4	G	3001	-	0,12,12	-	-	-		
15	F6C	a	1121	-	52,54,74	3.05	27 (51%)	59,90,114	3.70	31 (52%)
18	BCR	B	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.62	26 (46%)
14	CLA	H	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.77	23 (39%)
18	BCR	b	4010	-	41,41,41	2.75	6 (14%)	56,56,56	6.73	21 (37%)
14	CLA	A	1108	-	49,53,73	2.53	21 (42%)	58,89,113	2.76	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	1218	-	49,53,73	2.50	19 (38%)	58,89,113	2.83	21 (36%)
15	F6C	B	1237	-	67,69,74	2.79	25 (37%)	77,108,114	3.21	36 (46%)
21	LMT	a	6002	-	29,29,36	1.35	5 (17%)	40,40,47	1.42	8 (20%)
14	CLA	G	1122	-	59,63,73	2.37	21 (35%)	70,101,113	2.62	27 (38%)
14	CLA	H	1221	-	64,68,73	2.27	20 (31%)	76,107,113	2.49	27 (35%)
21	LMT	a	6001	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	4 (9%)
14	CLA	B	1023	-	69,73,73	2.19	22 (31%)	82,113,113	2.81	31 (37%)
14	CLA	a	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.58	27 (32%)
14	CLA	H	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.78	24 (41%)
14	CLA	a	1113	-	49,53,73	2.49	19 (38%)	58,89,113	2.86	23 (39%)
14	CLA	A	1129	-	49,53,73	2.50	18 (36%)	58,89,113	2.77	25 (43%)
14	CLA	A	1110	-	49,53,73	2.49	20 (40%)	58,89,113	2.91	23 (39%)
18	BCR	b	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.60	24 (42%)
14	CLA	B	1215	-	64,68,73	2.29	19 (29%)	76,107,113	2.53	30 (39%)
14	CLA	H	1206	-	49,53,73	2.49	19 (38%)	58,89,113	2.62	23 (39%)
14	CLA	A	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.36	27 (32%)
18	BCR	I	4018	-	41,41,41	2.86	7 (17%)	56,56,56	6.84	25 (44%)
14	CLA	G	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.57	27 (32%)
14	CLA	B	1203	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	28 (34%)
14	CLA	a	1112	-	49,53,73	2.51	22 (44%)	58,89,113	2.78	22 (37%)
14	CLA	l	1503	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	27 (32%)
14	CLA	b	1204	-	69,73,73	2.24	20 (28%)	82,113,113	2.50	27 (32%)
20	LMG	l	5007	-	50,50,55	1.44	7 (14%)	58,58,63	1.10	2 (3%)
18	BCR	a	4007	-	41,41,41	2.77	7 (17%)	56,56,56	6.81	24 (42%)
14	CLA	A	1124	-	59,63,73	2.37	20 (33%)	70,101,113	2.69	28 (40%)
14	CLA	b	1222	-	69,73,73	2.23	21 (30%)	82,113,113	2.58	32 (39%)
14	CLA	a	1138	-	64,68,73	2.30	22 (34%)	76,107,113	2.61	30 (39%)
14	CLA	G	1012	-	69,73,73	2.21	20 (28%)	82,113,113	2.51	29 (35%)
14	CLA	G	1105	-	49,53,73	2.53	20 (40%)	58,89,113	2.76	22 (37%)
14	CLA	G	1106	-	49,53,73	2.48	20 (40%)	58,89,113	2.91	25 (43%)
18	BCR	H	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.62	25 (44%)
15	F6C	A	1121	-	52,54,74	3.05	27 (51%)	59,90,114	3.69	30 (50%)
14	CLA	a	1123	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	29 (38%)
14	CLA	b	1223	-	69,73,73	2.20	21 (30%)	82,113,113	2.47	26 (31%)
14	CLA	A	1136	-	59,63,73	2.35	21 (35%)	70,101,113	2.76	28 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	G	1132	-	69,73,73	2.21	20 (28%)	82,113,113	2.56	28 (34%)
21	LMT	A	6002	-	29,29,36	1.35	5 (17%)	40,40,47	1.42	8 (20%)
15	F6C	G	1121	-	52,54,74	3.05	27 (51%)	59,90,114	3.69	30 (50%)
14	CLA	a	1118	-	59,63,73	2.37	20 (33%)	70,101,113	2.73	29 (41%)
18	BCR	R	4020	-	41,41,41	2.87	7 (17%)	56,56,56	6.44	24 (42%)
18	BCR	A	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.30	23 (41%)
14	CLA	G	1112	-	49,53,73	2.50	22 (44%)	58,89,113	2.78	22 (37%)
14	CLA	A	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.57	27 (32%)
14	CLA	b	1232	-	49,53,73	2.51	22 (44%)	58,89,113	2.70	23 (39%)
14	CLA	G	1140	-	69,73,73	2.21	21 (30%)	82,113,113	2.41	27 (32%)
14	CLA	H	1023	-	69,73,73	2.20	22 (31%)	82,113,113	2.80	32 (39%)
14	CLA	H	1232	-	49,53,73	2.51	20 (40%)	58,89,113	2.70	23 (39%)
20	LMG	i	5006	-	37,37,55	1.16	3 (8%)	45,45,63	1.22	4 (8%)
14	CLA	A	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.57	29 (38%)
19	LHG	A	5001	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	4 (9%)
14	CLA	H	1236	-	49,53,73	2.49	20 (40%)	58,89,113	2.80	23 (39%)
20	LMG	I	5006	-	37,37,55	1.15	3 (8%)	45,45,63	1.22	4 (8%)
14	CLA	B	1223	-	69,73,73	2.21	21 (30%)	82,113,113	2.47	26 (31%)
14	CLA	G	1101	-	49,53,73	2.47	19 (38%)	58,89,113	2.79	25 (43%)
14	CLA	a	1131	-	64,68,73	2.27	21 (32%)	76,107,113	2.58	25 (32%)
14	CLA	A	1111	-	64,68,73	2.29	22 (34%)	76,107,113	2.62	29 (38%)
14	CLA	B	1208	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	H	1231	-	59,63,73	2.42	20 (33%)	70,101,113	2.66	26 (37%)
14	CLA	b	1224	-	69,73,73	2.21	19 (27%)	82,113,113	2.48	29 (35%)
18	BCR	a	4003	-	41,41,41	2.70	6 (14%)	56,56,56	6.66	23 (41%)
14	CLA	B	1238	-	69,73,73	2.25	19 (27%)	82,113,113	2.60	32 (39%)
14	CLA	G	1102	-	64,68,73	2.33	20 (31%)	76,107,113	2.59	27 (35%)
14	CLA	H	1212	-	49,53,73	2.51	20 (40%)	58,89,113	2.81	23 (39%)
18	BCR	a	4011	-	41,41,41	2.75	7 (17%)	56,56,56	6.68	25 (44%)
19	LHG	H	5004	-	43,43,48	0.98	2 (4%)	46,49,54	1.21	3 (6%)
14	CLA	b	1214	-	64,68,73	2.33	20 (31%)	76,107,113	2.53	34 (44%)
14	CLA	b	1203	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	28 (34%)
18	BCR	m	4021	-	41,41,41	2.72	6 (14%)	56,56,56	6.70	23 (41%)
14	CLA	B	1235	-	64,68,73	2.29	19 (29%)	76,107,113	2.65	27 (35%)
14	CLA	a	1012	-	69,73,73	2.21	20 (28%)	82,113,113	2.51	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	1013	-	64,68,73	2.35	22 (34%)	76,107,113	2.67	30 (39%)
14	CLA	H	1220	-	59,63,73	2.38	20 (33%)	70,101,113	2.64	25 (35%)
14	CLA	H	1205	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
18	BCR	a	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.63	22 (39%)
21	LMT	G	6002	-	29,29,36	1.35	5 (17%)	40,40,47	1.42	8 (20%)
14	CLA	H	1012	-	69,73,73	2.20	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	a	1114	-	49,53,73	2.55	21 (42%)	58,89,113	2.74	24 (41%)
14	CLA	b	1208	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	B	1210	-	69,73,73	2.23	21 (30%)	82,113,113	2.56	32 (39%)
18	BCR	b	4009	-	41,41,41	2.71	6 (14%)	56,56,56	6.72	25 (44%)
14	CLA	B	1234	-	59,63,73	2.34	20 (33%)	70,101,113	2.66	27 (38%)
14	CLA	x	1701	-	49,53,73	2.48	19 (38%)	58,89,113	2.76	23 (39%)
14	CLA	a	1109	-	49,53,73	2.46	21 (42%)	58,89,113	2.84	22 (37%)
14	CLA	b	1202	-	64,68,73	2.26	20 (31%)	76,107,113	2.59	28 (36%)
14	CLA	a	1013	-	64,68,73	2.35	22 (34%)	76,107,113	2.67	30 (39%)
14	CLA	B	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.77	24 (41%)
14	CLA	a	1117	-	69,73,73	2.19	21 (30%)	82,113,113	2.41	28 (34%)
14	CLA	a	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.70	22 (37%)
14	CLA	H	1228	-	49,53,73	2.51	21 (42%)	58,89,113	2.75	26 (44%)
14	CLA	b	1239	-	69,73,73	2.23	22 (31%)	82,113,113	2.63	30 (36%)
17	SF4	N	3003	-	0,12,12	-	-	-		
14	CLA	B	1227	-	49,53,73	2.56	19 (38%)	58,89,113	2.64	24 (41%)
18	BCR	B	4005	-	41,41,41	2.66	7 (17%)	56,56,56	6.77	27 (48%)
19	LHG	a	5001	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	4 (9%)
18	BCR	b	4013	-	41,41,41	2.63	6 (14%)	56,56,56	6.72	23 (41%)
14	CLA	a	1124	-	59,63,73	2.37	20 (33%)	70,101,113	2.68	27 (38%)
14	CLA	A	1109	-	49,53,73	2.47	21 (42%)	58,89,113	2.85	23 (39%)
14	CLA	A	1104	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	25 (30%)
14	CLA	a	1105	-	49,53,73	2.53	20 (40%)	58,89,113	2.76	22 (37%)
14	CLA	B	1214	-	64,68,73	2.33	21 (32%)	76,107,113	2.53	34 (44%)
14	CLA	A	1128	-	64,68,73	2.33	19 (29%)	76,107,113	2.48	30 (39%)
18	BCR	b	4016	-	41,41,41	2.66	6 (14%)	56,56,56	6.65	18 (32%)
14	CLA	B	1218	-	49,53,73	2.50	19 (38%)	58,89,113	2.83	21 (36%)
18	BCR	B	4012	-	41,41,41	2.59	6 (14%)	56,56,56	6.78	27 (48%)
14	CLA	H	1021	-	69,73,73	2.20	21 (30%)	82,113,113	2.56	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	1226	-	69,73,73	2.26	21 (30%)	82,113,113	2.39	27 (32%)
14	CLA	H	1238	-	69,73,73	2.26	19 (27%)	82,113,113	2.60	32 (39%)
14	CLA	U	1503	-	69,73,73	2.19	20 (28%)	82,113,113	2.46	26 (31%)
14	CLA	b	1229	-	64,68,73	2.29	21 (32%)	76,107,113	2.64	26 (34%)
14	CLA	H	1203	-	69,73,73	2.16	20 (28%)	82,113,113	2.55	28 (34%)
20	LMG	U	5007	-	50,50,55	1.44	7 (14%)	58,58,63	1.10	2 (3%)
18	BCR	G	4003	-	41,41,41	2.70	6 (14%)	56,56,56	6.66	23 (41%)
14	CLA	a	1116	-	59,63,73	2.40	20 (33%)	70,101,113	2.67	28 (40%)
19	LHG	B	5004	-	43,43,48	0.98	2 (4%)	46,49,54	1.21	3 (6%)
14	CLA	b	1217	-	59,63,73	2.38	21 (35%)	70,101,113	2.64	25 (35%)
14	CLA	b	1238	-	69,73,73	2.25	20 (28%)	82,113,113	2.60	32 (39%)
18	BCR	l	4022	-	41,41,41	2.82	6 (14%)	56,56,56	6.63	24 (42%)
14	CLA	a	1101	-	49,53,73	2.47	19 (38%)	58,89,113	2.79	25 (43%)
14	CLA	G	1110	-	49,53,73	2.48	20 (40%)	58,89,113	2.90	23 (39%)
14	CLA	B	1236	-	49,53,73	2.49	20 (40%)	58,89,113	2.79	23 (39%)
18	BCR	U	4022	-	41,41,41	2.82	6 (14%)	56,56,56	6.62	24 (42%)
14	CLA	A	1012	-	69,73,73	2.21	20 (28%)	82,113,113	2.52	29 (35%)
17	SF4	A	3001	-	0,12,12	-	-	-		
14	CLA	W	1701	-	49,53,73	2.48	19 (38%)	58,89,113	2.75	23 (39%)
18	BCR	b	4006	-	41,41,41	2.65	6 (14%)	56,56,56	6.71	23 (41%)
14	CLA	b	1220	-	59,63,73	2.39	20 (33%)	70,101,113	2.64	25 (35%)
14	CLA	k	1401	-	49,53,73	2.55	22 (44%)	58,89,113	2.77	21 (36%)
14	CLA	G	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.70	22 (37%)
18	BCR	L	4019	-	41,41,41	2.68	6 (14%)	56,56,56	6.70	24 (42%)
14	CLA	A	1114	-	49,53,73	2.56	22 (44%)	58,89,113	2.74	24 (41%)
14	CLA	A	1113	-	49,53,73	2.49	19 (38%)	58,89,113	2.86	23 (39%)
18	BCR	G	4011	-	41,41,41	2.75	7 (17%)	56,56,56	6.68	26 (46%)
14	CLA	a	1132	-	69,73,73	2.21	20 (28%)	82,113,113	2.57	28 (34%)
14	CLA	G	1103	-	64,68,73	2.22	20 (31%)	76,107,113	2.63	26 (34%)
14	CLA	A	1122	-	59,63,73	2.37	21 (35%)	70,101,113	2.62	27 (38%)
18	BCR	i	4018	-	41,41,41	2.86	7 (17%)	56,56,56	6.85	25 (44%)
18	BCR	B	4013	-	41,41,41	2.63	6 (14%)	56,56,56	6.72	23 (41%)
18	BCR	B	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.59	24 (42%)
14	CLA	B	1212	-	49,53,73	2.51	20 (40%)	58,89,113	2.82	23 (39%)
14	CLA	G	1113	-	49,53,73	2.48	19 (38%)	58,89,113	2.85	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	1127	-	69,73,73	2.24	21 (30%)	82,113,113	2.40	28 (34%)
18	BCR	A	4003	-	41,41,41	2.70	6 (14%)	56,56,56	6.65	23 (41%)
14	CLA	B	1213	-	59,63,73	2.40	21 (35%)	70,101,113	2.72	26 (37%)
14	CLA	b	1201	-	59,63,73	2.37	21 (35%)	70,101,113	2.83	27 (38%)
18	BCR	A	4008	-	41,41,41	2.89	7 (17%)	56,56,56	6.49	22 (39%)
14	CLA	L	1501	-	64,68,73	2.28	21 (32%)	76,107,113	2.72	27 (35%)
14	CLA	L	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
15	F6C	H	1237	-	67,69,74	2.78	25 (37%)	77,108,114	3.21	36 (46%)
14	CLA	H	1227	-	49,53,73	2.55	20 (40%)	58,89,113	2.65	24 (41%)
14	CLA	a	1106	-	49,53,73	2.49	20 (40%)	58,89,113	2.91	25 (43%)
20	LMG	G	5005	-	46,46,55	1.36	5 (10%)	54,54,63	1.16	3 (5%)
18	BCR	H	4016	-	41,41,41	2.67	6 (14%)	56,56,56	6.65	18 (32%)
15	F6C	A	1120	-	52,54,74	3.10	25 (48%)	59,90,114	3.71	28 (47%)
18	BCR	b	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.62	26 (46%)
14	CLA	H	1226	-	69,73,73	2.26	21 (30%)	82,113,113	2.39	27 (32%)
14	CLA	H	1215	-	64,68,73	2.29	19 (29%)	76,107,113	2.52	30 (39%)
14	CLA	A	1105	-	49,53,73	2.53	21 (42%)	58,89,113	2.76	22 (37%)
14	CLA	H	1229	-	64,68,73	2.30	21 (32%)	76,107,113	2.65	26 (34%)
14	CLA	a	1136	-	59,63,73	2.35	22 (37%)	70,101,113	2.76	28 (40%)
18	BCR	b	4017	-	41,41,41	2.76	6 (14%)	56,56,56	6.75	18 (32%)
18	BCR	V	4021	-	41,41,41	2.72	6 (14%)	56,56,56	6.70	23 (41%)
21	LMT	G	6001	-	32,32,36	1.26	6 (18%)	43,43,47	1.04	4 (9%)
14	CLA	G	1117	-	69,73,73	2.19	22 (31%)	82,113,113	2.42	28 (34%)
14	CLA	B	1216	-	59,63,73	2.40	22 (37%)	70,101,113	2.60	31 (44%)
14	CLA	b	1021	-	69,73,73	2.18	21 (30%)	82,113,113	2.56	30 (36%)
14	CLA	H	1222	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	32 (39%)
14	CLA	H	1239	-	69,73,73	2.23	22 (31%)	82,113,113	2.63	30 (36%)
14	CLA	b	1022	-	69,73,73	2.20	20 (28%)	82,113,113	2.48	28 (34%)
14	CLA	A	1112	-	49,53,73	2.50	22 (44%)	58,89,113	2.78	22 (37%)
14	CLA	B	1217	-	59,63,73	2.38	21 (35%)	70,101,113	2.64	25 (35%)
14	CLA	H	1210	-	69,73,73	2.23	21 (30%)	82,113,113	2.57	32 (39%)
13	CL0	a	1011	-	58,73,73	3.15	21 (36%)	60,113,113	3.12	24 (40%)
14	CLA	A	1140	-	69,73,73	2.21	21 (30%)	82,113,113	2.42	27 (32%)
18	BCR	l	4019	-	41,41,41	2.68	6 (14%)	56,56,56	6.70	24 (42%)
18	BCR	H	4012	-	41,41,41	2.59	6 (14%)	56,56,56	6.78	27 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	1102	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	28 (36%)
14	CLA	H	1214	-	64,68,73	2.33	20 (31%)	76,107,113	2.53	35 (46%)
14	CLA	B	1224	-	69,73,73	2.21	20 (28%)	82,113,113	2.48	29 (35%)
16	PQN	B	2002	-	34,34,34	1.52	2 (5%)	43,45,45	1.18	1 (2%)
20	LMG	A	5005	-	46,46,55	1.36	5 (10%)	54,54,63	1.17	2 (3%)
17	SF4	C	3003	-	0,12,12	-	-	-		
20	LMG	b	5002	-	46,46,55	1.35	5 (10%)	54,54,63	1.18	3 (5%)
14	CLA	U	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	b	1207	-	49,53,73	2.48	20 (40%)	58,89,113	2.84	23 (39%)
14	CLA	b	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.78	23 (39%)
14	CLA	b	1205	-	69,73,73	2.19	20 (28%)	82,113,113	2.64	29 (35%)
14	CLA	H	1211	-	69,73,73	2.21	20 (28%)	82,113,113	2.39	26 (31%)
14	CLA	a	1108	-	49,53,73	2.52	21 (42%)	58,89,113	2.75	23 (39%)
14	CLA	G	1116	-	59,63,73	2.39	20 (33%)	70,101,113	2.67	28 (40%)
14	CLA	b	1221	-	64,68,73	2.27	20 (31%)	76,107,113	2.49	27 (35%)
18	BCR	I	4020	-	41,41,41	2.87	7 (17%)	56,56,56	6.44	24 (42%)
14	CLA	l	1501	-	64,68,73	2.28	21 (32%)	76,107,113	2.71	28 (36%)
18	BCR	G	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.30	24 (42%)
18	BCR	H	4014	-	41,41,41	2.75	6 (14%)	56,56,56	6.60	23 (41%)
14	CLA	a	1110	-	49,53,73	2.49	20 (40%)	58,89,113	2.90	23 (39%)
14	CLA	A	1131	-	64,68,73	2.27	21 (32%)	76,107,113	2.59	25 (32%)
14	CLA	G	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.58	28 (40%)
14	CLA	H	1213	-	59,63,73	2.40	21 (35%)	70,101,113	2.72	26 (37%)
14	CLA	H	1223	-	69,73,73	2.20	21 (30%)	82,113,113	2.48	26 (31%)
15	F6C	b	1230	-	52,54,74	3.07	27 (51%)	59,90,114	3.57	32 (54%)
14	CLA	b	1219	-	49,53,73	2.51	20 (40%)	58,89,113	2.75	22 (37%)
18	BCR	H	4006	-	41,41,41	2.65	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	G	1108	-	49,53,73	2.53	21 (42%)	58,89,113	2.75	23 (39%)
14	CLA	b	1215	-	64,68,73	2.30	19 (29%)	76,107,113	2.52	30 (39%)
18	BCR	H	4013	-	41,41,41	2.63	6 (14%)	56,56,56	6.72	23 (41%)
14	CLA	B	1202	-	64,68,73	2.25	20 (31%)	76,107,113	2.59	28 (36%)
14	CLA	B	1204	-	69,73,73	2.24	20 (28%)	82,113,113	2.49	27 (32%)
14	CLA	G	1109	-	49,53,73	2.47	21 (42%)	58,89,113	2.85	23 (39%)
14	CLA	G	1013	-	64,68,73	2.36	22 (34%)	76,107,113	2.67	30 (39%)
14	CLA	b	1216	-	59,63,73	2.40	22 (37%)	70,101,113	2.61	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	H	1204	-	69,73,73	2.24	20 (28%)	82,113,113	2.49	27 (32%)
14	CLA	l	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	25 (32%)
14	CLA	B	1225	-	69,73,73	2.25	20 (28%)	82,113,113	2.25	21 (25%)
18	BCR	H	4010	-	41,41,41	2.75	6 (14%)	56,56,56	6.74	22 (39%)
16	PQN	G	2001	-	34,34,34	1.48	2 (5%)	43,45,45	1.12	2 (4%)
15	F6C	G	1120	-	52,54,74	3.10	26 (50%)	59,90,114	3.72	28 (47%)
14	CLA	a	1129	-	49,53,73	2.51	18 (36%)	58,89,113	2.77	25 (43%)
14	CLA	X	1701	-	49,53,73	2.48	19 (38%)	58,89,113	2.75	23 (39%)
20	LMG	a	5005	-	46,46,55	1.37	5 (10%)	54,54,63	1.16	3 (5%)
20	LMG	H	5002	-	46,46,55	1.36	5 (10%)	54,54,63	1.18	3 (5%)
18	BCR	B	4016	-	41,41,41	2.67	6 (14%)	56,56,56	6.65	18 (32%)
14	CLA	B	1220	-	59,63,73	2.39	20 (33%)	70,101,113	2.64	25 (35%)
14	CLA	a	1103	-	64,68,73	2.22	20 (31%)	76,107,113	2.63	26 (34%)
14	CLA	A	1116	-	59,63,73	2.39	20 (33%)	70,101,113	2.66	28 (40%)
14	CLA	B	1229	-	64,68,73	2.30	21 (32%)	76,107,113	2.64	26 (34%)
14	CLA	L	1503	-	69,73,73	2.19	20 (28%)	82,113,113	2.46	26 (31%)
14	CLA	b	1225	-	69,73,73	2.25	20 (28%)	82,113,113	2.25	21 (25%)
14	CLA	A	1118	-	59,63,73	2.37	20 (33%)	70,101,113	2.73	28 (40%)
14	CLA	a	1107	-	49,53,73	2.48	19 (38%)	58,89,113	2.69	24 (41%)
14	CLA	B	1222	-	69,73,73	2.23	20 (28%)	82,113,113	2.58	32 (39%)
14	CLA	a	1137	-	49,53,73	2.48	19 (38%)	58,89,113	2.95	25 (43%)
14	CLA	H	1219	-	49,53,73	2.51	20 (40%)	58,89,113	2.76	22 (37%)
14	CLA	A	1132	-	69,73,73	2.21	20 (28%)	82,113,113	2.56	28 (34%)
19	LHG	G	5001	-	41,41,48	1.02	2 (4%)	44,47,54	1.12	4 (9%)
18	BCR	A	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.63	22 (39%)
14	CLA	H	1208	-	69,73,73	2.22	22 (31%)	82,113,113	2.45	25 (30%)
14	CLA	H	1225	-	69,73,73	2.25	20 (28%)	82,113,113	2.25	21 (25%)
14	CLA	A	1107	-	49,53,73	2.48	19 (38%)	58,89,113	2.70	24 (41%)
14	CLA	B	1232	-	49,53,73	2.52	22 (44%)	58,89,113	2.70	23 (39%)
18	BCR	G	4008	-	41,41,41	2.89	7 (17%)	56,56,56	6.49	22 (39%)
18	BCR	H	4009	-	41,41,41	2.71	6 (14%)	56,56,56	6.71	25 (44%)
14	CLA	H	1216	-	59,63,73	2.40	22 (37%)	70,101,113	2.60	30 (42%)
14	CLA	G	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	26 (34%)
16	PQN	H	2002	-	34,34,34	1.52	2 (5%)	43,45,45	1.18	1 (2%)
14	CLA	B	1226	-	69,73,73	2.26	21 (30%)	82,113,113	2.39	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	G	1127	-	69,73,73	2.23	21 (30%)	82,113,113	2.41	28 (34%)
14	CLA	G	1137	-	49,53,73	2.48	19 (38%)	58,89,113	2.96	25 (43%)
14	CLA	G	1107	-	49,53,73	2.48	19 (38%)	58,89,113	2.69	24 (41%)
16	PQN	a	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.12	2 (4%)
14	CLA	G	1124	-	59,63,73	2.37	21 (35%)	70,101,113	2.69	28 (40%)
18	BCR	a	4002	-	41,41,41	2.70	6 (14%)	56,56,56	6.30	24 (42%)
14	CLA	A	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.70	22 (37%)
14	CLA	a	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.59	27 (35%)
14	CLA	A	1102	-	64,68,73	2.33	21 (32%)	76,107,113	2.60	27 (35%)
14	CLA	B	1207	-	49,53,73	2.48	20 (40%)	58,89,113	2.83	24 (41%)
14	CLA	B	1022	-	69,73,73	2.20	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	a	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.58	27 (38%)
17	SF4	N	3002	-	0,12,12	-	-	-		
14	CLA	a	1122	-	59,63,73	2.37	21 (35%)	70,101,113	2.63	28 (40%)
17	SF4	c	3003	-	0,12,12	-	-	-		
15	F6C	b	1237	-	67,69,74	2.78	26 (38%)	77,108,114	3.21	36 (46%)
14	CLA	G	1115	-	59,63,73	2.39	21 (35%)	70,101,113	2.71	26 (37%)
14	CLA	H	1235	-	64,68,73	2.29	19 (29%)	76,107,113	2.65	27 (35%)
14	CLA	U	1501	-	64,68,73	2.28	21 (32%)	76,107,113	2.72	27 (35%)
14	CLA	B	1205	-	69,73,73	2.19	21 (30%)	82,113,113	2.64	29 (35%)
14	CLA	H	1218	-	49,53,73	2.50	19 (38%)	58,89,113	2.83	21 (36%)
14	CLA	b	1234	-	59,63,73	2.34	20 (33%)	70,101,113	2.66	27 (38%)
14	CLA	A	1103	-	64,68,73	2.23	20 (31%)	76,107,113	2.63	26 (34%)
14	CLA	G	1135	-	54,58,73	2.53	21 (38%)	64,95,113	2.84	28 (43%)
18	BCR	R	4018	-	41,41,41	2.86	7 (17%)	56,56,56	6.84	25 (44%)
14	CLA	b	1233	-	49,53,73	2.52	21 (42%)	58,89,113	2.78	24 (41%)
18	BCR	A	4011	-	41,41,41	2.75	7 (17%)	56,56,56	6.67	25 (44%)
14	CLA	A	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.59	27 (35%)
14	CLA	A	1106	-	49,53,73	2.49	20 (40%)	58,89,113	2.91	24 (41%)
18	BCR	H	4017	-	41,41,41	2.76	6 (14%)	56,56,56	6.76	18 (32%)
14	CLA	B	1219	-	49,53,73	2.51	20 (40%)	58,89,113	2.76	23 (39%)
14	CLA	G	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.60	27 (35%)
14	CLA	H	1201	-	59,63,73	2.37	21 (35%)	70,101,113	2.83	27 (38%)
18	BCR	i	4020	-	41,41,41	2.86	7 (17%)	56,56,56	6.44	24 (42%)
18	BCR	H	4005	-	41,41,41	2.66	7 (17%)	56,56,56	6.76	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	G	1119	-	69,73,73	2.22	19 (27%)	82,113,113	2.35	28 (34%)
14	CLA	a	1111	-	64,68,73	2.29	22 (34%)	76,107,113	2.62	29 (38%)
14	CLA	b	1023	-	69,73,73	2.20	22 (31%)	82,113,113	2.80	31 (37%)
14	CLA	K	1401	-	49,53,73	2.55	22 (44%)	58,89,113	2.76	21 (36%)
14	CLA	a	1104	-	69,73,73	2.16	20 (28%)	82,113,113	2.56	25 (30%)
15	F6C	a	1120	-	52,54,74	3.10	25 (48%)	59,90,114	3.72	27 (45%)
14	CLA	b	1213	-	59,63,73	2.40	21 (35%)	70,101,113	2.72	26 (37%)
14	CLA	B	1228	-	49,53,73	2.51	21 (42%)	58,89,113	2.75	26 (44%)
19	LHG	b	5004	-	43,43,48	0.98	2 (4%)	46,49,54	1.21	3 (6%)
14	CLA	A	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.58	27 (38%)
13	CL0	G	1011	-	58,73,73	3.15	21 (36%)	60,113,113	3.11	24 (40%)
14	CLA	G	1129	-	49,53,73	2.51	18 (36%)	58,89,113	2.77	25 (43%)
14	CLA	G	1136	-	59,63,73	2.34	21 (35%)	70,101,113	2.75	28 (40%)
18	BCR	a	4008	-	41,41,41	2.89	7 (17%)	56,56,56	6.48	22 (39%)
14	CLA	a	1128	-	64,68,73	2.33	20 (31%)	76,107,113	2.47	29 (38%)
20	LMG	B	5002	-	46,46,55	1.36	5 (10%)	54,54,63	1.18	3 (5%)
14	CLA	A	1117	-	69,73,73	2.19	21 (30%)	82,113,113	2.41	28 (34%)
14	CLA	b	1227	-	49,53,73	2.55	19 (38%)	58,89,113	2.64	24 (41%)
14	CLA	a	1126	-	64,68,73	2.33	20 (31%)	76,107,113	2.60	27 (35%)
14	CLA	a	1127	-	69,73,73	2.24	20 (28%)	82,113,113	2.41	28 (34%)
14	CLA	b	1228	-	49,53,73	2.50	21 (42%)	58,89,113	2.75	26 (44%)
18	BCR	B	4009	-	41,41,41	2.71	6 (14%)	56,56,56	6.72	25 (44%)
14	CLA	b	1231	-	59,63,73	2.42	20 (33%)	70,101,113	2.66	26 (37%)
14	CLA	a	1115	-	59,63,73	2.39	21 (35%)	70,101,113	2.71	26 (37%)
14	CLA	G	1123	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	29 (38%)
15	F6C	H	1230	-	52,54,74	3.08	27 (51%)	59,90,114	3.55	32 (54%)
14	CLA	G	1128	-	64,68,73	2.33	20 (31%)	76,107,113	2.48	29 (38%)
14	CLA	G	1111	-	64,68,73	2.29	22 (34%)	76,107,113	2.62	29 (38%)
14	CLA	b	1212	-	49,53,73	2.51	20 (40%)	58,89,113	2.81	23 (39%)
14	CLA	B	1206	-	49,53,73	2.49	19 (38%)	58,89,113	2.62	22 (37%)
14	CLA	H	1217	-	59,63,73	2.38	21 (35%)	70,101,113	2.64	25 (35%)
18	BCR	M	4021	-	41,41,41	2.72	6 (14%)	56,56,56	6.71	23 (41%)
14	CLA	B	1239	-	69,73,73	2.23	22 (31%)	82,113,113	2.62	30 (36%)
14	CLA	A	1101	-	49,53,73	2.48	19 (38%)	58,89,113	2.80	25 (43%)
16	PQN	A	2001	-	34,34,34	1.48	2 (5%)	43,45,45	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BCR	L	4022	-	41,41,41	2.82	6 (14%)	56,56,56	6.63	25 (44%)
14	CLA	H	1202	-	64,68,73	2.25	20 (31%)	76,107,113	2.59	27 (35%)
14	CLA	B	1201	-	59,63,73	2.37	21 (35%)	70,101,113	2.83	27 (38%)
14	CLA	A	1137	-	49,53,73	2.48	19 (38%)	58,89,113	2.95	25 (43%)
14	CLA	H	1207	-	49,53,73	2.49	20 (40%)	58,89,113	2.84	23 (39%)
14	CLA	a	1140	-	69,73,73	2.20	21 (30%)	82,113,113	2.40	27 (32%)
14	CLA	a	1135	-	54,58,73	2.52	21 (38%)	64,95,113	2.83	29 (45%)
14	CLA	b	1236	-	49,53,73	2.48	20 (40%)	58,89,113	2.79	23 (39%)
18	BCR	G	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.64	22 (39%)
14	CLA	b	1235	-	64,68,73	2.30	19 (29%)	76,107,113	2.65	27 (35%)
18	BCR	A	4007	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	24 (42%)

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
20	LMG	R	5006	-	-	13/32/52/70	0/1/1/1
18	BCR	G	4007	-	-	13/29/63/63	0/2/2/2
18	BCR	B	4017	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1224	-	1/1/15/20	12/39/115/115	-
14	CLA	G	1118	-	1/1/13/20	14/27/103/115	-
14	CLA	B	1021	-	1/1/15/20	14/39/115/115	-
21	LMT	A	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	B	1231	-	1/1/13/20	5/27/103/115	-
14	CLA	a	1119	-	1/1/15/20	15/39/115/115	-
17	SF4	c	3002	-	-	-	0/6/5/5
14	CLA	b	1206	-	1/1/11/20	5/15/91/115	-
14	CLA	G	1104	-	1/1/15/20	13/39/115/115	-
14	CLA	B	1211	-	1/1/15/20	16/39/115/115	-
14	CLA	B	1209	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1234	-	1/1/13/20	9/27/103/115	-
13	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	G	1131	-	1/1/14/20	17/33/109/115	-
18	BCR	B	4010	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1138	-	1/1/14/20	14/33/109/115	-
14	CLA	B	1221	-	1/1/14/20	13/33/109/115	-
17	SF4	a	3001	-	-	-	0/6/5/5
14	CLA	G	1114	-	1/1/11/20	7/15/91/115	-
14	CLA	A	1126	-	1/1/14/20	24/33/109/115	-
14	CLA	A	1115	-	1/1/13/20	9/27/103/115	-
18	BCR	U	4019	-	-	8/29/63/63	0/2/2/2
20	LMG	L	5007	-	-	13/45/65/70	0/1/1/1
18	BCR	b	4012	-	-	20/29/63/63	0/2/2/2
14	CLA	G	1138	-	1/1/14/20	14/33/109/115	-
14	CLA	b	1211	-	1/1/15/20	16/39/115/115	-
14	CLA	b	1210	-	1/1/15/20	9/39/115/115	-
17	SF4	C	3002	-	-	-	0/6/5/5
16	PQN	b	2002	-	-	11/23/43/43	0/2/2/2
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
15	F6C	B	1230	-	1/1/6/16	8/17/73/97	-
18	BCR	b	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	A	1135	-	1/1/12/20	6/21/97/115	-
14	CLA	T	1401	-	1/1/11/20	6/15/91/115	-
17	SF4	G	3001	-	-	-	0/6/5/5
15	F6C	a	1121	-	1/1/6/16	8/17/73/97	-
18	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	H	1209	-	1/1/11/20	4/15/91/115	-
18	BCR	b	4010	-	-	9/29/63/63	0/2/2/2
14	CLA	A	1108	-	1/1/11/20	6/15/91/115	-
14	CLA	b	1218	-	1/1/11/20	6/15/91/115	-
15	F6C	B	1237	-	1/1/9/16	17/35/91/97	-
21	LMT	a	6002	-	-	3/14/54/61	0/2/2/2
14	CLA	G	1122	-	1/1/13/20	9/27/103/115	-
14	CLA	H	1221	-	1/1/14/20	13/33/109/115	-
21	LMT	a	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	B	1023	-	1/1/15/20	15/39/115/115	-
14	CLA	a	1125	-	1/1/15/20	23/39/115/115	-
14	CLA	H	1233	-	1/1/11/20	9/15/91/115	-
14	CLA	a	1113	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	1129	-	1/1/11/20	4/15/91/115	-
14	CLA	A	1110	-	1/1/11/20	8/15/91/115	-
18	BCR	b	4014	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1215	-	1/1/14/20	14/33/109/115	-
14	CLA	H	1206	-	1/1/11/20	5/15/91/115	-
14	CLA	A	1119	-	1/1/15/20	15/39/115/115	-
18	BCR	I	4018	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1125	-	1/1/15/20	23/39/115/115	-
14	CLA	B	1203	-	1/1/15/20	18/39/115/115	-
14	CLA	a	1112	-	1/1/11/20	7/15/91/115	-
14	CLA	l	1503	-	1/1/15/20	12/39/115/115	-
14	CLA	b	1204	-	1/1/15/20	19/39/115/115	-
20	LMG	l	5007	-	-	13/45/65/70	0/1/1/1
18	BCR	a	4007	-	-	13/29/63/63	0/2/2/2
14	CLA	A	1124	-	1/1/13/20	9/27/103/115	-
14	CLA	b	1222	-	1/1/15/20	16/39/115/115	-
14	CLA	a	1138	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1012	-	1/1/15/20	14/39/115/115	-
14	CLA	G	1105	-	1/1/11/20	7/15/91/115	-
14	CLA	G	1106	-	1/1/11/20	9/15/91/115	-
18	BCR	H	4004	-	-	8/29/63/63	0/2/2/2
15	F6C	A	1121	-	1/1/6/16	8/17/73/97	-
14	CLA	a	1123	-	1/1/14/20	7/33/109/115	-
14	CLA	b	1223	-	1/1/15/20	11/39/115/115	-
14	CLA	A	1136	-	1/1/13/20	15/27/103/115	-
14	CLA	G	1132	-	1/1/15/20	20/39/115/115	-
21	LMT	A	6002	-	-	3/14/54/61	0/2/2/2
15	F6C	G	1121	-	1/1/6/16	8/17/73/97	-
14	CLA	a	1118	-	1/1/13/20	14/27/103/115	-
18	BCR	R	4020	-	-	11/29/63/63	0/2/2/2
18	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
14	CLA	G	1112	-	1/1/11/20	7/15/91/115	-
14	CLA	A	1125	-	1/1/15/20	23/39/115/115	-
14	CLA	b	1232	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1140	-	1/1/15/20	19/39/115/115	-
14	CLA	H	1023	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1232	-	1/1/11/20	4/15/91/115	-
20	LMG	i	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	A	1123	-	1/1/14/20	7/33/109/115	-
19	LHG	A	5001	-	-	20/46/46/53	-
14	CLA	H	1236	-	1/1/11/20	5/15/91/115	-
20	LMG	I	5006	-	-	13/32/52/70	0/1/1/1
14	CLA	B	1223	-	1/1/15/20	11/39/115/115	-
14	CLA	G	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	a	1131	-	1/1/14/20	17/33/109/115	-
14	CLA	A	1111	-	1/1/14/20	15/33/109/115	-
14	CLA	B	1208	-	1/1/15/20	10/39/115/115	-
14	CLA	H	1231	-	1/1/13/20	5/27/103/115	-
14	CLA	b	1224	-	1/1/15/20	12/39/115/115	-
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1238	-	1/1/15/20	15/39/115/115	-
14	CLA	G	1102	-	1/1/14/20	11/33/109/115	-
14	CLA	H	1212	-	1/1/11/20	11/15/91/115	-
18	BCR	a	4011	-	-	15/29/63/63	0/2/2/2
19	LHG	H	5004	-	-	19/48/48/53	-
14	CLA	b	1214	-	1/1/14/20	17/33/109/115	-
14	CLA	b	1203	-	1/1/15/20	18/39/115/115	-
18	BCR	m	4021	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1235	-	1/1/14/20	9/33/109/115	-
14	CLA	a	1012	-	1/1/15/20	14/39/115/115	-
14	CLA	A	1013	-	1/1/14/20	13/33/109/115	-
14	CLA	H	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	H	1205	-	1/1/15/20	14/39/115/115	-
18	BCR	a	4001	-	-	12/29/63/63	0/2/2/2
21	LMT	G	6002	-	-	3/14/54/61	0/2/2/2
14	CLA	H	1012	-	1/1/15/20	17/39/115/115	-
14	CLA	a	1114	-	1/1/11/20	7/15/91/115	-
14	CLA	b	1208	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	1210	-	1/1/15/20	9/39/115/115	-
18	BCR	b	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	B	1234	-	1/1/13/20	9/27/103/115	-
14	CLA	x	1701	-	1/1/11/20	8/15/91/115	-
14	CLA	a	1109	-	1/1/11/20	7/15/91/115	-
14	CLA	b	1202	-	1/1/14/20	11/33/109/115	-
14	CLA	a	1013	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1233	-	1/1/11/20	9/15/91/115	-
14	CLA	a	1117	-	1/1/15/20	15/39/115/115	-
14	CLA	a	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1228	-	1/1/11/20	6/15/91/115	-
14	CLA	b	1239	-	1/1/15/20	20/39/115/115	-
17	SF4	N	3003	-	-	-	0/6/5/5
14	CLA	B	1227	-	1/1/11/20	7/15/91/115	-
18	BCR	B	4005	-	-	4/29/63/63	0/2/2/2
19	LHG	a	5001	-	-	20/46/46/53	-
18	BCR	b	4013	-	-	19/29/63/63	0/2/2/2
14	CLA	a	1124	-	1/1/13/20	9/27/103/115	-
14	CLA	A	1109	-	1/1/11/20	7/15/91/115	-
14	CLA	A	1104	-	1/1/15/20	13/39/115/115	-
14	CLA	a	1105	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1214	-	1/1/14/20	17/33/109/115	-
14	CLA	A	1128	-	1/1/14/20	11/33/109/115	-
18	BCR	b	4016	-	-	15/29/63/63	0/2/2/2
14	CLA	B	1218	-	1/1/11/20	6/15/91/115	-
18	BCR	B	4012	-	-	20/29/63/63	0/2/2/2
14	CLA	H	1021	-	1/1/15/20	13/39/115/115	-
14	CLA	b	1226	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1238	-	1/1/15/20	15/39/115/115	-
14	CLA	U	1503	-	1/1/15/20	12/39/115/115	-
14	CLA	b	1229	-	1/1/14/20	15/33/109/115	-
14	CLA	H	1203	-	1/1/15/20	18/39/115/115	-
20	LMG	U	5007	-	-	13/45/65/70	0/1/1/1
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1116	-	1/1/13/20	12/27/103/115	-
19	LHG	B	5004	-	-	19/48/48/53	-
14	CLA	b	1217	-	1/1/13/20	10/27/103/115	-
14	CLA	b	1238	-	1/1/15/20	15/39/115/115	-
18	BCR	l	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	a	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	G	1110	-	1/1/11/20	8/15/91/115	-
14	CLA	B	1236	-	1/1/11/20	5/15/91/115	-
18	BCR	U	4022	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1012	-	1/1/15/20	14/39/115/115	-
17	SF4	A	3001	-	-	-	0/6/5/5
14	CLA	W	1701	-	1/1/11/20	8/15/91/115	-
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	b	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	k	1401	-	1/1/11/20	6/15/91/115	-
14	CLA	G	1139	-	1/1/11/20	4/15/91/115	-
18	BCR	L	4019	-	-	8/29/63/63	0/2/2/2
14	CLA	A	1114	-	1/1/11/20	7/15/91/115	-
14	CLA	A	1113	-	1/1/11/20	6/15/91/115	-
18	BCR	G	4011	-	-	15/29/63/63	0/2/2/2
14	CLA	a	1132	-	1/1/15/20	20/39/115/115	-
14	CLA	G	1103	-	1/1/14/20	17/33/109/115	-
14	CLA	A	1122	-	1/1/13/20	9/27/103/115	-
18	BCR	i	4018	-	-	11/29/63/63	0/2/2/2
18	BCR	B	4013	-	-	19/29/63/63	0/2/2/2
18	BCR	B	4014	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1212	-	1/1/11/20	11/15/91/115	-
14	CLA	G	1113	-	1/1/11/20	6/15/91/115	-
14	CLA	A	1127	-	1/1/15/20	15/39/115/115	-
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1213	-	1/1/13/20	14/27/103/115	-
14	CLA	b	1201	-	1/1/13/20	12/27/103/115	-
18	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
14	CLA	L	1501	-	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L	1502	-	1/1/14/20	12/33/109/115	-
15	F6C	H	1237	-	1/1/9/16	17/35/91/97	-
14	CLA	H	1227	-	1/1/11/20	7/15/91/115	-
14	CLA	a	1106	-	1/1/11/20	9/15/91/115	-
20	LMG	G	5005	-	-	17/41/61/70	0/1/1/1
18	BCR	H	4016	-	-	15/29/63/63	0/2/2/2
15	F6C	A	1120	-	1/1/6/16	8/17/73/97	-
18	BCR	b	4004	-	-	8/29/63/63	0/2/2/2
14	CLA	H	1226	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1215	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1105	-	1/1/11/20	7/15/91/115	-
14	CLA	H	1229	-	1/1/14/20	15/33/109/115	-
14	CLA	a	1136	-	1/1/13/20	15/27/103/115	-
18	BCR	b	4017	-	-	11/29/63/63	0/2/2/2
18	BCR	V	4021	-	-	11/29/63/63	0/2/2/2
21	LMT	G	6001	-	-	9/17/57/61	0/2/2/2
14	CLA	G	1117	-	1/1/15/20	15/39/115/115	-
14	CLA	B	1216	-	1/1/13/20	10/27/103/115	-
14	CLA	b	1021	-	1/1/15/20	13/39/115/115	-
14	CLA	H	1222	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1239	-	1/1/15/20	20/39/115/115	-
14	CLA	b	1022	-	1/1/15/20	17/39/115/115	-
14	CLA	A	1112	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1217	-	1/1/13/20	10/27/103/115	-
14	CLA	H	1210	-	1/1/15/20	9/39/115/115	-
13	CL0	a	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	A	1140	-	1/1/15/20	19/39/115/115	-
18	BCR	l	4019	-	-	8/29/63/63	0/2/2/2
18	BCR	H	4012	-	-	20/29/63/63	0/2/2/2
14	CLA	a	1102	-	1/1/14/20	11/33/109/115	-
14	CLA	H	1214	-	1/1/14/20	17/33/109/115	-
14	CLA	B	1224	-	1/1/15/20	12/39/115/115	-
16	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
20	LMG	A	5005	-	-	17/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	C	3003	-	-	-	0/6/5/5
20	LMG	b	5002	-	-	17/41/61/70	0/1/1/1
14	CLA	U	1502	-	1/1/14/20	12/33/109/115	-
14	CLA	b	1207	-	1/1/11/20	7/15/91/115	-
14	CLA	b	1209	-	1/1/11/20	4/15/91/115	-
14	CLA	b	1205	-	1/1/15/20	14/39/115/115	-
14	CLA	H	1211	-	1/1/15/20	16/39/115/115	-
14	CLA	a	1108	-	1/1/11/20	6/15/91/115	-
14	CLA	G	1116	-	1/1/13/20	12/27/103/115	-
14	CLA	b	1221	-	1/1/14/20	13/33/109/115	-
18	BCR	I	4020	-	-	11/29/63/63	0/2/2/2
14	CLA	l	1501	-	1/1/14/20	12/33/109/115	-
18	BCR	G	4002	-	-	7/29/63/63	0/2/2/2
18	BCR	H	4014	-	-	11/29/63/63	0/2/2/2
14	CLA	a	1110	-	1/1/11/20	8/15/91/115	-
14	CLA	A	1131	-	1/1/14/20	17/33/109/115	-
14	CLA	G	1130	-	1/1/13/20	10/27/103/115	-
14	CLA	H	1213	-	1/1/13/20	14/27/103/115	-
14	CLA	H	1223	-	1/1/15/20	11/39/115/115	-
15	F6C	b	1230	-	1/1/6/16	3/17/73/97	-
14	CLA	b	1219	-	1/1/11/20	7/15/91/115	-
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	G	1108	-	1/1/11/20	6/15/91/115	-
14	CLA	b	1215	-	1/1/14/20	14/33/109/115	-
18	BCR	H	4013	-	-	19/29/63/63	0/2/2/2
14	CLA	B	1202	-	1/1/14/20	11/33/109/115	-
14	CLA	B	1204	-	1/1/15/20	19/39/115/115	-
14	CLA	G	1109	-	1/1/11/20	7/15/91/115	-
14	CLA	G	1013	-	1/1/14/20	13/33/109/115	-
14	CLA	b	1216	-	1/1/13/20	10/27/103/115	-
14	CLA	H	1204	-	1/1/15/20	19/39/115/115	-
14	CLA	l	1502	-	1/1/14/20	12/33/109/115	-
14	CLA	B	1225	-	1/1/15/20	14/39/115/115	-
18	BCR	H	4010	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
15	F6C	G	1120	-	1/1/6/16	8/17/73/97	-
14	CLA	a	1129	-	1/1/11/20	4/15/91/115	-
14	CLA	X	1701	-	1/1/11/20	8/15/91/115	-
20	LMG	a	5005	-	-	17/41/61/70	0/1/1/1
20	LMG	H	5002	-	-	17/41/61/70	0/1/1/1
18	BCR	B	4016	-	-	15/29/63/63	0/2/2/2
14	CLA	B	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	a	1103	-	1/1/14/20	17/33/109/115	-
14	CLA	A	1116	-	1/1/13/20	12/27/103/115	-
14	CLA	B	1229	-	1/1/14/20	15/33/109/115	-
14	CLA	L	1503	-	1/1/15/20	12/39/115/115	-
14	CLA	b	1225	-	1/1/15/20	14/39/115/115	-
14	CLA	A	1118	-	1/1/13/20	14/27/103/115	-
14	CLA	a	1107	-	1/1/11/20	5/15/91/115	-
14	CLA	B	1222	-	1/1/15/20	16/39/115/115	-
14	CLA	a	1137	-	1/1/11/20	7/15/91/115	-
14	CLA	H	1219	-	1/1/11/20	7/15/91/115	-
14	CLA	A	1132	-	1/1/15/20	20/39/115/115	-
19	LHG	G	5001	-	-	20/46/46/53	-
18	BCR	A	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	H	1208	-	1/1/15/20	10/39/115/115	-
14	CLA	H	1225	-	1/1/15/20	14/39/115/115	-
14	CLA	A	1107	-	1/1/11/20	5/15/91/115	-
14	CLA	B	1232	-	1/1/11/20	4/15/91/115	-
18	BCR	G	4008	-	-	10/29/63/63	0/2/2/2
18	BCR	H	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	H	1216	-	1/1/13/20	10/27/103/115	-
14	CLA	G	1126	-	1/1/14/20	24/33/109/115	-
16	PQN	H	2002	-	-	11/23/43/43	0/2/2/2
14	CLA	B	1226	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1127	-	1/1/15/20	15/39/115/115	-
14	CLA	G	1137	-	1/1/11/20	7/15/91/115	-
14	CLA	G	1107	-	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	G	1124	-	1/1/13/20	9/27/103/115	-
18	BCR	a	4002	-	-	7/29/63/63	0/2/2/2
14	CLA	A	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	a	1133	-	1/1/14/20	19/33/109/115	-
14	CLA	A	1102	-	1/1/14/20	11/33/109/115	-
14	CLA	B	1207	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1022	-	1/1/15/20	17/39/115/115	-
14	CLA	a	1130	-	1/1/13/20	10/27/103/115	-
17	SF4	N	3002	-	-	-	0/6/5/5
14	CLA	a	1122	-	1/1/13/20	9/27/103/115	-
17	SF4	c	3003	-	-	-	0/6/5/5
15	F6C	b	1237	-	1/1/9/16	17/35/91/97	-
14	CLA	G	1115	-	1/1/13/20	9/27/103/115	-
14	CLA	H	1235	-	1/1/14/20	9/33/109/115	-
14	CLA	U	1501	-	1/1/14/20	12/33/109/115	-
14	CLA	B	1205	-	1/1/15/20	14/39/115/115	-
14	CLA	H	1218	-	1/1/11/20	6/15/91/115	-
14	CLA	b	1234	-	1/1/13/20	9/27/103/115	-
14	CLA	A	1103	-	1/1/14/20	17/33/109/115	-
14	CLA	G	1135	-	1/1/12/20	6/21/97/115	-
18	BCR	R	4018	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1233	-	1/1/11/20	9/15/91/115	-
18	BCR	A	4011	-	-	15/29/63/63	0/2/2/2
14	CLA	A	1133	-	1/1/14/20	19/33/109/115	-
14	CLA	A	1106	-	1/1/11/20	9/15/91/115	-
18	BCR	H	4017	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1219	-	1/1/11/20	7/15/91/115	-
14	CLA	G	1133	-	1/1/14/20	19/33/109/115	-
14	CLA	H	1201	-	1/1/13/20	12/27/103/115	-
18	BCR	i	4020	-	-	11/29/63/63	0/2/2/2
18	BCR	H	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	G	1119	-	1/1/15/20	15/39/115/115	-
14	CLA	a	1111	-	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1023	-	1/1/15/20	15/39/115/115	-
14	CLA	K	1401	-	1/1/11/20	6/15/91/115	-
14	CLA	a	1104	-	1/1/15/20	13/39/115/115	-
15	F6C	a	1120	-	1/1/6/16	8/17/73/97	-
14	CLA	b	1213	-	1/1/13/20	14/27/103/115	-
14	CLA	B	1228	-	1/1/11/20	6/15/91/115	-
19	LHG	b	5004	-	-	19/48/48/53	-
14	CLA	A	1130	-	1/1/13/20	10/27/103/115	-
13	CL0	G	1011	-	3/3/20/25	11/37/135/135	-
14	CLA	G	1129	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1136	-	1/1/13/20	15/27/103/115	-
18	BCR	a	4008	-	-	10/29/63/63	0/2/2/2
14	CLA	a	1128	-	1/1/14/20	11/33/109/115	-
20	LMG	B	5002	-	-	17/41/61/70	0/1/1/1
14	CLA	A	1117	-	1/1/15/20	15/39/115/115	-
14	CLA	b	1227	-	1/1/11/20	7/15/91/115	-
14	CLA	a	1126	-	1/1/14/20	24/33/109/115	-
14	CLA	a	1127	-	1/1/15/20	15/39/115/115	-
14	CLA	b	1228	-	1/1/11/20	6/15/91/115	-
18	BCR	B	4009	-	-	4/29/63/63	0/2/2/2
14	CLA	b	1231	-	1/1/13/20	5/27/103/115	-
14	CLA	a	1115	-	1/1/13/20	9/27/103/115	-
14	CLA	G	1123	-	1/1/14/20	7/33/109/115	-
15	F6C	H	1230	-	1/1/6/16	5/17/73/97	-
14	CLA	G	1128	-	1/1/14/20	11/33/109/115	-
14	CLA	G	1111	-	1/1/14/20	15/33/109/115	-
14	CLA	b	1212	-	1/1/11/20	11/15/91/115	-
14	CLA	B	1206	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1217	-	1/1/13/20	10/27/103/115	-
18	BCR	M	4021	-	-	11/29/63/63	0/2/2/2
14	CLA	B	1239	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1101	-	1/1/11/20	8/15/91/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
18	BCR	L	4022	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1202	-	1/1/14/20	11/33/109/115	-
14	CLA	B	1201	-	1/1/13/20	12/27/103/115	-
14	CLA	A	1137	-	1/1/11/20	7/15/91/115	-
14	CLA	H	1207	-	1/1/11/20	7/15/91/115	-
14	CLA	a	1140	-	1/1/15/20	19/39/115/115	-
14	CLA	a	1135	-	1/1/12/20	6/21/97/115	-
14	CLA	b	1236	-	1/1/11/20	5/15/91/115	-
18	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1235	-	1/1/14/20	9/33/109/115	-
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2

All (6027) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1237	F6C	C1A-CHA	9.88	1.51	1.35
15	b	1237	F6C	C1A-CHA	9.88	1.51	1.35
15	G	1120	F6C	C1A-CHA	9.87	1.51	1.35
15	A	1120	F6C	C1A-CHA	9.86	1.51	1.35
15	a	1120	F6C	C1A-CHA	9.86	1.51	1.35
15	H	1237	F6C	C1A-CHA	9.84	1.51	1.35
15	a	1121	F6C	C1A-CHA	9.44	1.50	1.35
15	G	1121	F6C	C1A-CHA	9.43	1.50	1.35
15	A	1121	F6C	C1A-CHA	9.41	1.50	1.35
13	A	1011	CL0	C1A-CHA	9.21	1.50	1.40
13	a	1011	CL0	C1A-CHA	9.15	1.50	1.40
13	G	1011	CL0	C1A-CHA	9.14	1.50	1.40
15	H	1230	F6C	MG-NA	9.12	2.23	2.05
15	B	1230	F6C	MG-NA	9.10	2.23	2.05
15	b	1230	F6C	MG-NA	9.04	2.23	2.05
15	a	1121	F6C	MG-NA	8.97	2.23	2.05
15	G	1121	F6C	MG-NA	8.96	2.23	2.05
13	a	1011	CL0	C1B-C2B	8.95	1.49	1.39
15	A	1121	F6C	MG-NA	8.94	2.23	2.05
15	a	1120	F6C	MG-NA	8.90	2.23	2.05
15	A	1120	F6C	MG-NA	8.88	2.23	2.05
15	G	1120	F6C	MG-NA	8.88	2.23	2.05
13	G	1011	CL0	C1B-C2B	8.86	1.49	1.39
13	A	1011	CL0	C1B-C2B	8.86	1.49	1.39
18	a	4008	BCR	C8-C9	-8.84	1.27	1.46
15	B	1237	F6C	MG-NA	8.83	2.23	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1237	F6C	MG-NA	8.83	2.23	2.05
18	A	4008	BCR	C8-C9	-8.82	1.27	1.46
18	G	4008	BCR	C8-C9	-8.81	1.27	1.46
15	B	1230	F6C	C1A-CHA	8.79	1.49	1.35
15	H	1237	F6C	MG-NA	8.78	2.23	2.05
15	b	1230	F6C	C1A-CHA	8.78	1.49	1.35
15	H	1230	F6C	C1A-CHA	8.74	1.49	1.35
18	l	4022	BCR	C8-C9	-8.68	1.27	1.46
18	L	4022	BCR	C8-C9	-8.67	1.27	1.46
18	U	4022	BCR	C8-C9	-8.65	1.27	1.46
18	I	4018	BCR	C8-C9	-8.64	1.27	1.46
18	a	4007	BCR	C8-C9	-8.62	1.27	1.46
18	R	4018	BCR	C8-C9	-8.62	1.27	1.46
18	i	4018	BCR	C8-C9	-8.61	1.27	1.46
18	G	4008	BCR	C11-C10	-8.61	1.16	1.43
18	V	4021	BCR	C8-C9	-8.60	1.27	1.46
18	G	4007	BCR	C8-C9	-8.60	1.27	1.46
18	G	4011	BCR	C8-C9	-8.60	1.27	1.46
18	A	4008	BCR	C11-C10	-8.59	1.16	1.43
18	A	4007	BCR	C8-C9	-8.59	1.27	1.46
18	A	4011	BCR	C8-C9	-8.59	1.27	1.46
18	a	4008	BCR	C11-C10	-8.59	1.16	1.43
18	m	4021	BCR	C8-C9	-8.59	1.27	1.46
18	a	4002	BCR	C8-C9	-8.55	1.27	1.46
18	M	4021	BCR	C8-C9	-8.55	1.27	1.46
18	a	4011	BCR	C8-C9	-8.55	1.27	1.46
18	A	4001	BCR	C8-C9	-8.54	1.27	1.46
18	G	4001	BCR	C8-C9	-8.54	1.27	1.46
18	R	4020	BCR	C8-C9	-8.53	1.27	1.46
18	a	4001	BCR	C8-C9	-8.53	1.27	1.46
18	G	4002	BCR	C8-C9	-8.52	1.27	1.46
18	I	4020	BCR	C8-C9	-8.52	1.27	1.46
18	A	4002	BCR	C8-C9	-8.50	1.27	1.46
18	L	4022	BCR	C11-C10	-8.50	1.16	1.43
18	U	4022	BCR	C11-C10	-8.49	1.16	1.43
18	i	4018	BCR	C11-C10	-8.47	1.16	1.43
18	B	4010	BCR	C8-C9	-8.47	1.27	1.46
18	b	4017	BCR	C8-C9	-8.47	1.27	1.46
18	i	4020	BCR	C8-C9	-8.47	1.27	1.46
18	B	4017	BCR	C8-C9	-8.47	1.27	1.46
18	H	4010	BCR	C8-C9	-8.47	1.27	1.46
18	l	4022	BCR	C11-C10	-8.46	1.16	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	4010	BCR	C8-C9	-8.46	1.27	1.46
18	I	4018	BCR	C11-C10	-8.45	1.17	1.43
18	R	4018	BCR	C11-C10	-8.44	1.17	1.43
18	H	4017	BCR	C8-C9	-8.42	1.27	1.46
18	B	4014	BCR	C8-C9	-8.38	1.28	1.46
18	H	4014	BCR	C8-C9	-8.38	1.28	1.46
18	b	4014	BCR	C8-C9	-8.38	1.28	1.46
18	G	4003	BCR	C8-C9	-8.38	1.28	1.46
18	a	4003	BCR	C8-C9	-8.38	1.28	1.46
18	b	4012	BCR	C8-C9	-8.38	1.28	1.46
18	H	4006	BCR	C8-C9	-8.37	1.28	1.46
18	A	4003	BCR	C8-C9	-8.37	1.28	1.46
18	R	4020	BCR	C11-C10	-8.35	1.17	1.43
18	b	4006	BCR	C8-C9	-8.34	1.28	1.46
18	b	4004	BCR	C8-C9	-8.32	1.28	1.46
18	B	4012	BCR	C8-C9	-8.32	1.28	1.46
18	H	4016	BCR	C8-C9	-8.32	1.28	1.46
18	H	4012	BCR	C8-C9	-8.32	1.28	1.46
18	B	4016	BCR	C8-C9	-8.32	1.28	1.46
18	i	4020	BCR	C11-C10	-8.32	1.17	1.43
18	I	4020	BCR	C11-C10	-8.31	1.17	1.43
18	H	4004	BCR	C8-C9	-8.31	1.28	1.46
18	a	4007	BCR	C11-C10	-8.31	1.17	1.43
18	B	4004	BCR	C8-C9	-8.30	1.28	1.46
18	b	4016	BCR	C8-C9	-8.30	1.28	1.46
18	M	4021	BCR	C11-C10	-8.30	1.17	1.43
18	B	4006	BCR	C8-C9	-8.30	1.28	1.46
18	G	4007	BCR	C11-C10	-8.29	1.17	1.43
18	H	4017	BCR	C11-C10	-8.29	1.17	1.43
18	B	4017	BCR	C11-C10	-8.29	1.17	1.43
18	V	4021	BCR	C11-C10	-8.28	1.17	1.43
18	b	4017	BCR	C11-C10	-8.28	1.17	1.43
18	l	4019	BCR	C8-C9	-8.28	1.28	1.46
18	m	4021	BCR	C11-C10	-8.27	1.17	1.43
18	G	4001	BCR	C11-C10	-8.26	1.17	1.43
18	A	4007	BCR	C11-C10	-8.26	1.17	1.43
18	b	4014	BCR	C11-C10	-8.26	1.17	1.43
18	B	4014	BCR	C11-C10	-8.26	1.17	1.43
18	a	4001	BCR	C11-C10	-8.26	1.17	1.43
18	A	4001	BCR	C11-C10	-8.25	1.17	1.43
18	H	4014	BCR	C11-C10	-8.24	1.17	1.43
18	b	4013	BCR	C8-C9	-8.24	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	4016	BCR	C11-C10	-8.24	1.17	1.43
18	L	4019	BCR	C8-C9	-8.23	1.28	1.46
18	H	4013	BCR	C8-C9	-8.23	1.28	1.46
18	U	4019	BCR	C8-C9	-8.22	1.28	1.46
18	A	4011	BCR	C11-C10	-8.22	1.17	1.43
18	B	4013	BCR	C8-C9	-8.22	1.28	1.46
18	H	4016	BCR	C11-C10	-8.21	1.17	1.43
18	G	4011	BCR	C11-C10	-8.20	1.17	1.43
18	B	4016	BCR	C11-C10	-8.20	1.17	1.43
18	a	4011	BCR	C11-C10	-8.19	1.17	1.43
18	B	4010	BCR	C11-C10	-8.17	1.17	1.43
18	B	4009	BCR	C11-C10	-8.16	1.17	1.43
18	H	4009	BCR	C8-C9	-8.16	1.28	1.46
18	b	4009	BCR	C11-C10	-8.16	1.17	1.43
18	b	4010	BCR	C11-C10	-8.16	1.17	1.43
18	H	4009	BCR	C11-C10	-8.15	1.17	1.43
18	H	4010	BCR	C11-C10	-8.15	1.17	1.43
18	B	4009	BCR	C8-C9	-8.15	1.28	1.46
18	b	4009	BCR	C8-C9	-8.13	1.28	1.46
18	A	4003	BCR	C11-C10	-8.10	1.18	1.43
18	a	4003	BCR	C11-C10	-8.08	1.18	1.43
18	G	4003	BCR	C11-C10	-8.08	1.18	1.43
18	b	4004	BCR	C11-C10	-8.08	1.18	1.43
18	U	4019	BCR	C11-C10	-8.07	1.18	1.43
18	B	4004	BCR	C11-C10	-8.07	1.18	1.43
18	H	4004	BCR	C11-C10	-8.06	1.18	1.43
18	L	4019	BCR	C11-C10	-8.05	1.18	1.43
18	l	4019	BCR	C11-C10	-8.04	1.18	1.43
18	H	4005	BCR	C11-C10	-8.04	1.18	1.43
18	b	4005	BCR	C11-C10	-8.04	1.18	1.43
18	H	4013	BCR	C11-C10	-8.03	1.18	1.43
18	B	4005	BCR	C11-C10	-8.03	1.18	1.43
18	B	4013	BCR	C11-C10	-8.02	1.18	1.43
18	b	4013	BCR	C11-C10	-8.02	1.18	1.43
18	H	4005	BCR	C8-C9	-7.99	1.28	1.46
18	B	4005	BCR	C8-C9	-7.98	1.28	1.46
18	b	4005	BCR	C8-C9	-7.96	1.28	1.46
18	H	4006	BCR	C11-C10	-7.95	1.18	1.43
18	B	4006	BCR	C11-C10	-7.95	1.18	1.43
18	b	4006	BCR	C11-C10	-7.95	1.18	1.43
18	A	4008	BCR	C20-C21	-7.88	1.18	1.43
18	A	4002	BCR	C11-C10	-7.87	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	a	4002	BCR	C11-C10	-7.86	1.18	1.43
18	G	4002	BCR	C11-C10	-7.85	1.18	1.43
18	G	4008	BCR	C20-C21	-7.82	1.18	1.43
18	a	4008	BCR	C20-C21	-7.82	1.18	1.43
13	A	1011	CL0	C3A-C2A	-7.82	1.47	1.54
13	G	1011	CL0	C3A-C2A	-7.81	1.48	1.54
18	I	4020	BCR	C16-C17	-7.80	1.19	1.43
18	R	4020	BCR	C16-C17	-7.80	1.19	1.43
18	i	4020	BCR	C16-C17	-7.79	1.19	1.43
18	U	4022	BCR	C20-C21	-7.78	1.19	1.43
18	L	4022	BCR	C20-C21	-7.77	1.19	1.43
18	b	4012	BCR	C11-C10	-7.77	1.19	1.43
13	a	1011	CL0	C3A-C2A	-7.77	1.48	1.54
18	H	4012	BCR	C11-C10	-7.77	1.19	1.43
18	R	4018	BCR	C20-C21	-7.77	1.19	1.43
18	l	4022	BCR	C20-C21	-7.76	1.19	1.43
18	B	4012	BCR	C11-C10	-7.76	1.19	1.43
18	A	4008	BCR	C16-C17	-7.75	1.19	1.43
18	G	4011	BCR	C20-C21	-7.75	1.19	1.43
18	G	4008	BCR	C16-C17	-7.75	1.19	1.43
18	I	4018	BCR	C20-C21	-7.74	1.19	1.43
18	a	4008	BCR	C16-C17	-7.74	1.19	1.43
18	i	4018	BCR	C20-C21	-7.73	1.19	1.43
18	A	4011	BCR	C20-C21	-7.72	1.19	1.43
18	a	4011	BCR	C20-C21	-7.72	1.19	1.43
18	H	4009	BCR	C20-C21	-7.71	1.19	1.43
18	B	4009	BCR	C20-C21	-7.70	1.19	1.43
18	b	4009	BCR	C20-C21	-7.69	1.19	1.43
18	L	4022	BCR	C16-C17	-7.68	1.19	1.43
18	U	4022	BCR	C16-C17	-7.67	1.19	1.43
18	I	4020	BCR	C20-C21	-7.65	1.19	1.43
18	i	4020	BCR	C20-C21	-7.65	1.19	1.43
18	R	4020	BCR	C20-C21	-7.64	1.19	1.43
18	l	4022	BCR	C16-C17	-7.64	1.19	1.43
18	i	4018	BCR	C16-C17	-7.64	1.19	1.43
18	H	4010	BCR	C16-C17	-7.63	1.19	1.43
18	B	4017	BCR	C20-C21	-7.63	1.19	1.43
18	I	4018	BCR	C16-C17	-7.62	1.19	1.43
18	R	4018	BCR	C16-C17	-7.61	1.19	1.43
18	H	4017	BCR	C20-C21	-7.61	1.19	1.43
18	B	4010	BCR	C20-C21	-7.61	1.19	1.43
18	H	4014	BCR	C16-C17	-7.61	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	4014	BCR	C16-C17	-7.60	1.19	1.43
18	b	4017	BCR	C20-C21	-7.60	1.19	1.43
18	B	4010	BCR	C16-C17	-7.60	1.19	1.43
18	H	4010	BCR	C20-C21	-7.60	1.19	1.43
18	b	4010	BCR	C16-C17	-7.60	1.19	1.43
18	B	4014	BCR	C20-C21	-7.60	1.19	1.43
18	B	4014	BCR	C16-C17	-7.59	1.19	1.43
18	b	4010	BCR	C20-C21	-7.58	1.19	1.43
16	b	2002	PQN	C3-C2	7.58	1.48	1.35
14	B	1223	CLA	MG-NA	7.57	2.24	2.06
14	K	1401	CLA	MG-NA	7.57	2.24	2.06
18	H	4014	BCR	C20-C21	-7.57	1.19	1.43
14	T	1401	CLA	MG-NA	7.57	2.24	2.06
18	b	4014	BCR	C20-C21	-7.57	1.19	1.43
16	B	2002	PQN	C3-C2	7.57	1.48	1.35
18	H	4017	BCR	C16-C17	-7.56	1.19	1.43
16	H	2002	PQN	C3-C2	7.55	1.48	1.35
14	k	1401	CLA	MG-NA	7.55	2.24	2.06
18	b	4017	BCR	C16-C17	-7.54	1.19	1.43
18	a	4003	BCR	C20-C21	-7.54	1.19	1.43
14	b	1233	CLA	MG-NA	7.54	2.24	2.06
14	H	1223	CLA	MG-NA	7.54	2.24	2.06
18	B	4017	BCR	C16-C17	-7.53	1.19	1.43
18	G	4003	BCR	C20-C21	-7.53	1.19	1.43
18	A	4003	BCR	C20-C21	-7.52	1.19	1.43
14	b	1223	CLA	MG-NA	7.52	2.24	2.06
14	B	1232	CLA	MG-NA	7.52	2.24	2.06
14	H	1233	CLA	MG-NA	7.51	2.24	2.06
18	b	4009	BCR	C16-C17	-7.51	1.19	1.43
14	B	1233	CLA	MG-NA	7.51	2.24	2.06
18	B	4009	BCR	C16-C17	-7.51	1.19	1.43
14	A	1110	CLA	MG-NA	7.49	2.24	2.06
18	A	4002	BCR	C20-C21	-7.49	1.20	1.43
18	H	4009	BCR	C16-C17	-7.49	1.20	1.43
18	b	4005	BCR	C20-C21	-7.48	1.20	1.43
14	B	1212	CLA	MG-NA	7.48	2.24	2.06
18	H	4016	BCR	C20-C21	-7.48	1.20	1.43
14	A	1123	CLA	MG-NA	7.48	2.24	2.06
18	A	4001	BCR	C20-C21	-7.47	1.20	1.43
14	b	1232	CLA	MG-NA	7.47	2.24	2.06
14	G	1111	CLA	MG-NA	7.47	2.24	2.06
18	a	4001	BCR	C16-C17	-7.47	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1232	CLA	MG-NA	7.47	2.24	2.06
14	G	1123	CLA	MG-NA	7.47	2.24	2.06
18	G	4003	BCR	C16-C17	-7.47	1.20	1.43
18	H	4004	BCR	C20-C21	-7.46	1.20	1.43
18	a	4001	BCR	C20-C21	-7.46	1.20	1.43
15	H	1230	F6C	C2A-C3A	7.46	1.52	1.36
14	a	1110	CLA	MG-NA	7.46	2.24	2.06
18	A	4007	BCR	C16-C17	-7.46	1.20	1.43
14	A	1111	CLA	MG-NA	7.46	2.24	2.06
18	G	4002	BCR	C20-C21	-7.46	1.20	1.43
14	G	1110	CLA	MG-NA	7.46	2.24	2.06
18	A	4003	BCR	C16-C17	-7.46	1.20	1.43
14	H	1212	CLA	MG-NA	7.46	2.24	2.06
18	b	4004	BCR	C20-C21	-7.45	1.20	1.43
18	G	4001	BCR	C20-C21	-7.45	1.20	1.43
18	G	4001	BCR	C16-C17	-7.45	1.20	1.43
18	a	4002	BCR	C20-C21	-7.45	1.20	1.43
18	B	4005	BCR	C20-C21	-7.45	1.20	1.43
18	A	4001	BCR	C16-C17	-7.45	1.20	1.43
18	U	4019	BCR	C20-C21	-7.45	1.20	1.43
18	G	4007	BCR	C16-C17	-7.45	1.20	1.43
14	b	1212	CLA	MG-NA	7.45	2.24	2.06
14	B	1214	CLA	MG-NA	7.45	2.24	2.06
18	B	4016	BCR	C20-C21	-7.45	1.20	1.43
18	b	4016	BCR	C20-C21	-7.44	1.20	1.43
18	H	4005	BCR	C20-C21	-7.44	1.20	1.43
18	a	4002	BCR	C16-C17	-7.44	1.20	1.43
18	L	4019	BCR	C20-C21	-7.44	1.20	1.43
18	B	4004	BCR	C20-C21	-7.44	1.20	1.43
18	l	4019	BCR	C20-C21	-7.44	1.20	1.43
14	a	1111	CLA	MG-NA	7.44	2.23	2.06
18	a	4003	BCR	C16-C17	-7.44	1.20	1.43
14	a	1123	CLA	MG-NA	7.43	2.23	2.06
18	a	4007	BCR	C16-C17	-7.43	1.20	1.43
18	A	4007	BCR	C20-C21	-7.42	1.20	1.43
14	H	1214	CLA	MG-NA	7.42	2.23	2.06
14	b	1214	CLA	MG-NA	7.42	2.23	2.06
18	A	4002	BCR	C16-C17	-7.42	1.20	1.43
18	a	4007	BCR	C20-C21	-7.41	1.20	1.43
14	G	1135	CLA	MG-NA	7.41	2.23	2.06
14	W	1701	CLA	MG-NA	7.41	2.23	2.06
15	B	1230	F6C	C2A-C3A	7.41	1.52	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	4002	BCR	C16-C17	-7.41	1.20	1.43
14	G	1133	CLA	MG-NA	7.40	2.23	2.06
18	G	4007	BCR	C20-C21	-7.40	1.20	1.43
18	A	4011	BCR	C16-C17	-7.40	1.20	1.43
14	a	1135	CLA	MG-NA	7.40	2.23	2.06
15	b	1230	F6C	C2A-C3A	7.40	1.52	1.36
14	A	1135	CLA	MG-NA	7.39	2.23	2.06
18	l	4019	BCR	C16-C17	-7.39	1.20	1.43
18	L	4019	BCR	C16-C17	-7.39	1.20	1.43
14	G	1140	CLA	MG-NA	7.39	2.23	2.06
14	a	1114	CLA	MG-NA	7.39	2.23	2.06
14	A	1140	CLA	MG-NA	7.39	2.23	2.06
14	a	1140	CLA	MG-NA	7.39	2.23	2.06
18	U	4019	BCR	C16-C17	-7.38	1.20	1.43
14	H	1217	CLA	MG-NA	7.38	2.23	2.06
18	G	4011	BCR	C16-C17	-7.38	1.20	1.43
14	a	1116	CLA	MG-NA	7.38	2.23	2.06
14	a	1133	CLA	MG-NA	7.38	2.23	2.06
14	A	1114	CLA	MG-NA	7.38	2.23	2.06
18	b	4005	BCR	C16-C17	-7.38	1.20	1.43
14	G	1012	CLA	MG-NA	7.38	2.23	2.06
14	G	1114	CLA	MG-NA	7.38	2.23	2.06
14	G	1116	CLA	MG-NA	7.38	2.23	2.06
14	A	1133	CLA	MG-NA	7.38	2.23	2.06
14	A	1116	CLA	MG-NA	7.37	2.23	2.06
14	B	1217	CLA	MG-NA	7.37	2.23	2.06
18	a	4011	BCR	C16-C17	-7.37	1.20	1.43
14	B	1239	CLA	MG-NA	7.37	2.23	2.06
14	b	1218	CLA	MG-NA	7.37	2.23	2.06
18	B	4006	BCR	C20-C21	-7.37	1.20	1.43
14	b	1217	CLA	MG-NA	7.37	2.23	2.06
18	V	4021	BCR	C16-C17	-7.37	1.20	1.43
14	X	1701	CLA	MG-NA	7.37	2.23	2.06
14	b	1239	CLA	MG-NA	7.37	2.23	2.06
18	b	4013	BCR	C20-C21	-7.36	1.20	1.43
14	b	1213	CLA	MG-NA	7.36	2.23	2.06
14	H	1239	CLA	MG-NA	7.36	2.23	2.06
18	B	4005	BCR	C16-C17	-7.36	1.20	1.43
14	x	1701	CLA	MG-NA	7.36	2.23	2.06
18	M	4021	BCR	C16-C17	-7.35	1.20	1.43
18	b	4006	BCR	C20-C21	-7.35	1.20	1.43
14	H	1227	CLA	MG-NA	7.35	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4006	BCR	C20-C21	-7.35	1.20	1.43
18	m	4021	BCR	C16-C17	-7.35	1.20	1.43
14	B	1218	CLA	MG-NA	7.34	2.23	2.06
14	b	1209	CLA	MG-NA	7.34	2.23	2.06
18	H	4005	BCR	C16-C17	-7.34	1.20	1.43
14	H	1218	CLA	MG-NA	7.34	2.23	2.06
14	H	1213	CLA	MG-NA	7.34	2.23	2.06
14	A	1012	CLA	MG-NA	7.33	2.23	2.06
18	H	4013	BCR	C20-C21	-7.33	1.20	1.43
18	B	4013	BCR	C20-C21	-7.33	1.20	1.43
14	B	1224	CLA	MG-NA	7.33	2.23	2.06
18	H	4004	BCR	C16-C17	-7.33	1.20	1.43
14	H	1224	CLA	MG-NA	7.32	2.23	2.06
14	A	1136	CLA	MG-NA	7.32	2.23	2.06
14	a	1130	CLA	MG-NA	7.32	2.23	2.06
14	H	1209	CLA	MG-NA	7.32	2.23	2.06
14	a	1012	CLA	MG-NA	7.32	2.23	2.06
14	a	1112	CLA	MG-NA	7.32	2.23	2.06
14	A	1127	CLA	MG-NA	7.32	2.23	2.06
14	b	1227	CLA	MG-NA	7.32	2.23	2.06
14	B	1227	CLA	MG-NA	7.31	2.23	2.06
14	A	1139	CLA	MG-NA	7.31	2.23	2.06
14	A	1105	CLA	MG-NA	7.31	2.23	2.06
14	B	1213	CLA	MG-NA	7.31	2.23	2.06
14	G	1139	CLA	MG-NA	7.31	2.23	2.06
14	B	1210	CLA	MG-NA	7.31	2.23	2.06
14	G	1130	CLA	MG-NA	7.31	2.23	2.06
14	a	1136	CLA	MG-NA	7.30	2.23	2.06
18	B	4004	BCR	C16-C17	-7.30	1.20	1.43
18	b	4004	BCR	C16-C17	-7.30	1.20	1.43
14	A	1115	CLA	MG-NA	7.30	2.23	2.06
14	B	1209	CLA	MG-NA	7.30	2.23	2.06
14	H	1210	CLA	MG-NA	7.30	2.23	2.06
14	A	1130	CLA	MG-NA	7.30	2.23	2.06
18	B	4006	BCR	C16-C17	-7.30	1.20	1.43
14	H	1231	CLA	MG-NA	7.30	2.23	2.06
14	H	1238	CLA	MG-NA	7.30	2.23	2.06
14	B	1022	CLA	MG-NA	7.30	2.23	2.06
14	A	1107	CLA	MG-NA	7.30	2.23	2.06
18	H	4006	BCR	C16-C17	-7.30	1.20	1.43
14	G	1105	CLA	MG-NA	7.29	2.23	2.06
14	b	1224	CLA	MG-NA	7.29	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	G	2001	PQN	C3-C2	7.29	1.48	1.35
14	A	1112	CLA	MG-NA	7.29	2.23	2.06
14	b	1238	CLA	MG-NA	7.29	2.23	2.06
14	B	1238	CLA	MG-NA	7.29	2.23	2.06
14	G	1136	CLA	MG-NA	7.29	2.23	2.06
18	b	4006	BCR	C16-C17	-7.29	1.20	1.43
14	a	1115	CLA	MG-NA	7.29	2.23	2.06
14	a	1105	CLA	MG-NA	7.29	2.23	2.06
18	B	4016	BCR	C16-C17	-7.28	1.20	1.43
18	H	4016	BCR	C16-C17	-7.28	1.20	1.43
14	A	1108	CLA	MG-NA	7.28	2.23	2.06
14	H	1012	CLA	MG-NA	7.28	2.23	2.06
14	U	1501	CLA	MG-NA	7.28	2.23	2.06
14	H	1234	CLA	MG-NA	7.28	2.23	2.06
14	B	1231	CLA	MG-NA	7.28	2.23	2.06
14	A	1101	CLA	MG-NA	7.28	2.23	2.06
14	b	1225	CLA	MG-NA	7.28	2.23	2.06
18	b	4016	BCR	C16-C17	-7.28	1.20	1.43
14	a	1129	CLA	MG-NA	7.27	2.23	2.06
14	G	1127	CLA	MG-NA	7.27	2.23	2.06
14	G	1112	CLA	MG-NA	7.27	2.23	2.06
14	b	1022	CLA	MG-NA	7.27	2.23	2.06
14	b	1231	CLA	MG-NA	7.27	2.23	2.06
14	H	1225	CLA	MG-NA	7.27	2.23	2.06
14	a	1139	CLA	MG-NA	7.27	2.23	2.06
14	b	1210	CLA	MG-NA	7.27	2.23	2.06
16	A	2001	PQN	C3-C2	7.27	1.48	1.35
14	G	1115	CLA	MG-NA	7.27	2.23	2.06
14	B	1225	CLA	MG-NA	7.27	2.23	2.06
16	a	2001	PQN	C3-C2	7.27	1.48	1.35
14	a	1127	CLA	MG-NA	7.27	2.23	2.06
14	G	1129	CLA	MG-NA	7.27	2.23	2.06
13	G	1011	CL0	C1D-C2D	7.26	1.47	1.39
14	L	1501	CLA	MG-NA	7.26	2.23	2.06
14	A	1129	CLA	MG-NA	7.26	2.23	2.06
14	B	1234	CLA	MG-NA	7.26	2.23	2.06
18	H	4012	BCR	C20-C21	-7.26	1.20	1.43
14	b	1234	CLA	MG-NA	7.25	2.23	2.06
18	B	4012	BCR	C20-C21	-7.25	1.20	1.43
14	a	1107	CLA	MG-NA	7.25	2.23	2.06
13	a	1011	CL0	C1D-C2D	7.25	1.47	1.39
18	B	4013	BCR	C16-C17	-7.25	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1229	CLA	MG-NA	7.25	2.23	2.06
14	G	1107	CLA	MG-NA	7.24	2.23	2.06
18	b	4013	BCR	C16-C17	-7.24	1.20	1.43
14	a	1101	CLA	MG-NA	7.24	2.23	2.06
14	a	1137	CLA	MG-NA	7.24	2.23	2.06
14	G	1137	CLA	MG-NA	7.24	2.23	2.06
14	A	1138	CLA	MG-NA	7.24	2.23	2.06
14	B	1229	CLA	MG-NA	7.23	2.23	2.06
18	b	4012	BCR	C20-C21	-7.23	1.20	1.43
14	a	1102	CLA	MG-NA	7.23	2.23	2.06
14	G	1108	CLA	MG-NA	7.23	2.23	2.06
14	a	1108	CLA	MG-NA	7.23	2.23	2.06
14	l	1501	CLA	MG-NA	7.23	2.23	2.06
14	b	1229	CLA	MG-NA	7.23	2.23	2.06
14	G	1101	CLA	MG-NA	7.23	2.23	2.06
14	A	1102	CLA	MG-NA	7.22	2.23	2.06
14	H	1236	CLA	MG-NA	7.22	2.23	2.06
14	b	1220	CLA	MG-NA	7.22	2.23	2.06
18	H	4013	BCR	C16-C17	-7.22	1.20	1.43
14	G	1102	CLA	MG-NA	7.22	2.23	2.06
18	V	4021	BCR	C20-C21	-7.22	1.20	1.43
14	a	1138	CLA	MG-NA	7.22	2.23	2.06
14	A	1137	CLA	MG-NA	7.21	2.23	2.06
18	M	4021	BCR	C20-C21	-7.21	1.20	1.43
14	B	1220	CLA	MG-NA	7.21	2.23	2.06
14	a	1106	CLA	MG-NA	7.21	2.23	2.06
18	m	4021	BCR	C20-C21	-7.20	1.20	1.43
14	G	1138	CLA	MG-NA	7.19	2.23	2.06
14	H	1220	CLA	MG-NA	7.19	2.23	2.06
14	B	1219	CLA	MG-NA	7.19	2.23	2.06
14	A	1106	CLA	MG-NA	7.19	2.23	2.06
14	H	1207	CLA	MG-NA	7.18	2.23	2.06
14	H	1219	CLA	MG-NA	7.18	2.23	2.06
13	A	1011	CL0	C1D-C2D	7.18	1.47	1.39
14	b	1207	CLA	MG-NA	7.18	2.23	2.06
14	B	1207	CLA	MG-NA	7.18	2.23	2.06
14	B	1236	CLA	MG-NA	7.17	2.23	2.06
14	B	1208	CLA	MG-NA	7.17	2.23	2.06
14	G	1106	CLA	MG-NA	7.17	2.23	2.06
14	H	1208	CLA	MG-NA	7.16	2.23	2.06
14	b	1236	CLA	MG-NA	7.16	2.23	2.06
14	a	1122	CLA	MG-NA	7.16	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1219	CLA	MG-NA	7.16	2.23	2.06
14	A	1119	CLA	MG-NA	7.15	2.23	2.06
14	b	1208	CLA	MG-NA	7.15	2.23	2.06
14	G	1122	CLA	MG-NA	7.15	2.23	2.06
14	H	1204	CLA	MG-NA	7.14	2.23	2.06
14	b	1204	CLA	MG-NA	7.14	2.23	2.06
14	A	1122	CLA	MG-NA	7.14	2.23	2.06
14	G	1131	CLA	MG-NA	7.14	2.23	2.06
14	G	1119	CLA	MG-NA	7.14	2.23	2.06
14	b	1228	CLA	MG-NA	7.13	2.23	2.06
14	B	1204	CLA	MG-NA	7.13	2.23	2.06
14	H	1228	CLA	MG-NA	7.12	2.23	2.06
14	G	1128	CLA	MG-NA	7.12	2.23	2.06
14	A	1113	CLA	MG-NA	7.12	2.23	2.06
14	a	1132	CLA	MG-NA	7.12	2.23	2.06
14	A	1131	CLA	MG-NA	7.12	2.23	2.06
14	a	1119	CLA	MG-NA	7.11	2.23	2.06
14	a	1113	CLA	MG-NA	7.11	2.23	2.06
14	a	1131	CLA	MG-NA	7.11	2.23	2.06
14	G	1113	CLA	MG-NA	7.11	2.23	2.06
14	A	1132	CLA	MG-NA	7.10	2.23	2.06
14	a	1118	CLA	MG-NA	7.10	2.23	2.06
14	a	1126	CLA	MG-NA	7.10	2.23	2.06
14	b	1211	CLA	MG-NA	7.10	2.23	2.06
14	A	1126	CLA	MG-NA	7.10	2.23	2.06
14	a	1128	CLA	MG-NA	7.10	2.23	2.06
14	b	1215	CLA	MG-NA	7.09	2.23	2.06
14	H	1215	CLA	MG-NA	7.09	2.23	2.06
14	B	1226	CLA	MG-NA	7.09	2.23	2.06
15	a	1120	F6C	C2A-C3A	7.09	1.52	1.36
14	B	1203	CLA	MG-NA	7.08	2.23	2.06
14	B	1211	CLA	MG-NA	7.08	2.23	2.06
15	A	1120	F6C	C2A-C3A	7.08	1.52	1.36
14	G	1126	CLA	MG-NA	7.08	2.23	2.06
14	B	1228	CLA	MG-NA	7.08	2.23	2.06
15	G	1120	F6C	C2A-C3A	7.08	1.52	1.36
14	A	1128	CLA	MG-NA	7.08	2.23	2.06
14	H	1203	CLA	MG-NA	7.08	2.23	2.06
14	H	1202	CLA	MG-NA	7.08	2.23	2.06
18	H	4012	BCR	C16-C17	-7.07	1.21	1.43
14	B	1222	CLA	MG-NA	7.07	2.23	2.06
18	B	4012	BCR	C16-C17	-7.07	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1211	CLA	MG-NA	7.07	2.23	2.06
14	B	1215	CLA	MG-NA	7.07	2.23	2.06
14	b	1203	CLA	MG-NA	7.07	2.23	2.06
14	G	1118	CLA	MG-NA	7.07	2.23	2.06
18	b	4012	BCR	C16-C17	-7.07	1.21	1.43
14	H	1206	CLA	MG-NA	7.06	2.23	2.06
14	A	1118	CLA	MG-NA	7.06	2.23	2.06
14	G	1132	CLA	MG-NA	7.06	2.23	2.06
14	a	1117	CLA	MG-NA	7.06	2.23	2.06
14	b	1222	CLA	MG-NA	7.05	2.23	2.06
14	H	1222	CLA	MG-NA	7.05	2.23	2.06
14	b	1226	CLA	MG-NA	7.05	2.23	2.06
14	G	1117	CLA	MG-NA	7.05	2.23	2.06
14	b	1202	CLA	MG-NA	7.05	2.23	2.06
14	A	1117	CLA	MG-NA	7.04	2.23	2.06
14	B	1221	CLA	MG-NA	7.04	2.23	2.06
14	B	1206	CLA	MG-NA	7.04	2.23	2.06
14	b	1206	CLA	MG-NA	7.04	2.23	2.06
14	H	1226	CLA	MG-NA	7.04	2.23	2.06
14	B	1202	CLA	MG-NA	7.04	2.23	2.06
14	a	1125	CLA	MG-NA	7.03	2.23	2.06
14	b	1235	CLA	MG-NA	7.02	2.22	2.06
14	A	1125	CLA	MG-NA	7.01	2.22	2.06
14	L	1503	CLA	MG-NA	7.01	2.22	2.06
14	G	1125	CLA	MG-NA	7.00	2.22	2.06
14	A	1124	CLA	MG-NA	7.00	2.22	2.06
14	l	1503	CLA	MG-NA	7.00	2.22	2.06
14	B	1201	CLA	MG-NA	7.00	2.22	2.06
14	b	1201	CLA	MG-NA	7.00	2.22	2.06
14	G	1124	CLA	MG-NA	6.99	2.22	2.06
14	b	1221	CLA	MG-NA	6.99	2.22	2.06
14	H	1221	CLA	MG-NA	6.99	2.22	2.06
14	H	1201	CLA	MG-NA	6.99	2.22	2.06
14	a	1124	CLA	MG-NA	6.99	2.22	2.06
14	H	1235	CLA	MG-NA	6.98	2.22	2.06
14	U	1503	CLA	MG-NA	6.98	2.22	2.06
14	B	1235	CLA	MG-NA	6.97	2.22	2.06
14	H	1216	CLA	MG-NA	6.97	2.22	2.06
14	B	1216	CLA	MG-NA	6.97	2.22	2.06
14	G	1109	CLA	MG-NA	6.96	2.22	2.06
14	a	1109	CLA	MG-NA	6.95	2.22	2.06
14	b	1216	CLA	MG-NA	6.95	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1109	CLA	MG-NA	6.93	2.22	2.06
14	U	1502	CLA	MG-NA	6.92	2.22	2.06
14	l	1502	CLA	MG-NA	6.91	2.22	2.06
14	L	1502	CLA	MG-NA	6.91	2.22	2.06
14	H	1021	CLA	MG-NA	6.90	2.22	2.06
14	b	1021	CLA	MG-NA	6.89	2.22	2.06
14	B	1021	CLA	MG-NA	6.89	2.22	2.06
14	G	1104	CLA	MG-NA	6.84	2.22	2.06
14	a	1104	CLA	MG-NA	6.83	2.22	2.06
14	H	1205	CLA	MG-NA	6.83	2.22	2.06
14	A	1104	CLA	MG-NA	6.82	2.22	2.06
14	B	1205	CLA	MG-NA	6.82	2.22	2.06
15	H	1237	F6C	C2A-C3A	6.80	1.51	1.36
14	b	1205	CLA	MG-NA	6.80	2.22	2.06
15	b	1237	F6C	C2A-C3A	6.79	1.51	1.36
15	B	1237	F6C	C2A-C3A	6.77	1.51	1.36
14	G	1103	CLA	MG-NA	6.65	2.22	2.06
14	a	1103	CLA	MG-NA	6.64	2.22	2.06
14	A	1103	CLA	MG-NA	6.64	2.22	2.06
14	a	1013	CLA	MG-NA	6.62	2.22	2.06
14	G	1013	CLA	MG-NA	6.61	2.22	2.06
15	a	1121	F6C	C2A-C3A	6.60	1.51	1.36
15	G	1121	F6C	C2A-C3A	6.60	1.51	1.36
14	A	1013	CLA	MG-NA	6.59	2.21	2.06
15	A	1121	F6C	C2A-C3A	6.58	1.51	1.36
14	b	1023	CLA	MG-NA	6.57	2.21	2.06
14	H	1023	CLA	MG-NA	6.57	2.21	2.06
14	B	1023	CLA	MG-NA	6.54	2.21	2.06
14	H	1215	CLA	O2A-C1	5.64	1.61	1.46
14	b	1215	CLA	O2A-C1	5.62	1.61	1.46
14	B	1215	CLA	O2A-C1	5.60	1.61	1.46
14	A	1102	CLA	O2A-C1	5.60	1.61	1.46
14	a	1102	CLA	O2A-C1	5.60	1.61	1.46
14	G	1102	CLA	O2A-C1	5.57	1.61	1.46
14	G	1118	CLA	O2A-C1	5.55	1.61	1.46
14	A	1116	CLA	O2A-C1	5.54	1.61	1.46
14	b	1216	CLA	O2A-C1	5.54	1.61	1.46
14	a	1133	CLA	O2A-C1	5.53	1.61	1.46
14	H	1216	CLA	O2A-C1	5.53	1.61	1.46
14	B	1216	CLA	O2A-C1	5.53	1.61	1.46
14	a	1118	CLA	O2A-C1	5.52	1.61	1.46
14	A	1118	CLA	O2A-C1	5.52	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1013	CLA	O2A-C1	5.51	1.61	1.46
14	A	1133	CLA	O2A-C1	5.51	1.61	1.46
14	G	1133	CLA	O2A-C1	5.51	1.61	1.46
14	a	1116	CLA	O2A-C1	5.51	1.60	1.46
13	A	1011	CL0	O2A-C1	5.50	1.60	1.46
14	G	1116	CLA	O2A-C1	5.50	1.60	1.46
13	G	1011	CL0	O2A-C1	5.50	1.60	1.46
14	G	1013	CLA	O2A-C1	5.50	1.60	1.46
13	a	1011	CL0	O2A-C1	5.49	1.60	1.46
14	a	1013	CLA	O2A-C1	5.48	1.60	1.46
14	A	1111	CLA	O2A-C1	5.46	1.60	1.46
14	G	1013	CLA	C1D-ND	-5.46	1.30	1.37
14	G	1111	CLA	O2A-C1	5.44	1.60	1.46
14	a	1111	CLA	O2A-C1	5.44	1.60	1.46
14	G	1140	CLA	O2A-C1	5.43	1.60	1.46
14	A	1125	CLA	O2A-C1	5.42	1.60	1.46
14	B	1213	CLA	O2A-C1	5.42	1.60	1.46
14	A	1140	CLA	O2A-C1	5.42	1.60	1.46
14	B	1225	CLA	O2A-C1	5.42	1.60	1.46
14	H	1225	CLA	O2A-C1	5.42	1.60	1.46
14	G	1136	CLA	O2A-C1	5.42	1.60	1.46
14	b	1213	CLA	O2A-C1	5.42	1.60	1.46
14	a	1125	CLA	O2A-C1	5.42	1.60	1.46
14	b	1221	CLA	O2A-C1	5.42	1.60	1.46
14	B	1221	CLA	O2A-C1	5.42	1.60	1.46
14	H	1213	CLA	O2A-C1	5.42	1.60	1.46
14	a	1130	CLA	O2A-C1	5.42	1.60	1.46
14	B	1022	CLA	O2A-C1	5.42	1.60	1.46
14	H	1205	CLA	O2A-C1	5.42	1.60	1.46
14	G	1125	CLA	O2A-C1	5.41	1.60	1.46
14	a	1013	CLA	C1D-ND	-5.41	1.30	1.37
14	a	1136	CLA	O2A-C1	5.41	1.60	1.46
14	b	1225	CLA	O2A-C1	5.41	1.60	1.46
14	H	1221	CLA	O2A-C1	5.41	1.60	1.46
14	b	1022	CLA	O2A-C1	5.41	1.60	1.46
14	B	1239	CLA	O2A-C1	5.41	1.60	1.46
14	H	1012	CLA	O2A-C1	5.40	1.60	1.46
14	A	1136	CLA	O2A-C1	5.40	1.60	1.46
14	a	1119	CLA	O2A-C1	5.40	1.60	1.46
14	a	1140	CLA	O2A-C1	5.40	1.60	1.46
14	G	1119	CLA	O2A-C1	5.39	1.60	1.46
14	G	1130	CLA	O2A-C1	5.39	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1130	CLA	O2A-C1	5.39	1.60	1.46
14	B	1217	CLA	O2A-C1	5.39	1.60	1.46
14	b	1239	CLA	O2A-C1	5.38	1.60	1.46
14	U	1502	CLA	O2A-C1	5.38	1.60	1.46
14	b	1205	CLA	O2A-C1	5.38	1.60	1.46
14	H	1217	CLA	O2A-C1	5.38	1.60	1.46
14	b	1217	CLA	O2A-C1	5.37	1.60	1.46
14	A	1119	CLA	O2A-C1	5.37	1.60	1.46
14	l	1502	CLA	O2A-C1	5.37	1.60	1.46
14	B	1220	CLA	O2A-C1	5.36	1.60	1.46
14	B	1201	CLA	O2A-C1	5.36	1.60	1.46
14	b	1201	CLA	O2A-C1	5.36	1.60	1.46
14	B	1205	CLA	O2A-C1	5.36	1.60	1.46
14	H	1239	CLA	O2A-C1	5.36	1.60	1.46
14	A	1013	CLA	C1D-ND	-5.36	1.30	1.37
18	R	4020	BCR	C10-C9	-5.35	1.23	1.35
14	L	1502	CLA	O2A-C1	5.35	1.60	1.46
14	a	1127	CLA	O2A-C1	5.35	1.60	1.46
14	H	1220	CLA	O2A-C1	5.35	1.60	1.46
14	A	1127	CLA	O2A-C1	5.35	1.60	1.46
14	b	1220	CLA	O2A-C1	5.35	1.60	1.46
14	H	1201	CLA	O2A-C1	5.35	1.60	1.46
18	i	4020	BCR	C10-C9	-5.34	1.23	1.35
18	I	4020	BCR	C10-C9	-5.34	1.23	1.35
13	A	1011	CL0	C3D-C4D	-5.33	1.33	1.41
14	G	1127	CLA	O2A-C1	5.33	1.60	1.46
14	A	1012	CLA	O2A-C1	5.33	1.60	1.46
14	a	1012	CLA	O2A-C1	5.33	1.60	1.46
15	b	1237	F6C	O2A-C1	5.32	1.60	1.46
14	A	1135	CLA	O2A-C1	5.31	1.60	1.46
15	H	1237	F6C	O2A-C1	5.31	1.60	1.46
14	a	1135	CLA	O2A-C1	5.31	1.60	1.46
14	G	1135	CLA	O2A-C1	5.31	1.60	1.46
14	G	1012	CLA	O2A-C1	5.31	1.60	1.46
15	B	1237	F6C	O2A-C1	5.31	1.60	1.46
14	A	1128	CLA	O2A-C1	5.31	1.60	1.46
14	H	1208	CLA	O2A-C1	5.31	1.60	1.46
14	A	1115	CLA	O2A-C1	5.30	1.60	1.46
14	G	1115	CLA	O2A-C1	5.30	1.60	1.46
14	H	1211	CLA	O2A-C1	5.30	1.60	1.46
18	A	4008	BCR	C10-C9	-5.29	1.23	1.35
14	A	1117	CLA	O2A-C1	5.29	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	1011	CL0	C3D-C4D	-5.28	1.33	1.41
14	a	1123	CLA	O2A-C1	5.28	1.60	1.46
18	G	4008	BCR	C10-C9	-5.28	1.23	1.35
14	A	1132	CLA	O2A-C1	5.28	1.60	1.46
14	a	1128	CLA	O2A-C1	5.28	1.60	1.46
14	b	1208	CLA	O2A-C1	5.28	1.60	1.46
14	a	1132	CLA	O2A-C1	5.28	1.60	1.46
13	G	1011	CL0	C3D-C4D	-5.28	1.33	1.41
14	G	1117	CLA	O2A-C1	5.28	1.60	1.46
14	H	1238	CLA	O2A-C1	5.28	1.60	1.46
14	H	1229	CLA	O2A-C1	5.27	1.60	1.46
14	B	1208	CLA	O2A-C1	5.27	1.60	1.46
14	b	1229	CLA	O2A-C1	5.27	1.60	1.46
14	G	1128	CLA	O2A-C1	5.27	1.60	1.46
14	a	1115	CLA	O2A-C1	5.27	1.60	1.46
14	a	1117	CLA	O2A-C1	5.27	1.60	1.46
14	b	1211	CLA	O2A-C1	5.26	1.60	1.46
14	b	1204	CLA	O2A-C1	5.26	1.60	1.46
14	B	1211	CLA	O2A-C1	5.26	1.60	1.46
14	B	1229	CLA	O2A-C1	5.25	1.60	1.46
18	a	4008	BCR	C10-C9	-5.25	1.23	1.35
14	B	1235	CLA	O2A-C1	5.25	1.60	1.46
14	B	1238	CLA	O2A-C1	5.25	1.60	1.46
14	A	1123	CLA	O2A-C1	5.25	1.60	1.46
14	H	1235	CLA	O2A-C1	5.24	1.60	1.46
14	b	1235	CLA	O2A-C1	5.24	1.60	1.46
14	b	1223	CLA	O2A-C1	5.24	1.60	1.46
14	H	1204	CLA	O2A-C1	5.24	1.60	1.46
14	b	1238	CLA	O2A-C1	5.24	1.60	1.46
14	G	1123	CLA	O2A-C1	5.23	1.60	1.46
14	B	1223	CLA	O2A-C1	5.23	1.60	1.46
14	B	1204	CLA	O2A-C1	5.22	1.60	1.46
14	G	1132	CLA	O2A-C1	5.22	1.60	1.46
13	G	1011	CL0	CHB-C1B	5.22	1.48	1.39
14	H	1223	CLA	O2A-C1	5.21	1.60	1.46
14	l	1503	CLA	O2A-C1	5.21	1.60	1.46
14	G	1138	CLA	O2A-C1	5.21	1.60	1.46
14	H	1231	CLA	O2A-C1	5.21	1.60	1.46
14	G	1103	CLA	O2A-C1	5.20	1.60	1.46
14	b	1202	CLA	O2A-C1	5.20	1.60	1.46
14	L	1503	CLA	O2A-C1	5.20	1.60	1.46
14	b	1231	CLA	O2A-C1	5.20	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1138	CLA	O2A-C1	5.20	1.60	1.46
14	U	1503	CLA	O2A-C1	5.19	1.60	1.46
14	A	1103	CLA	O2A-C1	5.19	1.60	1.46
13	A	1011	CL0	CHB-C1B	5.19	1.48	1.39
14	b	1214	CLA	O2A-C1	5.19	1.60	1.46
14	B	1202	CLA	O2A-C1	5.19	1.60	1.46
14	A	1138	CLA	O2A-C1	5.18	1.60	1.46
14	B	1214	CLA	O2A-C1	5.18	1.60	1.46
14	H	1202	CLA	O2A-C1	5.17	1.60	1.46
14	B	1231	CLA	O2A-C1	5.17	1.60	1.46
14	a	1103	CLA	O2A-C1	5.17	1.60	1.46
14	H	1214	CLA	O2A-C1	5.17	1.60	1.46
14	G	1104	CLA	O2A-C1	5.16	1.60	1.46
18	i	4018	BCR	C10-C9	-5.16	1.23	1.35
14	A	1124	CLA	O2A-C1	5.16	1.60	1.46
14	H	1203	CLA	O2A-C1	5.16	1.60	1.46
14	a	1124	CLA	O2A-C1	5.16	1.60	1.46
14	L	1501	CLA	O2A-C1	5.15	1.60	1.46
14	a	1104	CLA	O2A-C1	5.15	1.60	1.46
14	G	1124	CLA	O2A-C1	5.15	1.60	1.46
14	B	1203	CLA	O2A-C1	5.15	1.60	1.46
18	I	4018	BCR	C10-C9	-5.15	1.23	1.35
14	A	1122	CLA	O2A-C1	5.15	1.60	1.46
14	U	1501	CLA	O2A-C1	5.15	1.60	1.46
14	H	1210	CLA	O2A-C1	5.14	1.60	1.46
14	H	1226	CLA	O2A-C1	5.14	1.60	1.46
14	A	1104	CLA	O2A-C1	5.14	1.60	1.46
18	R	4018	BCR	C10-C9	-5.14	1.23	1.35
14	l	1501	CLA	O2A-C1	5.14	1.60	1.46
14	b	1226	CLA	O2A-C1	5.14	1.60	1.46
14	b	1210	CLA	O2A-C1	5.14	1.60	1.46
13	a	1011	CL0	CHB-C1B	5.14	1.47	1.39
14	B	1210	CLA	O2A-C1	5.13	1.59	1.46
14	B	1226	CLA	O2A-C1	5.12	1.59	1.46
14	A	1122	CLA	O2D-CGD	5.12	1.45	1.33
14	B	1021	CLA	O2A-C1	5.12	1.59	1.46
14	G	1122	CLA	O2A-C1	5.11	1.59	1.46
14	a	1122	CLA	O2A-C1	5.11	1.59	1.46
14	a	1130	CLA	C3D-C4D	-5.10	1.32	1.44
14	b	1224	CLA	O2A-C1	5.10	1.59	1.46
14	A	1130	CLA	C3D-C4D	-5.10	1.32	1.44
14	B	1224	CLA	O2A-C1	5.10	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1130	CLA	C3D-C4D	-5.10	1.32	1.44
14	H	1224	CLA	O2A-C1	5.10	1.59	1.46
14	b	1203	CLA	O2A-C1	5.10	1.59	1.46
14	G	1122	CLA	O2D-CGD	5.09	1.45	1.33
14	H	1021	CLA	O2A-C1	5.09	1.59	1.46
18	G	4002	BCR	C10-C9	-5.08	1.24	1.35
14	b	1021	CLA	O2A-C1	5.08	1.59	1.46
14	a	1131	CLA	O2A-C1	5.08	1.59	1.46
14	A	1131	CLA	O2A-C1	5.08	1.59	1.46
15	b	1237	F6C	C4A-NA	-5.08	1.31	1.37
14	a	1122	CLA	O2D-CGD	5.08	1.45	1.33
14	k	1401	CLA	O2D-CGD	5.08	1.45	1.33
14	G	1131	CLA	O2A-C1	5.07	1.59	1.46
18	a	4002	BCR	C10-C9	-5.07	1.24	1.35
14	T	1401	CLA	O2D-CGD	5.07	1.45	1.33
18	A	4002	BCR	C10-C9	-5.06	1.24	1.35
14	A	1126	CLA	O2A-C1	5.06	1.59	1.46
15	B	1237	F6C	C4A-NA	-5.06	1.31	1.37
14	b	1234	CLA	O2A-C1	5.06	1.59	1.46
14	H	1234	CLA	O2A-C1	5.05	1.59	1.46
14	G	1013	CLA	CHC-C1C	5.05	1.48	1.38
15	H	1237	F6C	C4A-NA	-5.04	1.31	1.37
14	K	1401	CLA	O2D-CGD	5.04	1.45	1.33
14	B	1220	CLA	O2D-CGD	5.04	1.45	1.33
14	B	1023	CLA	O2A-C1	5.04	1.59	1.46
14	G	1126	CLA	O2A-C1	5.04	1.59	1.46
14	a	1126	CLA	O2A-C1	5.04	1.59	1.46
14	B	1234	CLA	O2A-C1	5.04	1.59	1.46
14	H	1023	CLA	O2A-C1	5.04	1.59	1.46
14	G	1129	CLA	C3D-C4D	-5.03	1.32	1.44
14	A	1013	CLA	CHC-C1C	5.02	1.48	1.38
14	b	1023	CLA	O2A-C1	5.02	1.59	1.46
14	a	1013	CLA	CHC-C1C	5.02	1.48	1.38
14	G	1012	CLA	C3D-C4D	-5.02	1.32	1.44
14	b	1220	CLA	O2D-CGD	5.02	1.45	1.33
14	H	1220	CLA	O2D-CGD	5.01	1.45	1.33
14	B	1227	CLA	O2D-CGD	5.01	1.45	1.33
14	a	1012	CLA	C3D-C4D	-5.01	1.32	1.44
14	b	1238	CLA	O2D-CGD	5.01	1.45	1.33
14	G	1138	CLA	O2D-CGD	5.00	1.45	1.33
14	A	1138	CLA	O2D-CGD	5.00	1.45	1.33
14	B	1238	CLA	O2D-CGD	5.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1012	CLA	C3D-C4D	-4.99	1.33	1.44
14	b	1227	CLA	O2D-CGD	4.99	1.45	1.33
14	a	1129	CLA	C3D-C4D	-4.99	1.33	1.44
14	A	1114	CLA	O2D-CGD	4.99	1.45	1.33
14	H	1227	CLA	O2D-CGD	4.98	1.45	1.33
14	H	1238	CLA	O2D-CGD	4.98	1.45	1.33
14	a	1138	CLA	O2D-CGD	4.98	1.45	1.33
14	b	1219	CLA	O2D-CGD	4.97	1.45	1.33
14	b	1218	CLA	O2D-CGD	4.97	1.45	1.33
14	H	1222	CLA	O2A-C1	4.97	1.59	1.46
13	A	1011	CL0	C3B-C4B	4.97	1.46	1.41
13	a	1011	CL0	C3B-C4B	4.96	1.46	1.41
14	B	1219	CLA	O2D-CGD	4.96	1.45	1.33
14	H	1219	CLA	O2D-CGD	4.96	1.45	1.33
13	G	1011	CL0	C3B-C4B	4.96	1.46	1.41
14	b	1233	CLA	O2D-CGD	4.95	1.45	1.33
14	b	1222	CLA	O2A-C1	4.95	1.59	1.46
14	A	1129	CLA	C3D-C4D	-4.95	1.33	1.44
14	B	1218	CLA	O2D-CGD	4.95	1.45	1.33
14	G	1114	CLA	O2D-CGD	4.95	1.45	1.33
14	H	1218	CLA	O2D-CGD	4.95	1.45	1.33
14	H	1233	CLA	O2D-CGD	4.95	1.45	1.33
15	b	1230	F6C	O2D-CGD	4.95	1.45	1.33
14	G	1105	CLA	O2D-CGD	4.95	1.45	1.33
14	b	1228	CLA	O2D-CGD	4.94	1.45	1.33
14	B	1222	CLA	O2A-C1	4.94	1.59	1.46
14	a	1114	CLA	O2D-CGD	4.94	1.45	1.33
14	G	1108	CLA	O2D-CGD	4.94	1.45	1.33
14	a	1108	CLA	O2D-CGD	4.94	1.45	1.33
15	H	1237	F6C	O2D-CGD	4.94	1.45	1.33
15	G	1121	F6C	O2D-CGD	4.94	1.45	1.33
15	a	1121	F6C	O2D-CGD	4.93	1.45	1.33
14	B	1233	CLA	O2D-CGD	4.93	1.45	1.33
15	B	1237	F6C	O2D-CGD	4.93	1.45	1.33
14	A	1108	CLA	O2D-CGD	4.93	1.45	1.33
14	b	1216	CLA	O2D-CGD	4.93	1.45	1.33
15	H	1230	F6C	O2D-CGD	4.93	1.45	1.33
15	b	1237	F6C	O2D-CGD	4.92	1.45	1.33
14	H	1216	CLA	O2D-CGD	4.92	1.45	1.33
14	G	1119	CLA	O2D-CGD	4.92	1.45	1.33
15	A	1121	F6C	O2D-CGD	4.92	1.45	1.33
14	a	1105	CLA	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1109	CLA	O2D-CGD	4.92	1.45	1.33
14	A	1105	CLA	O2D-CGD	4.92	1.45	1.33
14	a	1125	CLA	C3D-C4D	-4.91	1.33	1.44
15	B	1230	F6C	O2D-CGD	4.91	1.45	1.33
14	B	1216	CLA	O2D-CGD	4.91	1.45	1.33
14	H	1228	CLA	O2D-CGD	4.91	1.45	1.33
15	G	1121	F6C	C4A-NA	-4.91	1.31	1.37
14	A	1109	CLA	O2D-CGD	4.91	1.45	1.33
14	G	1115	CLA	O2D-CGD	4.91	1.45	1.33
14	G	1125	CLA	C3D-C4D	-4.90	1.33	1.44
14	B	1203	CLA	C3D-C4D	-4.89	1.33	1.44
14	a	1109	CLA	O2D-CGD	4.89	1.45	1.33
18	l	4022	BCR	C10-C9	-4.89	1.24	1.35
14	b	1203	CLA	C3D-C4D	-4.89	1.33	1.44
14	a	1119	CLA	O2D-CGD	4.89	1.45	1.33
14	A	1125	CLA	C3D-C4D	-4.89	1.33	1.44
14	A	1119	CLA	O2D-CGD	4.88	1.45	1.33
14	B	1207	CLA	O2D-CGD	4.88	1.45	1.33
14	B	1228	CLA	O2D-CGD	4.88	1.45	1.33
14	B	1232	CLA	O2D-CGD	4.88	1.45	1.33
18	U	4022	BCR	C10-C9	-4.88	1.24	1.35
15	A	1121	F6C	C4A-NA	-4.87	1.31	1.37
14	H	1203	CLA	C3D-C4D	-4.87	1.33	1.44
14	b	1204	CLA	O2D-CGD	4.87	1.45	1.33
14	A	1115	CLA	O2D-CGD	4.87	1.45	1.33
14	b	1232	CLA	O2D-CGD	4.87	1.45	1.33
18	L	4022	BCR	C10-C9	-4.87	1.24	1.35
14	H	1232	CLA	O2D-CGD	4.86	1.45	1.33
14	H	1214	CLA	O2D-CGD	4.86	1.45	1.33
18	m	4021	BCR	C10-C9	-4.86	1.24	1.35
14	H	1207	CLA	O2D-CGD	4.86	1.45	1.33
14	a	1116	CLA	O2D-CGD	4.86	1.45	1.33
14	a	1115	CLA	O2D-CGD	4.86	1.45	1.33
14	b	1207	CLA	O2D-CGD	4.86	1.45	1.33
14	b	1023	CLA	C1D-ND	-4.85	1.31	1.37
15	a	1121	F6C	C4A-NA	-4.85	1.31	1.37
14	H	1204	CLA	O2D-CGD	4.85	1.45	1.33
18	M	4021	BCR	C10-C9	-4.85	1.24	1.35
14	H	1224	CLA	C3D-C4D	-4.85	1.33	1.44
14	b	1224	CLA	C3D-C4D	-4.85	1.33	1.44
14	A	1104	CLA	O2D-CGD	4.85	1.45	1.33
14	b	1239	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	4021	BCR	C10-C9	-4.84	1.24	1.35
14	B	1213	CLA	O2D-CGD	4.84	1.45	1.33
14	B	1204	CLA	O2D-CGD	4.84	1.45	1.33
14	b	1213	CLA	O2D-CGD	4.84	1.45	1.33
14	H	1213	CLA	O2D-CGD	4.83	1.45	1.33
14	B	1023	CLA	C1D-ND	-4.83	1.31	1.37
14	B	1239	CLA	O2D-CGD	4.83	1.45	1.33
14	G	1104	CLA	O2D-CGD	4.83	1.45	1.33
14	a	1104	CLA	O2D-CGD	4.83	1.45	1.33
14	H	1239	CLA	O2D-CGD	4.82	1.45	1.33
14	B	1224	CLA	C3D-C4D	-4.82	1.33	1.44
14	H	1214	CLA	C3D-C4D	-4.82	1.33	1.44
14	b	1202	CLA	C3D-C4D	-4.82	1.33	1.44
18	G	4007	BCR	C10-C9	-4.82	1.24	1.35
14	B	1214	CLA	O2D-CGD	4.82	1.45	1.33
18	A	4007	BCR	C10-C9	-4.82	1.24	1.35
14	B	1214	CLA	C3D-C4D	-4.81	1.33	1.44
14	b	1214	CLA	O2D-CGD	4.81	1.45	1.33
14	H	1023	CLA	C1D-ND	-4.81	1.31	1.37
15	B	1230	F6C	CHC-C4B	4.81	1.48	1.38
14	B	1226	CLA	C3D-C4D	-4.81	1.33	1.44
14	b	1206	CLA	O2D-CGD	4.80	1.45	1.33
18	H	4017	BCR	C10-C9	-4.80	1.24	1.35
14	b	1214	CLA	C3D-C4D	-4.80	1.33	1.44
14	A	1113	CLA	O2D-CGD	4.80	1.45	1.33
14	G	1127	CLA	C3D-C4D	-4.80	1.33	1.44
14	B	1235	CLA	O2D-CGD	4.80	1.45	1.33
14	b	1226	CLA	C3D-C4D	-4.80	1.33	1.44
14	b	1235	CLA	O2D-CGD	4.80	1.45	1.33
14	b	1210	CLA	C3D-C4D	-4.79	1.33	1.44
14	A	1116	CLA	O2D-CGD	4.79	1.45	1.33
14	B	1204	CLA	C3D-C4D	-4.79	1.33	1.44
14	G	1126	CLA	C3D-C4D	-4.79	1.33	1.44
14	B	1209	CLA	O2D-CGD	4.79	1.45	1.33
18	a	4007	BCR	C10-C9	-4.79	1.24	1.35
14	B	1202	CLA	C3D-C4D	-4.79	1.33	1.44
14	G	1137	CLA	C3D-C4D	-4.79	1.33	1.44
14	b	1209	CLA	O2D-CGD	4.79	1.45	1.33
18	H	4010	BCR	C10-C9	-4.79	1.24	1.35
18	b	4010	BCR	C10-C9	-4.79	1.24	1.35
14	B	1210	CLA	C3D-C4D	-4.79	1.33	1.44
14	H	1208	CLA	O2D-CGD	4.79	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1230	F6C	CHC-C4B	4.79	1.48	1.38
14	a	1101	CLA	O2D-CGD	4.79	1.45	1.33
14	H	1226	CLA	C3D-C4D	-4.79	1.33	1.44
14	G	1101	CLA	O2D-CGD	4.78	1.45	1.33
14	a	1127	CLA	C3D-C4D	-4.78	1.33	1.44
14	H	1235	CLA	O2D-CGD	4.78	1.45	1.33
18	B	4010	BCR	C10-C9	-4.78	1.24	1.35
14	a	1107	CLA	C3D-C4D	-4.78	1.33	1.44
14	G	1113	CLA	O2D-CGD	4.78	1.45	1.33
14	H	1206	CLA	O2D-CGD	4.78	1.45	1.33
14	a	1130	CLA	O2D-CGD	4.78	1.45	1.33
14	H	1209	CLA	O2D-CGD	4.78	1.45	1.33
14	A	1127	CLA	C3D-C4D	-4.78	1.33	1.44
14	G	1139	CLA	O2D-CGD	4.78	1.45	1.33
14	a	1113	CLA	O2D-CGD	4.78	1.45	1.33
14	b	1238	CLA	C3D-C4D	-4.78	1.33	1.44
14	H	1202	CLA	C3D-C4D	-4.78	1.33	1.44
14	A	1126	CLA	C3D-C4D	-4.78	1.33	1.44
14	b	1208	CLA	O2D-CGD	4.77	1.45	1.33
14	a	1138	CLA	C3D-C4D	-4.77	1.33	1.44
18	H	4014	BCR	C10-C9	-4.77	1.24	1.35
18	b	4017	BCR	C10-C9	-4.77	1.24	1.35
14	G	1116	CLA	O2D-CGD	4.77	1.45	1.33
14	B	1208	CLA	O2D-CGD	4.77	1.45	1.33
14	H	1215	CLA	O2D-CGD	4.77	1.45	1.33
14	a	1137	CLA	C3D-C4D	-4.77	1.33	1.44
14	A	1137	CLA	C3D-C4D	-4.77	1.33	1.44
14	b	1211	CLA	O2D-CGD	4.77	1.45	1.33
14	H	1225	CLA	O2D-CGD	4.77	1.45	1.33
14	H	1210	CLA	C3D-C4D	-4.77	1.33	1.44
14	B	1215	CLA	O2D-CGD	4.77	1.44	1.33
14	a	1118	CLA	O2D-CGD	4.77	1.44	1.33
14	b	1204	CLA	C3D-C4D	-4.77	1.33	1.44
15	G	1120	F6C	O2D-CGD	4.77	1.44	1.33
18	B	4014	BCR	C10-C9	-4.77	1.24	1.35
18	B	4017	BCR	C10-C9	-4.76	1.24	1.35
14	G	1114	CLA	CHD-C1D	4.76	1.47	1.38
14	A	1126	CLA	O2D-CGD	4.76	1.44	1.33
14	a	1113	CLA	C3D-C4D	-4.76	1.33	1.44
14	a	1126	CLA	C3D-C4D	-4.76	1.33	1.44
14	G	1132	CLA	C3D-C4D	-4.76	1.33	1.44
14	H	1225	CLA	C3D-C4D	-4.76	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	x	1701	CLA	O2D-CGD	4.76	1.44	1.33
14	B	1225	CLA	C3D-C4D	-4.76	1.33	1.44
14	H	1238	CLA	C3D-C4D	-4.76	1.33	1.44
14	a	1132	CLA	C3D-C4D	-4.76	1.33	1.44
14	G	1107	CLA	C3D-C4D	-4.76	1.33	1.44
14	b	1225	CLA	C3D-C4D	-4.76	1.33	1.44
14	H	1204	CLA	C3D-C4D	-4.76	1.33	1.44
14	G	1130	CLA	O2D-CGD	4.76	1.44	1.33
14	b	1215	CLA	O2D-CGD	4.76	1.44	1.33
14	H	1211	CLA	O2D-CGD	4.76	1.44	1.33
14	A	1101	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1132	CLA	C3D-C4D	-4.75	1.33	1.44
14	G	1127	CLA	O2D-CGD	4.75	1.44	1.33
14	G	1113	CLA	C3D-C4D	-4.75	1.33	1.44
14	B	1211	CLA	O2D-CGD	4.75	1.44	1.33
14	B	1238	CLA	C3D-C4D	-4.75	1.33	1.44
14	a	1123	CLA	C3D-C4D	-4.75	1.33	1.44
14	B	1206	CLA	O2D-CGD	4.75	1.44	1.33
14	W	1701	CLA	O2D-CGD	4.75	1.44	1.33
14	b	1225	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1125	CLA	O2D-CGD	4.75	1.44	1.33
14	A	1103	CLA	C3D-C4D	-4.75	1.33	1.44
14	A	1118	CLA	O2D-CGD	4.75	1.44	1.33
15	A	1120	F6C	O2D-CGD	4.75	1.44	1.33
14	A	1135	CLA	C3D-C4D	-4.74	1.33	1.44
14	G	1123	CLA	C3D-C4D	-4.74	1.33	1.44
14	G	1125	CLA	O2D-CGD	4.74	1.44	1.33
14	b	1203	CLA	O2D-CGD	4.74	1.44	1.33
14	b	1226	CLA	O2D-CGD	4.74	1.44	1.33
15	a	1120	F6C	O2D-CGD	4.74	1.44	1.33
14	A	1130	CLA	O2D-CGD	4.74	1.44	1.33
14	a	1123	CLA	O2D-CGD	4.74	1.44	1.33
14	A	1113	CLA	C3D-C4D	-4.74	1.33	1.44
14	A	1107	CLA	C3D-C4D	-4.74	1.33	1.44
14	X	1701	CLA	O2D-CGD	4.74	1.44	1.33
14	G	1126	CLA	O2D-CGD	4.74	1.44	1.33
14	H	1236	CLA	C3D-C4D	-4.74	1.33	1.44
14	H	1012	CLA	C3D-C4D	-4.74	1.33	1.44
14	A	1123	CLA	C3D-C4D	-4.74	1.33	1.44
14	a	1139	CLA	O2D-CGD	4.74	1.44	1.33
14	G	1135	CLA	C3D-C4D	-4.74	1.33	1.44
14	a	1103	CLA	C3D-C4D	-4.74	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	b	4014	BCR	C10-C9	-4.73	1.24	1.35
14	A	1127	CLA	O2D-CGD	4.73	1.44	1.33
14	b	1227	CLA	C3D-C4D	-4.73	1.33	1.44
13	a	1011	CL0	O2D-CGD	4.73	1.44	1.33
14	H	1203	CLA	O2D-CGD	4.73	1.44	1.33
14	a	1126	CLA	O2D-CGD	4.73	1.44	1.33
14	G	1118	CLA	O2D-CGD	4.73	1.44	1.33
14	H	1226	CLA	O2D-CGD	4.73	1.44	1.33
14	A	1139	CLA	O2D-CGD	4.73	1.44	1.33
14	G	1138	CLA	C3D-C4D	-4.73	1.33	1.44
14	B	1203	CLA	O2D-CGD	4.73	1.44	1.33
14	G	1106	CLA	O2D-CGD	4.73	1.44	1.33
13	A	1011	CL0	C3B-C2B	4.72	1.46	1.40
14	A	1138	CLA	C3D-C4D	-4.72	1.33	1.44
14	B	1022	CLA	C3D-C4D	-4.72	1.33	1.44
18	A	4001	BCR	C10-C9	-4.72	1.24	1.35
14	G	1103	CLA	C3D-C4D	-4.72	1.33	1.44
14	A	1114	CLA	CHD-C1D	4.72	1.47	1.38
14	a	1127	CLA	O2D-CGD	4.72	1.44	1.33
14	B	1226	CLA	O2D-CGD	4.72	1.44	1.33
18	a	4001	BCR	C10-C9	-4.72	1.24	1.35
14	H	1207	CLA	C3D-C4D	-4.72	1.33	1.44
14	b	1239	CLA	C3D-C4D	-4.72	1.33	1.44
14	B	1239	CLA	C3D-C4D	-4.72	1.33	1.44
14	B	1236	CLA	C3D-C4D	-4.72	1.33	1.44
14	a	1114	CLA	CHD-C1D	4.72	1.47	1.38
14	H	1227	CLA	C3D-C4D	-4.72	1.33	1.44
14	b	1235	CLA	C3D-C4D	-4.72	1.33	1.44
14	H	1239	CLA	C3D-C4D	-4.72	1.33	1.44
14	H	1023	CLA	O2D-CGD	4.71	1.44	1.33
14	G	1102	CLA	C3D-C4D	-4.71	1.33	1.44
14	U	1502	CLA	C3D-C4D	-4.71	1.33	1.44
14	A	1106	CLA	O2D-CGD	4.71	1.44	1.33
15	A	1120	F6C	C4A-NA	-4.71	1.31	1.37
14	L	1502	CLA	C3D-C4D	-4.71	1.33	1.44
14	A	1133	CLA	O2D-CGD	4.71	1.44	1.33
14	a	1135	CLA	C3D-C4D	-4.71	1.33	1.44
13	G	1011	CL0	O2D-CGD	4.71	1.44	1.33
14	l	1502	CLA	C3D-C4D	-4.71	1.33	1.44
13	G	1011	CL0	C3B-C2B	4.71	1.46	1.40
14	B	1225	CLA	O2D-CGD	4.71	1.44	1.33
14	B	1231	CLA	CHC-C1C	4.71	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1102	CLA	C3D-C4D	-4.71	1.33	1.44
14	A	1116	CLA	C3D-C4D	-4.71	1.33	1.44
14	B	1227	CLA	C3D-C4D	-4.70	1.33	1.44
14	a	1128	CLA	C3D-C4D	-4.70	1.33	1.44
14	A	1123	CLA	O2D-CGD	4.70	1.44	1.33
14	G	1123	CLA	O2D-CGD	4.70	1.44	1.33
14	b	1231	CLA	CHC-C1C	4.70	1.47	1.38
14	b	1238	CLA	CHC-C1C	4.70	1.47	1.38
14	G	1133	CLA	O2D-CGD	4.70	1.44	1.33
14	b	1023	CLA	O2D-CGD	4.70	1.44	1.33
14	b	1236	CLA	C3D-C4D	-4.70	1.33	1.44
14	a	1125	CLA	O2D-CGD	4.70	1.44	1.33
14	a	1102	CLA	C3D-C4D	-4.70	1.33	1.44
14	B	1206	CLA	C3D-C4D	-4.70	1.33	1.44
14	H	1021	CLA	C3D-C4D	-4.70	1.33	1.44
14	H	1217	CLA	O2D-CGD	4.70	1.44	1.33
15	a	1120	F6C	C4A-NA	-4.70	1.31	1.37
14	G	1128	CLA	C3D-C4D	-4.69	1.33	1.44
15	b	1230	F6C	CHC-C4B	4.69	1.47	1.38
14	a	1106	CLA	O2D-CGD	4.69	1.44	1.33
14	A	1112	CLA	O2D-CGD	4.69	1.44	1.33
14	H	1231	CLA	CHC-C1C	4.69	1.47	1.38
14	b	1217	CLA	O2D-CGD	4.69	1.44	1.33
14	l	1503	CLA	C3D-C4D	-4.69	1.33	1.44
14	a	1140	CLA	O2D-CGD	4.69	1.44	1.33
18	a	4011	BCR	C10-C9	-4.69	1.25	1.35
15	G	1120	F6C	C4A-NA	-4.69	1.31	1.37
13	A	1011	CL0	O2D-CGD	4.69	1.44	1.33
14	G	1140	CLA	O2D-CGD	4.68	1.44	1.33
18	G	4001	BCR	C10-C9	-4.68	1.25	1.35
14	a	1133	CLA	O2D-CGD	4.68	1.44	1.33
14	A	1128	CLA	C3D-C4D	-4.68	1.33	1.44
14	B	1235	CLA	C3D-C4D	-4.68	1.33	1.44
14	G	1104	CLA	C3D-C4D	-4.68	1.33	1.44
14	a	1102	CLA	O2D-CGD	4.68	1.44	1.33
14	G	1112	CLA	O2D-CGD	4.68	1.44	1.33
18	G	4011	BCR	C10-C9	-4.68	1.25	1.35
14	G	1131	CLA	O2D-CGD	4.68	1.44	1.33
14	b	1022	CLA	C3D-C4D	-4.68	1.33	1.44
14	B	1023	CLA	O2D-CGD	4.68	1.44	1.33
14	a	1116	CLA	C3D-C4D	-4.68	1.33	1.44
14	A	1126	CLA	C3C-C2C	4.68	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1211	CLA	C3D-C4D	-4.67	1.33	1.44
14	H	1235	CLA	C3D-C4D	-4.67	1.33	1.44
14	G	1116	CLA	C3D-C4D	-4.67	1.33	1.44
14	a	1104	CLA	C3D-C4D	-4.67	1.33	1.44
14	B	1211	CLA	C3D-C4D	-4.67	1.33	1.44
14	b	1224	CLA	O2D-CGD	4.67	1.44	1.33
14	b	1239	CLA	C3C-C2C	4.67	1.46	1.36
14	a	1112	CLA	O2D-CGD	4.67	1.44	1.33
14	L	1503	CLA	C3D-C4D	-4.67	1.33	1.44
14	b	1207	CLA	C3D-C4D	-4.67	1.33	1.44
14	H	1206	CLA	C3D-C4D	-4.67	1.33	1.44
14	B	1234	CLA	C3D-C4D	-4.67	1.33	1.44
14	b	1234	CLA	C3D-C4D	-4.67	1.33	1.44
14	A	1117	CLA	O2D-CGD	4.67	1.44	1.33
14	a	1126	CLA	C3C-C2C	4.67	1.46	1.36
14	A	1140	CLA	O2D-CGD	4.67	1.44	1.33
14	B	1217	CLA	O2D-CGD	4.67	1.44	1.33
14	B	1223	CLA	O2D-CGD	4.67	1.44	1.33
14	H	1224	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1102	CLA	O2D-CGD	4.66	1.44	1.33
14	B	1224	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1117	CLA	O2D-CGD	4.66	1.44	1.33
14	H	1212	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1126	CLA	C3C-C2C	4.66	1.46	1.36
14	a	1117	CLA	O2D-CGD	4.66	1.44	1.33
14	a	1131	CLA	O2D-CGD	4.65	1.44	1.33
14	A	1131	CLA	O2D-CGD	4.65	1.44	1.33
14	b	1021	CLA	C3D-C4D	-4.65	1.33	1.44
14	B	1207	CLA	C3D-C4D	-4.65	1.33	1.44
14	H	1238	CLA	CHC-C1C	4.65	1.47	1.38
14	B	1205	CLA	O2D-CGD	4.65	1.44	1.33
14	A	1102	CLA	O2D-CGD	4.65	1.44	1.33
14	b	1206	CLA	C3D-C4D	-4.64	1.33	1.44
14	B	1021	CLA	C3D-C4D	-4.64	1.33	1.44
13	a	1011	CL0	C3B-C2B	4.64	1.46	1.40
14	B	1222	CLA	C3D-C4D	-4.64	1.33	1.44
14	T	1401	CLA	C3C-C2C	4.64	1.46	1.36
14	H	1214	CLA	C3C-C2C	4.64	1.46	1.36
14	H	1223	CLA	O2D-CGD	4.64	1.44	1.33
14	G	1131	CLA	C3D-C4D	-4.64	1.33	1.44
14	G	1013	CLA	O2D-CGD	4.64	1.44	1.33
14	b	1223	CLA	O2D-CGD	4.64	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4011	BCR	C10-C9	-4.64	1.25	1.35
14	A	1104	CLA	C3D-C4D	-4.63	1.33	1.44
14	H	1239	CLA	C3C-C2C	4.63	1.46	1.36
14	b	1205	CLA	O2D-CGD	4.63	1.44	1.33
14	b	1211	CLA	C3D-C4D	-4.63	1.33	1.44
14	K	1401	CLA	C3C-C2C	4.63	1.46	1.36
14	b	1214	CLA	C3C-C2C	4.63	1.46	1.36
14	B	1238	CLA	CHC-C1C	4.63	1.47	1.38
14	B	1212	CLA	O2D-CGD	4.63	1.44	1.33
14	b	1212	CLA	O2D-CGD	4.63	1.44	1.33
14	A	1137	CLA	O2D-CGD	4.63	1.44	1.33
14	H	1234	CLA	C3D-C4D	-4.62	1.33	1.44
14	B	1239	CLA	C3C-C2C	4.62	1.46	1.36
14	H	1205	CLA	O2D-CGD	4.62	1.44	1.33
14	A	1140	CLA	C3D-C4D	-4.62	1.33	1.44
14	U	1503	CLA	C3D-C4D	-4.62	1.33	1.44
14	H	1201	CLA	O2D-CGD	4.62	1.44	1.33
14	a	1013	CLA	O2D-CGD	4.62	1.44	1.33
14	B	1214	CLA	C3C-C2C	4.62	1.46	1.36
14	A	1109	CLA	C3D-C4D	-4.62	1.33	1.44
14	A	1101	CLA	CHC-C1C	4.62	1.47	1.38
14	A	1013	CLA	C1B-NB	-4.61	1.31	1.37
14	A	1131	CLA	C3D-C4D	-4.61	1.33	1.44
14	a	1013	CLA	C1B-NB	-4.61	1.31	1.37
14	k	1401	CLA	C3C-C2C	4.61	1.46	1.36
14	b	1201	CLA	O2D-CGD	4.61	1.44	1.33
14	b	1222	CLA	C3D-C4D	-4.61	1.33	1.44
14	b	1221	CLA	O2D-CGD	4.60	1.44	1.33
14	B	1223	CLA	C3D-C4D	-4.60	1.33	1.44
14	a	1109	CLA	C3D-C4D	-4.60	1.33	1.44
14	b	1223	CLA	C3D-C4D	-4.60	1.33	1.44
14	G	1109	CLA	C3D-C4D	-4.60	1.33	1.44
14	a	1131	CLA	C3D-C4D	-4.60	1.33	1.44
14	B	1201	CLA	O2D-CGD	4.60	1.44	1.33
14	H	1222	CLA	C3D-C4D	-4.60	1.33	1.44
14	G	1137	CLA	O2D-CGD	4.60	1.44	1.33
14	H	1213	CLA	C3D-C4D	-4.60	1.33	1.44
14	A	1013	CLA	O2D-CGD	4.60	1.44	1.33
14	G	1101	CLA	CHC-C1C	4.60	1.47	1.38
14	H	1012	CLA	CHC-C1C	4.60	1.47	1.38
14	l	1503	CLA	O2D-CGD	4.59	1.44	1.33
14	H	1221	CLA	O2D-CGD	4.59	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1222	CLA	O2D-CGD	4.59	1.44	1.33
14	H	1222	CLA	CHC-C1C	4.59	1.47	1.38
14	H	1223	CLA	C3D-C4D	-4.59	1.33	1.44
14	a	1105	CLA	CHC-C1C	4.59	1.47	1.38
14	U	1501	CLA	O2D-CGD	4.59	1.44	1.33
14	B	1213	CLA	C3D-C4D	-4.59	1.33	1.44
14	B	1021	CLA	C1D-ND	-4.59	1.31	1.37
14	b	1208	CLA	C3D-C4D	-4.59	1.33	1.44
14	B	1236	CLA	O2D-CGD	4.59	1.44	1.33
14	B	1231	CLA	C3D-C4D	-4.59	1.33	1.44
14	H	1236	CLA	O2D-CGD	4.59	1.44	1.33
14	k	1401	CLA	CHD-C1D	4.58	1.47	1.38
14	H	1229	CLA	O2D-CGD	4.58	1.44	1.33
14	l	1501	CLA	O2D-CGD	4.58	1.44	1.33
14	B	1228	CLA	C3D-C4D	-4.58	1.33	1.44
14	B	1222	CLA	O2D-CGD	4.58	1.44	1.33
14	H	1021	CLA	C1D-ND	-4.58	1.31	1.37
14	B	1208	CLA	C3D-C4D	-4.58	1.33	1.44
14	b	1213	CLA	C3D-C4D	-4.58	1.33	1.44
14	b	1229	CLA	O2D-CGD	4.58	1.44	1.33
14	A	1105	CLA	CHC-C1C	4.58	1.47	1.38
14	A	1118	CLA	C3D-C4D	-4.58	1.33	1.44
14	H	1221	CLA	C3D-C4D	-4.58	1.33	1.44
14	b	1229	CLA	C3D-C4D	-4.58	1.33	1.44
14	B	1201	CLA	C3D-C4D	-4.58	1.33	1.44
14	b	1219	CLA	CHC-C1C	4.58	1.47	1.38
14	a	1140	CLA	C3D-C4D	-4.58	1.33	1.44
14	G	1124	CLA	C3D-C4D	-4.57	1.33	1.44
14	b	1222	CLA	CHC-C1C	4.57	1.47	1.38
14	A	1124	CLA	C3D-C4D	-4.57	1.33	1.44
14	G	1117	CLA	C3D-C4D	-4.57	1.33	1.44
14	a	1118	CLA	C3D-C4D	-4.57	1.33	1.44
14	T	1401	CLA	CHD-C1D	4.57	1.47	1.38
14	G	1108	CLA	CHC-C1C	4.57	1.47	1.38
14	b	1221	CLA	C3D-C4D	-4.57	1.33	1.44
14	L	1501	CLA	O2D-CGD	4.57	1.44	1.33
14	K	1401	CLA	CHD-C1D	4.57	1.47	1.38
14	H	1228	CLA	C3D-C4D	-4.57	1.33	1.44
14	a	1107	CLA	O2D-CGD	4.57	1.44	1.33
14	b	1236	CLA	O2D-CGD	4.57	1.44	1.33
14	B	1022	CLA	CHC-C1C	4.57	1.47	1.38
14	G	1140	CLA	C3D-C4D	-4.57	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	CHC-C1C	4.57	1.47	1.38
14	B	1221	CLA	O2D-CGD	4.57	1.44	1.33
14	b	1222	CLA	O2D-CGD	4.57	1.44	1.33
14	B	1214	CLA	CHD-C1D	4.57	1.47	1.38
14	a	1137	CLA	O2D-CGD	4.57	1.44	1.33
14	A	1122	CLA	C3D-C4D	-4.57	1.33	1.44
14	a	1117	CLA	C3D-C4D	-4.57	1.33	1.44
14	a	1136	CLA	C3D-C4D	-4.57	1.33	1.44
14	l	1501	CLA	C3D-C4D	-4.57	1.33	1.44
14	H	1229	CLA	C3D-C4D	-4.57	1.33	1.44
14	b	1214	CLA	CHD-C1D	4.57	1.47	1.38
14	H	1214	CLA	CHD-C1D	4.56	1.47	1.38
14	a	1110	CLA	O2D-CGD	4.56	1.44	1.33
14	G	1118	CLA	C3D-C4D	-4.56	1.33	1.44
14	B	1222	CLA	CHC-C1C	4.56	1.47	1.38
14	B	1221	CLA	C3D-C4D	-4.56	1.33	1.44
14	G	1105	CLA	CHC-C1C	4.56	1.47	1.38
14	b	1234	CLA	CHC-C1C	4.56	1.47	1.38
14	a	1111	CLA	C3D-C4D	-4.56	1.33	1.44
14	B	1234	CLA	CHC-C1C	4.56	1.47	1.38
14	a	1129	CLA	O2D-CGD	4.56	1.44	1.33
14	a	1101	CLA	CHC-C1C	4.56	1.47	1.38
14	U	1503	CLA	O2D-CGD	4.56	1.44	1.33
14	H	1216	CLA	CHD-C1D	4.56	1.47	1.38
14	b	1216	CLA	CHD-C1D	4.56	1.47	1.38
14	G	1136	CLA	C3D-C4D	-4.56	1.33	1.44
14	B	1205	CLA	C3D-C4D	-4.56	1.33	1.44
14	H	1208	CLA	C3D-C4D	-4.56	1.33	1.44
14	a	1108	CLA	CHC-C1C	4.56	1.47	1.38
14	a	1110	CLA	CHC-C1C	4.56	1.47	1.38
14	X	1701	CLA	C3D-C4D	-4.56	1.33	1.44
14	a	1124	CLA	C3D-C4D	-4.56	1.33	1.44
14	B	1204	CLA	C1D-ND	-4.56	1.31	1.37
18	l	4019	BCR	C10-C9	-4.56	1.25	1.35
14	G	1013	CLA	C1B-NB	-4.55	1.31	1.37
14	H	1234	CLA	CHC-C1C	4.55	1.47	1.38
14	L	1503	CLA	O2D-CGD	4.55	1.44	1.33
14	H	1231	CLA	C3D-C4D	-4.55	1.33	1.44
14	A	1129	CLA	O2D-CGD	4.55	1.44	1.33
14	x	1701	CLA	CHC-C1C	4.55	1.47	1.38
14	B	1229	CLA	C3D-C4D	-4.55	1.33	1.44
14	b	1022	CLA	CHC-C1C	4.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1110	CLA	O2D-CGD	4.55	1.44	1.33
14	G	1119	CLA	C3D-C4D	-4.55	1.33	1.44
14	b	1205	CLA	C3D-C4D	-4.55	1.33	1.44
14	G	1129	CLA	O2D-CGD	4.55	1.44	1.33
14	A	1110	CLA	O2D-CGD	4.55	1.44	1.33
14	X	1701	CLA	CHC-C1C	4.55	1.47	1.38
14	A	1136	CLA	C3D-C4D	-4.55	1.33	1.44
14	A	1107	CLA	O2D-CGD	4.55	1.44	1.33
14	a	1119	CLA	C3D-C4D	-4.55	1.33	1.44
14	b	1212	CLA	CHC-C1C	4.55	1.47	1.38
14	B	1229	CLA	O2D-CGD	4.55	1.44	1.33
14	G	1107	CLA	O2D-CGD	4.55	1.44	1.33
14	A	1111	CLA	C3D-C4D	-4.55	1.34	1.44
14	b	1228	CLA	C3D-C4D	-4.55	1.34	1.44
14	H	1219	CLA	CHC-C1C	4.54	1.47	1.38
14	A	1128	CLA	O2D-CGD	4.54	1.44	1.33
14	B	1212	CLA	CHC-C1C	4.54	1.47	1.38
15	G	1120	F6C	CHC-C4B	4.54	1.47	1.38
14	a	1128	CLA	O2D-CGD	4.54	1.44	1.33
14	b	1201	CLA	C3D-C4D	-4.54	1.34	1.44
14	A	1110	CLA	CHC-C1C	4.54	1.47	1.38
14	G	1111	CLA	C3D-C4D	-4.54	1.34	1.44
14	G	1117	CLA	CHD-C1D	4.54	1.47	1.38
14	H	1205	CLA	C3D-C4D	-4.54	1.34	1.44
14	G	1122	CLA	C3D-C4D	-4.54	1.34	1.44
14	G	1101	CLA	C3D-C4D	-4.54	1.34	1.44
14	H	1212	CLA	CHC-C1C	4.54	1.47	1.38
14	a	1105	CLA	C3D-C4D	-4.54	1.34	1.44
14	H	1211	CLA	CHC-C1C	4.54	1.47	1.38
14	a	1130	CLA	CHC-C1C	4.54	1.47	1.38
14	b	1231	CLA	C3D-C4D	-4.54	1.34	1.44
14	B	1216	CLA	CHD-C1D	4.53	1.47	1.38
14	A	1115	CLA	C3D-C4D	-4.53	1.34	1.44
14	A	1101	CLA	C3D-C4D	-4.53	1.34	1.44
18	L	4019	BCR	C10-C9	-4.53	1.25	1.35
14	B	1216	CLA	C3D-C4D	-4.53	1.34	1.44
14	A	1117	CLA	C3D-C4D	-4.53	1.34	1.44
18	U	4019	BCR	C10-C9	-4.53	1.25	1.35
14	B	1211	CLA	CHC-C1C	4.53	1.47	1.38
14	G	1115	CLA	C3D-C4D	-4.53	1.34	1.44
14	A	1105	CLA	C3D-C4D	-4.53	1.34	1.44
14	a	1139	CLA	C3D-C4D	-4.52	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1119	CLA	C3D-C4D	-4.52	1.34	1.44
14	A	1139	CLA	C3D-C4D	-4.52	1.34	1.44
14	b	1211	CLA	CHC-C1C	4.52	1.47	1.38
14	a	1101	CLA	C3D-C4D	-4.52	1.34	1.44
14	a	1122	CLA	C3D-C4D	-4.52	1.34	1.44
14	H	1216	CLA	C3D-C4D	-4.52	1.34	1.44
14	U	1501	CLA	C3D-C4D	-4.52	1.34	1.44
14	B	1219	CLA	CHC-C1C	4.52	1.47	1.38
15	H	1237	F6C	CHC-C4B	4.52	1.47	1.38
14	G	1119	CLA	CHC-C1C	4.52	1.47	1.38
14	b	1216	CLA	C3D-C4D	-4.52	1.34	1.44
18	b	4009	BCR	C10-C9	-4.51	1.25	1.35
15	b	1237	F6C	CHC-C4B	4.51	1.47	1.38
15	A	1120	F6C	CHC-C4B	4.51	1.47	1.38
14	b	1225	CLA	C1D-ND	-4.51	1.31	1.37
14	H	1217	CLA	C3D-C4D	-4.51	1.34	1.44
14	G	1139	CLA	C3D-C4D	-4.51	1.34	1.44
14	a	1124	CLA	CHC-C1C	4.51	1.47	1.38
18	B	4009	BCR	C10-C9	-4.51	1.25	1.35
14	G	1105	CLA	C3D-C4D	-4.51	1.34	1.44
14	A	1124	CLA	CHC-C1C	4.51	1.47	1.38
14	H	1204	CLA	C1D-ND	-4.50	1.31	1.37
14	x	1701	CLA	C3D-C4D	-4.50	1.34	1.44
14	H	1201	CLA	C3D-C4D	-4.50	1.34	1.44
18	H	4009	BCR	C10-C9	-4.50	1.25	1.35
14	B	1218	CLA	CHC-C1C	4.50	1.47	1.38
15	B	1237	F6C	CHC-C4B	4.50	1.47	1.38
15	a	1120	F6C	CHC-C4B	4.50	1.47	1.38
14	G	1128	CLA	O2D-CGD	4.50	1.44	1.33
14	a	1119	CLA	CHC-C1C	4.50	1.47	1.38
14	b	1217	CLA	C3D-C4D	-4.50	1.34	1.44
14	B	1217	CLA	CHC-C1C	4.50	1.47	1.38
14	L	1501	CLA	C3D-C4D	-4.50	1.34	1.44
14	B	1231	CLA	O2D-CGD	4.50	1.44	1.33
14	G	1103	CLA	O2D-CGD	4.49	1.44	1.33
14	G	1124	CLA	CHC-C1C	4.49	1.47	1.38
14	b	1021	CLA	C1D-ND	-4.49	1.32	1.37
14	W	1701	CLA	CHC-C1C	4.49	1.47	1.38
14	A	1102	CLA	CHC-C1C	4.49	1.47	1.38
14	a	1135	CLA	O2D-CGD	4.49	1.44	1.33
14	a	1117	CLA	CHD-C1D	4.49	1.47	1.38
14	a	1133	CLA	C3D-C4D	-4.49	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	5005	LMG	O8-C28	4.49	1.46	1.33
14	b	1231	CLA	O2D-CGD	4.49	1.44	1.33
14	H	1225	CLA	C1D-ND	-4.49	1.32	1.37
14	G	1130	CLA	CHC-C1C	4.49	1.47	1.38
14	H	1210	CLA	O2D-CGD	4.49	1.44	1.33
14	A	1117	CLA	CHD-C1D	4.49	1.47	1.38
14	H	1221	CLA	CHC-C1C	4.49	1.47	1.38
14	a	1115	CLA	C3D-C4D	-4.49	1.34	1.44
14	G	1110	CLA	CHC-C1C	4.49	1.47	1.38
14	a	1102	CLA	CHC-C1C	4.49	1.47	1.38
14	B	1217	CLA	C3D-C4D	-4.48	1.34	1.44
14	H	1217	CLA	CHC-C1C	4.48	1.47	1.38
14	G	1102	CLA	CHC-C1C	4.48	1.47	1.38
14	A	1106	CLA	C3D-C4D	-4.48	1.34	1.44
14	G	1135	CLA	O2D-CGD	4.48	1.44	1.33
14	b	1210	CLA	O2D-CGD	4.48	1.44	1.33
14	W	1701	CLA	C3D-C4D	-4.48	1.34	1.44
14	B	1213	CLA	CHC-C1C	4.48	1.47	1.38
14	H	1218	CLA	CHC-C1C	4.48	1.47	1.38
14	b	1221	CLA	CHC-C1C	4.48	1.47	1.38
14	b	1204	CLA	C1D-ND	-4.48	1.32	1.37
14	a	1106	CLA	C3D-C4D	-4.48	1.34	1.44
14	G	1106	CLA	C3D-C4D	-4.47	1.34	1.44
14	B	1221	CLA	CHC-C1C	4.47	1.47	1.38
14	H	1220	CLA	C3D-C4D	-4.47	1.34	1.44
14	A	1110	CLA	C3D-C4D	-4.47	1.34	1.44
14	A	1103	CLA	O2D-CGD	4.47	1.44	1.33
20	G	5005	LMG	O8-C28	4.47	1.46	1.33
14	a	1103	CLA	O2D-CGD	4.47	1.44	1.33
14	B	1235	CLA	CHC-C1C	4.47	1.47	1.38
14	a	1114	CLA	C3C-C2C	4.47	1.46	1.36
14	a	1108	CLA	C3D-C4D	-4.47	1.34	1.44
14	A	1130	CLA	CHC-C1C	4.47	1.47	1.38
14	b	1213	CLA	CHC-C1C	4.47	1.47	1.38
14	G	1132	CLA	O2D-CGD	4.47	1.44	1.33
14	G	1114	CLA	C3C-C2C	4.47	1.46	1.36
14	A	1119	CLA	CHC-C1C	4.46	1.47	1.38
14	B	1224	CLA	CHC-C1C	4.46	1.47	1.38
14	b	1233	CLA	CHC-C1C	4.46	1.47	1.38
14	H	1231	CLA	O2D-CGD	4.46	1.44	1.33
14	B	1220	CLA	C3D-C4D	-4.46	1.34	1.44
14	B	1205	CLA	CHC-C1C	4.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1108	CLA	C3D-C4D	-4.46	1.34	1.44
14	b	1229	CLA	CHC-C1C	4.46	1.47	1.38
20	A	5005	LMG	O8-C28	4.46	1.46	1.33
14	A	1135	CLA	O2D-CGD	4.46	1.44	1.33
14	H	1232	CLA	CHD-C1D	4.46	1.47	1.38
14	H	1232	CLA	C3D-C4D	-4.46	1.34	1.44
14	B	1232	CLA	CHD-C1D	4.46	1.47	1.38
14	A	1114	CLA	C3D-C4D	-4.46	1.34	1.44
14	b	1220	CLA	C3D-C4D	-4.46	1.34	1.44
14	a	1114	CLA	C3D-C4D	-4.45	1.34	1.44
18	a	4003	BCR	C10-C9	-4.45	1.25	1.35
14	G	1133	CLA	C3D-C4D	-4.45	1.34	1.44
14	A	1133	CLA	C3D-C4D	-4.45	1.34	1.44
14	A	1112	CLA	CHC-C1C	4.45	1.47	1.38
14	G	1129	CLA	CHC-C1C	4.45	1.47	1.38
14	H	1229	CLA	CHC-C1C	4.45	1.47	1.38
14	H	1235	CLA	CHC-C1C	4.45	1.47	1.38
14	b	1232	CLA	CHD-C1D	4.45	1.47	1.38
18	H	4006	BCR	C10-C9	-4.45	1.25	1.35
18	b	4006	BCR	C10-C9	-4.45	1.25	1.35
14	a	1129	CLA	CHC-C1C	4.45	1.47	1.38
14	A	1108	CLA	C3D-C4D	-4.45	1.34	1.44
14	B	1229	CLA	CHC-C1C	4.45	1.47	1.38
14	A	1129	CLA	CHC-C1C	4.45	1.47	1.38
14	b	1215	CLA	C3D-C4D	-4.45	1.34	1.44
14	A	1114	CLA	C3C-C2C	4.45	1.46	1.36
14	b	1218	CLA	CHC-C1C	4.45	1.47	1.38
18	A	4003	BCR	C10-C9	-4.45	1.25	1.35
14	b	1224	CLA	CHC-C1C	4.45	1.47	1.38
14	B	1210	CLA	O2D-CGD	4.44	1.44	1.33
14	b	1232	CLA	C3D-C4D	-4.44	1.34	1.44
14	H	1205	CLA	CHC-C1C	4.44	1.47	1.38
14	T	1401	CLA	CHC-C1C	4.44	1.47	1.38
14	a	1112	CLA	CHC-C1C	4.44	1.47	1.38
18	G	4003	BCR	C10-C9	-4.44	1.25	1.35
14	H	1023	CLA	C3D-C4D	-4.44	1.34	1.44
14	a	1132	CLA	O2D-CGD	4.44	1.44	1.33
14	G	1110	CLA	C3D-C4D	-4.44	1.34	1.44
14	B	1222	CLA	C3C-C2C	4.44	1.46	1.36
14	B	1233	CLA	CHC-C1C	4.44	1.47	1.38
14	b	1209	CLA	C3D-C4D	-4.44	1.34	1.44
14	B	1215	CLA	C3D-C4D	-4.44	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1227	CLA	CHD-C1D	4.44	1.47	1.38
14	H	1213	CLA	CHC-C1C	4.44	1.47	1.38
14	b	1218	CLA	C3D-C4D	-4.43	1.34	1.44
14	G	1112	CLA	CHC-C1C	4.43	1.47	1.38
14	G	1124	CLA	C3C-C2C	4.43	1.46	1.36
14	B	1227	CLA	CHD-C1D	4.43	1.47	1.38
14	b	1233	CLA	C3D-C4D	-4.43	1.34	1.44
14	B	1209	CLA	C3D-C4D	-4.43	1.34	1.44
14	b	1023	CLA	C3D-C4D	-4.43	1.34	1.44
14	H	1208	CLA	CHD-C1D	4.43	1.47	1.38
14	l	1502	CLA	O2D-CGD	4.43	1.44	1.33
14	A	1132	CLA	O2D-CGD	4.43	1.44	1.33
14	b	1227	CLA	CHD-C1D	4.43	1.47	1.38
14	a	1110	CLA	C3D-C4D	-4.42	1.34	1.44
14	B	1225	CLA	C1D-ND	-4.42	1.32	1.37
14	b	1226	CLA	CHD-C1D	4.42	1.47	1.38
14	b	1222	CLA	C3C-C2C	4.42	1.46	1.36
14	B	1232	CLA	C3D-C4D	-4.42	1.34	1.44
18	B	4006	BCR	C10-C9	-4.42	1.25	1.35
14	G	1114	CLA	C3D-C4D	-4.42	1.34	1.44
14	a	1124	CLA	C3C-C2C	4.42	1.46	1.36
14	H	1202	CLA	O2D-CGD	4.42	1.44	1.33
14	G	1106	CLA	CHC-C1C	4.42	1.47	1.38
14	A	1124	CLA	C3C-C2C	4.42	1.46	1.36
14	H	1021	CLA	O2D-CGD	4.42	1.44	1.33
14	b	1217	CLA	CHC-C1C	4.42	1.47	1.38
14	b	1233	CLA	CHD-C1D	4.42	1.47	1.38
14	b	1202	CLA	O2D-CGD	4.42	1.44	1.33
19	G	5001	LHG	O8-C23	4.42	1.46	1.33
14	H	1209	CLA	C3D-C4D	-4.42	1.34	1.44
14	H	1222	CLA	C3C-C2C	4.41	1.46	1.36
14	G	1013	CLA	C3D-C4D	-4.41	1.34	1.44
14	H	1224	CLA	CHC-C1C	4.41	1.47	1.38
14	H	1229	CLA	C3C-C2C	4.41	1.46	1.36
14	b	1235	CLA	CHC-C1C	4.41	1.47	1.38
14	H	1218	CLA	C3D-C4D	-4.41	1.34	1.44
14	b	1205	CLA	CHC-C1C	4.41	1.47	1.38
14	B	1218	CLA	C3D-C4D	-4.41	1.34	1.44
14	H	1233	CLA	C3D-C4D	-4.41	1.34	1.44
14	A	1138	CLA	CHD-C1D	4.41	1.47	1.38
14	K	1401	CLA	CHC-C1C	4.41	1.47	1.38
14	B	1023	CLA	C3D-C4D	-4.41	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1106	CLA	CHC-C1C	4.41	1.47	1.38
14	b	1209	CLA	CHC-C1C	4.41	1.47	1.38
14	H	1215	CLA	C3D-C4D	-4.41	1.34	1.44
14	H	1233	CLA	CHC-C1C	4.41	1.47	1.38
14	H	1205	CLA	C1D-ND	-4.41	1.32	1.37
18	H	4005	BCR	C10-C9	-4.40	1.25	1.35
14	a	1138	CLA	CHD-C1D	4.40	1.47	1.38
14	k	1401	CLA	CHC-C1C	4.40	1.47	1.38
18	b	4005	BCR	C10-C9	-4.40	1.25	1.35
18	b	4013	BCR	C10-C9	-4.40	1.25	1.35
14	U	1502	CLA	O2D-CGD	4.40	1.44	1.33
18	B	4005	BCR	C10-C9	-4.40	1.25	1.35
14	L	1502	CLA	O2D-CGD	4.40	1.44	1.33
14	a	1106	CLA	CHC-C1C	4.40	1.47	1.38
14	H	1233	CLA	CHD-C1D	4.39	1.47	1.38
14	B	1233	CLA	C3D-C4D	-4.39	1.34	1.44
20	l	5007	LMG	O8-C28	4.39	1.46	1.33
15	b	1230	F6C	CHD-C1D	4.39	1.47	1.38
14	b	1021	CLA	O2D-CGD	4.39	1.44	1.33
14	a	1013	CLA	C3D-C4D	-4.39	1.34	1.44
14	H	1209	CLA	CHC-C1C	4.39	1.47	1.38
14	B	1233	CLA	CHD-C1D	4.39	1.47	1.38
14	b	1203	CLA	CHC-C1C	4.39	1.47	1.38
14	B	1205	CLA	C1D-ND	-4.39	1.32	1.37
14	B	1208	CLA	CHD-C1D	4.39	1.47	1.38
19	A	5001	LHG	O8-C23	4.39	1.46	1.33
14	B	1219	CLA	C3D-C4D	-4.39	1.34	1.44
14	a	1112	CLA	C3D-C4D	-4.39	1.34	1.44
14	G	1112	CLA	C3D-C4D	-4.38	1.34	1.44
14	B	1229	CLA	C3C-C2C	4.38	1.46	1.36
14	G	1124	CLA	O2D-CGD	4.38	1.44	1.33
20	L	5007	LMG	O8-C28	4.38	1.46	1.33
19	a	5001	LHG	O8-C23	4.38	1.46	1.33
14	H	1209	CLA	CHD-C1D	4.38	1.47	1.38
14	B	1202	CLA	O2D-CGD	4.38	1.44	1.33
14	G	1108	CLA	C3C-C2C	4.38	1.46	1.36
14	H	1226	CLA	CHD-C1D	4.38	1.47	1.38
14	a	1123	CLA	CHC-C1C	4.38	1.47	1.38
14	a	1139	CLA	CHC-C1C	4.38	1.47	1.38
14	a	1108	CLA	C3C-C2C	4.38	1.46	1.36
14	b	1209	CLA	CHD-C1D	4.38	1.47	1.38
14	A	1124	CLA	O2D-CGD	4.38	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1227	CLA	CHC-C1C	4.38	1.47	1.38
14	B	1212	CLA	C3D-C4D	-4.38	1.34	1.44
14	A	1112	CLA	C3D-C4D	-4.38	1.34	1.44
14	H	1212	CLA	C3D-C4D	-4.38	1.34	1.44
14	b	1208	CLA	CHD-C1D	4.38	1.47	1.38
14	B	1021	CLA	O2D-CGD	4.38	1.44	1.33
14	A	1118	CLA	CHD-C1D	4.38	1.47	1.38
14	B	1226	CLA	CHD-C1D	4.37	1.47	1.38
18	B	4013	BCR	C10-C9	-4.37	1.25	1.35
14	A	1013	CLA	C3D-C4D	-4.37	1.34	1.44
20	U	5007	LMG	O8-C28	4.37	1.46	1.33
14	b	1205	CLA	C1D-ND	-4.37	1.32	1.37
14	G	1123	CLA	CHC-C1C	4.37	1.47	1.38
14	U	1501	CLA	CHC-C1C	4.37	1.47	1.38
18	b	4004	BCR	C10-C9	-4.37	1.25	1.35
18	H	4013	BCR	C10-C9	-4.37	1.25	1.35
14	b	1229	CLA	C3C-C2C	4.37	1.46	1.36
18	H	4004	BCR	C10-C9	-4.37	1.25	1.35
14	b	1212	CLA	C3D-C4D	-4.37	1.34	1.44
14	G	1138	CLA	CHD-C1D	4.37	1.46	1.38
18	B	4004	BCR	C10-C9	-4.36	1.25	1.35
14	l	1501	CLA	CHC-C1C	4.36	1.47	1.38
14	b	1227	CLA	CHC-C1C	4.36	1.47	1.38
14	A	1123	CLA	CHC-C1C	4.36	1.47	1.38
14	G	1118	CLA	CHD-C1D	4.36	1.46	1.38
14	G	1132	CLA	C3C-C2C	4.36	1.46	1.36
14	H	1228	CLA	C3C-C2C	4.36	1.46	1.36
14	a	1124	CLA	O2D-CGD	4.36	1.43	1.33
14	G	1115	CLA	CHC-C1C	4.36	1.47	1.38
14	B	1203	CLA	CHC-C1C	4.36	1.47	1.38
14	G	1139	CLA	CHC-C1C	4.36	1.47	1.38
14	H	1226	CLA	C1B-NB	-4.36	1.32	1.37
14	a	1138	CLA	CHC-C1C	4.36	1.47	1.38
14	H	1227	CLA	CHC-C1C	4.36	1.47	1.38
14	G	1128	CLA	C3C-C2C	4.35	1.46	1.36
14	A	1139	CLA	CHC-C1C	4.35	1.47	1.38
14	B	1229	CLA	CHD-C1D	4.35	1.46	1.38
14	H	1203	CLA	CHC-C1C	4.35	1.47	1.38
14	G	1126	CLA	CHC-C1C	4.35	1.47	1.38
14	H	1219	CLA	C3D-C4D	-4.35	1.34	1.44
14	A	1126	CLA	CHC-C1C	4.35	1.47	1.38
14	a	1102	CLA	CHD-C1D	4.35	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	U	1501	CLA	C3C-C2C	4.35	1.46	1.36
14	b	1219	CLA	C3D-C4D	-4.34	1.34	1.44
14	B	1226	CLA	C1B-NB	-4.34	1.32	1.37
14	A	1108	CLA	C3C-C2C	4.34	1.46	1.36
14	L	1501	CLA	CHC-C1C	4.34	1.47	1.38
14	a	1128	CLA	C3C-C2C	4.34	1.46	1.36
14	B	1228	CLA	C3C-C2C	4.34	1.46	1.36
14	A	1108	CLA	CHD-C1D	4.34	1.46	1.38
14	A	1128	CLA	C3C-C2C	4.34	1.46	1.36
14	A	1102	CLA	CHD-C1D	4.34	1.46	1.38
14	b	1228	CLA	C3C-C2C	4.34	1.46	1.36
14	b	1226	CLA	C1B-NB	-4.34	1.32	1.37
13	A	1011	CL0	OBD-CAD	4.34	1.28	1.22
14	a	1118	CLA	CHD-C1D	4.34	1.46	1.38
14	H	1229	CLA	CHD-C1D	4.34	1.46	1.38
14	G	1102	CLA	CHD-C1D	4.34	1.46	1.38
14	l	1501	CLA	C3C-C2C	4.33	1.46	1.36
14	b	1229	CLA	CHD-C1D	4.33	1.46	1.38
14	A	1132	CLA	CHC-C1C	4.33	1.47	1.38
13	a	1011	CL0	OBD-CAD	4.33	1.28	1.22
14	a	1108	CLA	CHD-C1D	4.33	1.46	1.38
14	B	1209	CLA	CHD-C1D	4.33	1.46	1.38
14	A	1115	CLA	CHC-C1C	4.32	1.47	1.38
14	B	1209	CLA	CHC-C1C	4.32	1.47	1.38
14	a	1115	CLA	CHC-C1C	4.32	1.47	1.38
14	B	1226	CLA	C1D-ND	-4.32	1.32	1.37
14	A	1138	CLA	CHC-C1C	4.32	1.47	1.38
14	H	1219	CLA	C3C-C2C	4.32	1.46	1.36
14	H	1201	CLA	CHC-C1C	4.31	1.47	1.38
14	a	1113	CLA	CHD-C1D	4.31	1.46	1.38
14	a	1132	CLA	C3C-C2C	4.31	1.46	1.36
15	a	1121	F6C	CHD-C1D	4.31	1.47	1.38
14	G	1118	CLA	C3C-C2C	4.31	1.46	1.36
14	G	1108	CLA	CHD-C1D	4.31	1.46	1.38
14	a	1132	CLA	CHC-C1C	4.31	1.47	1.38
14	H	1226	CLA	C3C-C2C	4.31	1.46	1.36
14	G	1138	CLA	CHC-C1C	4.31	1.47	1.38
14	b	1213	CLA	CHD-C1D	4.31	1.46	1.38
14	G	1114	CLA	CHC-C1C	4.31	1.47	1.38
14	a	1128	CLA	C1B-NB	-4.31	1.32	1.37
14	G	1112	CLA	CHD-C1D	4.31	1.46	1.38
14	L	1501	CLA	C3C-C2C	4.31	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1132	CLA	C3C-C2C	4.31	1.46	1.36
14	B	1201	CLA	CHC-C1C	4.31	1.47	1.38
14	a	1126	CLA	CHC-C1C	4.31	1.47	1.38
14	a	1129	CLA	C1D-ND	-4.30	1.32	1.37
14	B	1219	CLA	C3C-C2C	4.30	1.46	1.36
14	B	1216	CLA	C3C-C2C	4.30	1.46	1.36
14	B	1228	CLA	CHC-C1C	4.30	1.47	1.38
14	a	1114	CLA	CHC-C1C	4.30	1.47	1.38
14	b	1201	CLA	CHC-C1C	4.30	1.47	1.38
14	b	1216	CLA	C3C-C2C	4.30	1.46	1.36
14	H	1210	CLA	CHD-C1D	4.30	1.46	1.38
14	B	1213	CLA	CHD-C1D	4.30	1.46	1.38
14	H	1216	CLA	C3C-C2C	4.30	1.46	1.36
14	a	1102	CLA	C3C-C2C	4.30	1.46	1.36
14	b	1219	CLA	C3C-C2C	4.30	1.46	1.36
14	a	1133	CLA	CHD-C1D	4.30	1.46	1.38
14	A	1114	CLA	CHC-C1C	4.30	1.47	1.38
15	H	1230	F6C	CHD-C1D	4.30	1.47	1.38
14	a	1127	CLA	CHC-C1C	4.29	1.47	1.38
14	A	1112	CLA	CHD-C1D	4.29	1.46	1.38
14	H	1234	CLA	C3C-C2C	4.29	1.46	1.36
14	a	1112	CLA	CHD-C1D	4.29	1.46	1.38
14	b	1227	CLA	C3C-C2C	4.29	1.46	1.36
14	H	1226	CLA	C1D-ND	-4.29	1.32	1.37
14	G	1109	CLA	CHC-C1C	4.29	1.47	1.38
14	H	1208	CLA	C3C-C2C	4.29	1.46	1.36
14	b	1228	CLA	CHC-C1C	4.29	1.47	1.38
14	B	1226	CLA	C3C-C2C	4.29	1.46	1.36
14	G	1130	CLA	C3C-C2C	4.29	1.46	1.36
14	b	1231	CLA	CHD-C1D	4.29	1.46	1.38
20	R	5006	LMG	O8-C28	4.28	1.45	1.33
14	H	1217	CLA	CHD-C1D	4.28	1.46	1.38
14	b	1234	CLA	C3C-C2C	4.28	1.46	1.36
14	A	1119	CLA	CHD-C1D	4.28	1.46	1.38
14	G	1132	CLA	CHD-C1D	4.28	1.46	1.38
14	b	1226	CLA	C1D-ND	-4.28	1.32	1.37
14	H	1213	CLA	CHD-C1D	4.28	1.46	1.38
14	A	1113	CLA	CHD-C1D	4.28	1.46	1.38
14	H	1228	CLA	CHC-C1C	4.28	1.47	1.38
14	G	1102	CLA	C3C-C2C	4.28	1.46	1.36
14	G	1116	CLA	CHC-C1C	4.28	1.47	1.38
14	B	1217	CLA	CHD-C1D	4.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1133	CLA	CHD-C1D	4.28	1.46	1.38
14	A	1130	CLA	C3C-C2C	4.28	1.46	1.36
14	G	1132	CLA	CHC-C1C	4.28	1.47	1.38
14	a	1136	CLA	CHC-C1C	4.28	1.47	1.38
14	G	1119	CLA	CHD-C1D	4.28	1.46	1.38
14	G	1128	CLA	C1D-ND	-4.28	1.32	1.37
14	B	1234	CLA	C3C-C2C	4.28	1.46	1.36
14	A	1118	CLA	C3C-C2C	4.28	1.46	1.36
14	G	1133	CLA	CHD-C1D	4.27	1.46	1.38
14	G	1012	CLA	CHC-C1C	4.27	1.47	1.38
14	H	1209	CLA	C3C-C2C	4.27	1.46	1.36
14	b	1226	CLA	C3C-C2C	4.27	1.46	1.36
14	b	1235	CLA	C3C-C2C	4.27	1.46	1.36
14	a	1122	CLA	CHC-C1C	4.27	1.47	1.38
15	A	1121	F6C	CHD-C1D	4.27	1.47	1.38
14	A	1136	CLA	CHC-C1C	4.27	1.47	1.38
14	B	1208	CLA	C3C-C2C	4.27	1.46	1.36
14	G	1110	CLA	C3C-C2C	4.27	1.46	1.36
14	H	1227	CLA	C3C-C2C	4.27	1.46	1.36
14	B	1236	CLA	CHC-C1C	4.27	1.47	1.38
14	H	1236	CLA	CHC-C1C	4.27	1.47	1.38
14	A	1109	CLA	CHC-C1C	4.26	1.47	1.38
14	b	1217	CLA	CHD-C1D	4.26	1.46	1.38
14	b	1208	CLA	C3C-C2C	4.26	1.46	1.36
14	b	1209	CLA	C3C-C2C	4.26	1.46	1.36
14	a	1128	CLA	C1D-ND	-4.26	1.32	1.37
14	a	1118	CLA	C3C-C2C	4.26	1.46	1.36
14	B	1209	CLA	C3C-C2C	4.26	1.46	1.36
14	H	1235	CLA	C3C-C2C	4.26	1.46	1.36
14	a	1130	CLA	C3C-C2C	4.26	1.46	1.36
14	A	1116	CLA	CHC-C1C	4.26	1.47	1.38
14	a	1132	CLA	CHD-C1D	4.26	1.46	1.38
14	A	1135	CLA	CHC-C1C	4.26	1.47	1.38
14	G	1135	CLA	CHC-C1C	4.26	1.47	1.38
20	i	5006	LMG	O8-C28	4.26	1.45	1.33
14	A	1102	CLA	C3C-C2C	4.26	1.46	1.36
14	a	1104	CLA	CHC-C1C	4.26	1.47	1.38
14	B	1227	CLA	C3C-C2C	4.26	1.46	1.36
14	A	1012	CLA	CHC-C1C	4.26	1.47	1.38
14	G	1122	CLA	CHC-C1C	4.26	1.47	1.38
14	G	1127	CLA	CHC-C1C	4.26	1.47	1.38
14	A	1110	CLA	C3C-C2C	4.26	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1231	CLA	CHD-C1D	4.25	1.46	1.38
13	G	1011	CL0	OBD-CAD	4.25	1.27	1.22
14	a	1135	CLA	CHC-C1C	4.25	1.47	1.38
15	B	1230	F6C	CHD-C1D	4.25	1.47	1.38
14	G	1119	CLA	C3C-C2C	4.25	1.45	1.36
14	G	1105	CLA	CHD-C1D	4.25	1.46	1.38
14	B	1212	CLA	C3C-C2C	4.25	1.45	1.36
14	a	1116	CLA	CHC-C1C	4.25	1.47	1.38
14	B	1236	CLA	C3C-C2C	4.25	1.45	1.36
14	B	1210	CLA	CHD-C1D	4.25	1.46	1.38
19	b	5004	LHG	O8-C23	4.25	1.45	1.33
14	H	1232	CLA	CHC-C1C	4.25	1.47	1.38
14	b	1236	CLA	CHC-C1C	4.25	1.47	1.38
18	H	4016	BCR	C10-C9	-4.25	1.26	1.35
14	A	1119	CLA	C3C-C2C	4.24	1.45	1.36
14	G	1111	CLA	O2D-CGD	4.24	1.43	1.33
15	a	1121	F6C	CHC-C4B	4.24	1.47	1.38
14	A	1111	CLA	O2D-CGD	4.24	1.43	1.33
14	b	1210	CLA	CHD-C1D	4.24	1.46	1.38
18	B	4016	BCR	C10-C9	-4.24	1.26	1.35
14	H	1220	CLA	CHC-C1C	4.24	1.47	1.38
14	G	1128	CLA	C1B-NB	-4.24	1.32	1.37
15	G	1121	F6C	CHD-C1D	4.24	1.47	1.38
19	B	5004	LHG	O8-C23	4.24	1.45	1.33
20	I	5006	LMG	O8-C28	4.24	1.45	1.33
14	G	1113	CLA	CHD-C1D	4.24	1.46	1.38
14	B	1022	CLA	O2D-CGD	4.24	1.43	1.33
14	A	1132	CLA	CHD-C1D	4.23	1.46	1.38
14	b	1220	CLA	CHC-C1C	4.23	1.47	1.38
14	a	1119	CLA	C3C-C2C	4.23	1.45	1.36
14	A	1127	CLA	CHC-C1C	4.23	1.47	1.38
14	G	1128	CLA	CHD-C1D	4.23	1.46	1.38
14	a	1119	CLA	CHD-C1D	4.23	1.46	1.38
14	G	1104	CLA	CHC-C1C	4.23	1.47	1.38
14	A	1128	CLA	C1B-NB	-4.23	1.32	1.37
14	G	1129	CLA	C1D-ND	-4.23	1.32	1.37
14	x	1701	CLA	C3C-C2C	4.23	1.45	1.36
14	A	1109	CLA	CHD-C1D	4.23	1.46	1.38
14	H	1239	CLA	CHD-C1D	4.23	1.46	1.38
14	H	1201	CLA	C3C-C2C	4.23	1.45	1.36
14	a	1012	CLA	CHC-C1C	4.23	1.47	1.38
18	b	4016	BCR	C10-C9	-4.23	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1111	CLA	O2D-CGD	4.23	1.43	1.33
14	G	1136	CLA	CHC-C1C	4.23	1.47	1.38
14	a	1109	CLA	CHC-C1C	4.23	1.47	1.38
19	H	5004	LHG	O8-C23	4.23	1.45	1.33
14	B	1231	CLA	CHD-C1D	4.23	1.46	1.38
14	a	1126	CLA	CHD-C1D	4.23	1.46	1.38
14	a	1110	CLA	C3C-C2C	4.23	1.45	1.36
14	A	1122	CLA	CHC-C1C	4.23	1.47	1.38
14	A	1104	CLA	CHC-C1C	4.23	1.47	1.38
14	H	1236	CLA	C3C-C2C	4.23	1.45	1.36
14	b	1232	CLA	CHC-C1C	4.22	1.46	1.38
14	B	1223	CLA	CHC-C1C	4.22	1.46	1.38
15	H	1230	F6C	C4A-NA	-4.22	1.32	1.37
14	a	1105	CLA	CHD-C1D	4.22	1.46	1.38
14	H	1204	CLA	CHC-C1C	4.22	1.46	1.38
14	a	1115	CLA	CHD-C1D	4.22	1.46	1.38
14	G	1105	CLA	C3C-C2C	4.22	1.45	1.36
14	b	1204	CLA	CHC-C1C	4.22	1.46	1.38
14	G	1131	CLA	CHD-C1D	4.22	1.46	1.38
14	a	1131	CLA	CHD-C1D	4.22	1.46	1.38
14	A	1126	CLA	CHD-C1D	4.22	1.46	1.38
14	H	1223	CLA	C3C-C2C	4.22	1.45	1.36
14	B	1225	CLA	CHC-C1C	4.22	1.46	1.38
14	A	1140	CLA	CHC-C1C	4.22	1.46	1.38
14	H	1223	CLA	CHC-C1C	4.22	1.46	1.38
14	G	1126	CLA	CHD-C1D	4.22	1.46	1.38
14	b	1239	CLA	CHD-C1D	4.22	1.46	1.38
14	B	1232	CLA	CHC-C1C	4.21	1.46	1.38
14	H	1012	CLA	O2D-CGD	4.21	1.43	1.33
14	A	1129	CLA	C1D-ND	-4.21	1.32	1.37
14	B	1223	CLA	C3C-C2C	4.21	1.45	1.36
14	b	1236	CLA	C3C-C2C	4.21	1.45	1.36
14	b	1201	CLA	C3C-C2C	4.21	1.45	1.36
14	A	1128	CLA	C1D-ND	-4.21	1.32	1.37
14	G	1118	CLA	CHC-C1C	4.21	1.46	1.38
14	H	1023	CLA	C1C-NC	-4.21	1.31	1.37
14	B	1204	CLA	CHC-C1C	4.21	1.46	1.38
14	A	1105	CLA	CHD-C1D	4.21	1.46	1.38
20	a	5005	LMG	O7-C10	4.21	1.46	1.34
14	a	1140	CLA	CHC-C1C	4.21	1.46	1.38
15	G	1121	F6C	CHC-C4B	4.21	1.46	1.38
14	b	1233	CLA	C3C-C2C	4.21	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	1503	CLA	C3C-C2C	4.21	1.45	1.36
14	b	1212	CLA	C3C-C2C	4.21	1.45	1.36
14	B	1211	CLA	CHD-C1D	4.21	1.46	1.38
14	A	1113	CLA	CHC-C1C	4.21	1.46	1.38
14	B	1239	CLA	CHD-C1D	4.20	1.46	1.38
14	b	1211	CLA	CHD-C1D	4.20	1.46	1.38
14	B	1201	CLA	C3C-C2C	4.20	1.45	1.36
14	G	1111	CLA	CHD-C1D	4.20	1.46	1.38
14	B	1235	CLA	C3C-C2C	4.20	1.45	1.36
20	H	5002	LMG	O8-C28	4.20	1.45	1.33
14	H	1232	CLA	C3C-C2C	4.20	1.45	1.36
14	a	1111	CLA	CHD-C1D	4.20	1.46	1.38
14	B	1214	CLA	CHC-C1C	4.20	1.46	1.38
14	b	1223	CLA	CHC-C1C	4.20	1.46	1.38
14	a	1116	CLA	CHD-C1D	4.20	1.46	1.38
14	H	1214	CLA	CHC-C1C	4.20	1.46	1.38
14	a	1113	CLA	CHC-C1C	4.20	1.46	1.38
14	b	1235	CLA	CHD-C1D	4.20	1.46	1.38
14	A	1131	CLA	CHD-C1D	4.20	1.46	1.38
14	A	1111	CLA	CHC-C1C	4.20	1.46	1.38
14	a	1105	CLA	C3C-C2C	4.20	1.45	1.36
14	b	1223	CLA	C3C-C2C	4.20	1.45	1.36
14	G	1125	CLA	CHC-C1C	4.20	1.46	1.38
14	A	1133	CLA	C3C-C2C	4.20	1.45	1.36
14	G	1133	CLA	C3C-C2C	4.20	1.45	1.36
14	a	1106	CLA	C3C-C2C	4.20	1.45	1.36
14	X	1701	CLA	C3C-C2C	4.19	1.45	1.36
14	G	1135	CLA	C3C-C2C	4.19	1.45	1.36
14	H	1235	CLA	CHD-C1D	4.19	1.46	1.38
14	H	1219	CLA	CHD-C1D	4.19	1.46	1.38
14	H	1238	CLA	C1D-ND	-4.19	1.32	1.37
14	B	1233	CLA	C3C-C2C	4.19	1.45	1.36
14	G	1109	CLA	CHD-C1D	4.19	1.46	1.38
14	H	1212	CLA	C3C-C2C	4.19	1.45	1.36
14	A	1118	CLA	CHC-C1C	4.19	1.46	1.38
14	U	1502	CLA	C3C-C2C	4.19	1.45	1.36
14	B	1225	CLA	C1B-NB	-4.19	1.32	1.37
14	l	1502	CLA	C3C-C2C	4.19	1.45	1.36
14	a	1138	CLA	C3C-C2C	4.19	1.45	1.36
14	b	1022	CLA	O2D-CGD	4.19	1.43	1.33
14	G	1138	CLA	C3C-C2C	4.19	1.45	1.36
14	H	1225	CLA	CHC-C1C	4.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1214	CLA	CHC-C1C	4.18	1.46	1.38
20	G	5005	LMG	O7-C10	4.18	1.46	1.34
20	B	5002	LMG	O8-C28	4.18	1.45	1.33
14	G	1136	CLA	O2D-CGD	4.18	1.43	1.33
14	A	1105	CLA	C3C-C2C	4.18	1.45	1.36
14	B	1235	CLA	CHD-C1D	4.18	1.46	1.38
20	b	5002	LMG	O8-C28	4.18	1.45	1.33
14	G	1133	CLA	CHC-C1C	4.18	1.46	1.38
14	B	1208	CLA	CHC-C1C	4.18	1.46	1.38
15	A	1121	F6C	CHC-C4B	4.18	1.46	1.38
14	W	1701	CLA	C3C-C2C	4.18	1.45	1.36
14	G	1115	CLA	CHD-C1D	4.18	1.46	1.38
14	B	1224	CLA	C1D-ND	-4.18	1.32	1.37
14	B	1220	CLA	CHC-C1C	4.18	1.46	1.38
14	H	1233	CLA	C3C-C2C	4.18	1.45	1.36
14	U	1503	CLA	C3C-C2C	4.18	1.45	1.36
14	G	1111	CLA	CHC-C1C	4.18	1.46	1.38
14	B	1023	CLA	C1C-NC	-4.18	1.31	1.37
14	T	1401	CLA	C3D-C4D	-4.18	1.34	1.44
14	A	1138	CLA	C3C-C2C	4.18	1.45	1.36
14	L	1502	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1225	CLA	CHC-C1C	4.18	1.46	1.38
14	A	1128	CLA	CHD-C1D	4.18	1.46	1.38
14	A	1135	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1232	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1202	CLA	CHC-C1C	4.18	1.46	1.38
20	A	5005	LMG	O7-C10	4.18	1.46	1.34
14	G	1140	CLA	CHC-C1C	4.18	1.46	1.38
14	a	1125	CLA	CHC-C1C	4.18	1.46	1.38
14	B	1232	CLA	C3C-C2C	4.18	1.45	1.36
14	a	1133	CLA	C3C-C2C	4.18	1.45	1.36
14	a	1136	CLA	O2D-CGD	4.18	1.43	1.33
14	U	1503	CLA	CHC-C1C	4.18	1.46	1.38
14	A	1136	CLA	O2D-CGD	4.18	1.43	1.33
14	A	1115	CLA	CHD-C1D	4.17	1.46	1.38
14	G	1116	CLA	CHD-C1D	4.17	1.46	1.38
14	A	1112	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1116	CLA	CHD-C1D	4.17	1.46	1.38
14	K	1401	CLA	C3D-C4D	-4.17	1.34	1.44
14	a	1112	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1107	CLA	CHC-C1C	4.17	1.46	1.38
14	G	1106	CLA	C3C-C2C	4.17	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1131	CLA	C3C-C2C	4.17	1.45	1.36
14	B	1219	CLA	CHD-C1D	4.17	1.46	1.38
14	G	1131	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1125	CLA	CHC-C1C	4.17	1.46	1.38
14	b	1219	CLA	CHD-C1D	4.17	1.46	1.38
14	b	1208	CLA	CHC-C1C	4.16	1.46	1.38
14	a	1109	CLA	CHD-C1D	4.16	1.46	1.38
14	b	1224	CLA	C1D-ND	-4.16	1.32	1.37
14	H	1211	CLA	CHD-C1D	4.16	1.46	1.38
14	H	1238	CLA	C3C-C2C	4.16	1.45	1.36
14	B	1238	CLA	C1D-ND	-4.16	1.32	1.37
14	G	1137	CLA	C3C-C2C	4.16	1.45	1.36
14	a	1135	CLA	C3C-C2C	4.16	1.45	1.36
14	b	1238	CLA	C1D-ND	-4.16	1.32	1.37
14	L	1503	CLA	CHC-C1C	4.16	1.46	1.38
14	b	1023	CLA	C1C-NC	-4.16	1.31	1.37
14	a	1137	CLA	C3C-C2C	4.16	1.45	1.36
14	G	1113	CLA	CHC-C1C	4.16	1.46	1.38
14	H	1208	CLA	CHC-C1C	4.16	1.46	1.38
14	k	1401	CLA	C3D-C4D	-4.16	1.34	1.44
14	L	1503	CLA	C3C-C2C	4.16	1.45	1.36
20	L	5007	LMG	O7-C10	4.16	1.46	1.34
18	R	4018	BCR	C11-C12	-4.16	1.23	1.34
14	G	1127	CLA	C1D-ND	-4.15	1.32	1.37
14	b	1211	CLA	C3C-C2C	4.15	1.45	1.36
20	l	5007	LMG	O7-C10	4.15	1.46	1.34
14	b	1238	CLA	C3C-C2C	4.15	1.45	1.36
14	b	1225	CLA	C1B-NB	-4.15	1.32	1.37
14	a	1128	CLA	CHD-C1D	4.15	1.46	1.38
14	H	1210	CLA	CHC-C1C	4.15	1.46	1.38
20	U	5007	LMG	O7-C10	4.15	1.46	1.34
14	l	1503	CLA	CHC-C1C	4.15	1.46	1.38
14	a	1111	CLA	CHC-C1C	4.15	1.46	1.38
14	a	1131	CLA	C3C-C2C	4.15	1.45	1.36
14	G	1140	CLA	C3C-C2C	4.15	1.45	1.36
14	H	1217	CLA	C3C-C2C	4.15	1.45	1.36
14	A	1111	CLA	CHD-C1D	4.14	1.46	1.38
14	b	1228	CLA	CHD-C1D	4.14	1.46	1.38
14	G	1113	CLA	C3C-C2C	4.14	1.45	1.36
14	G	1122	CLA	CHD-C1D	4.14	1.46	1.38
14	a	1133	CLA	CHC-C1C	4.14	1.46	1.38
14	G	1109	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	1131	CLA	CHC-C1C	4.14	1.46	1.38
14	A	1137	CLA	C3C-C2C	4.14	1.45	1.36
14	A	1133	CLA	CHC-C1C	4.14	1.46	1.38
14	B	1228	CLA	CHD-C1D	4.14	1.46	1.38
14	H	1211	CLA	C3C-C2C	4.14	1.45	1.36
14	A	1113	CLA	C3C-C2C	4.14	1.45	1.36
14	B	1238	CLA	C3C-C2C	4.14	1.45	1.36
18	I	4018	BCR	C11-C12	-4.14	1.23	1.34
14	H	1202	CLA	CHC-C1C	4.14	1.46	1.38
14	H	1218	CLA	C3C-C2C	4.14	1.45	1.36
14	A	1106	CLA	C3C-C2C	4.14	1.45	1.36
14	B	1022	CLA	C3C-C2C	4.14	1.45	1.36
14	a	1127	CLA	C1D-ND	-4.14	1.32	1.37
14	a	1118	CLA	CHC-C1C	4.13	1.46	1.38
14	L	1503	CLA	CHD-C1D	4.13	1.46	1.38
18	i	4018	BCR	C11-C12	-4.13	1.23	1.34
14	H	1228	CLA	CHD-C1D	4.13	1.46	1.38
14	B	1215	CLA	CHC-C1C	4.13	1.46	1.38
14	B	1202	CLA	CHC-C1C	4.13	1.46	1.38
14	G	1107	CLA	CHC-C1C	4.13	1.46	1.38
14	G	1112	CLA	C3C-C2C	4.13	1.45	1.36
14	l	1503	CLA	CHD-C1D	4.13	1.46	1.38
14	H	1213	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1123	CLA	C3C-C2C	4.13	1.45	1.36
14	b	1231	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1109	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1115	CLA	C3C-C2C	4.13	1.45	1.36
14	H	1012	CLA	C3C-C2C	4.13	1.45	1.36
14	b	1201	CLA	CHD-C1D	4.13	1.46	1.38
14	b	1215	CLA	CHC-C1C	4.13	1.46	1.38
14	B	1211	CLA	C3C-C2C	4.13	1.45	1.36
14	B	1217	CLA	C3C-C2C	4.13	1.45	1.36
14	a	1113	CLA	C3C-C2C	4.13	1.45	1.36
14	b	1217	CLA	C3C-C2C	4.12	1.45	1.36
14	B	1201	CLA	CHD-C1D	4.12	1.46	1.38
14	B	1218	CLA	C3C-C2C	4.12	1.45	1.36
14	B	1213	CLA	C3C-C2C	4.12	1.45	1.36
14	A	1127	CLA	C1D-ND	-4.12	1.32	1.37
14	B	1231	CLA	C3C-C2C	4.12	1.45	1.36
14	U	1503	CLA	CHD-C1D	4.12	1.46	1.38
14	H	1215	CLA	CHC-C1C	4.12	1.46	1.38
14	b	1216	CLA	CHC-C1C	4.12	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1218	CLA	CHD-C1D	4.12	1.46	1.38
14	A	1127	CLA	C3C-C2C	4.11	1.45	1.36
14	B	1210	CLA	CHC-C1C	4.11	1.46	1.38
14	A	1122	CLA	CHD-C1D	4.11	1.46	1.38
14	b	1213	CLA	C3C-C2C	4.11	1.45	1.36
14	a	1122	CLA	CHD-C1D	4.11	1.46	1.38
14	b	1022	CLA	C3C-C2C	4.11	1.45	1.36
14	b	1210	CLA	CHC-C1C	4.11	1.46	1.38
14	H	1231	CLA	C3C-C2C	4.11	1.45	1.36
14	H	1012	CLA	C1D-ND	-4.11	1.32	1.37
14	b	1204	CLA	C3C-C2C	4.11	1.45	1.36
14	G	1130	CLA	CHD-C1D	4.11	1.46	1.38
14	B	1216	CLA	CHC-C1C	4.11	1.46	1.38
15	B	1230	F6C	C4A-NA	-4.10	1.32	1.37
14	a	1109	CLA	C3C-C2C	4.10	1.45	1.36
14	A	1123	CLA	CHD-C1D	4.10	1.46	1.38
15	b	1230	F6C	C4A-NA	-4.10	1.32	1.37
18	H	4012	BCR	C10-C9	-4.10	1.26	1.35
14	a	1140	CLA	C3C-C2C	4.10	1.45	1.36
14	H	1201	CLA	CHD-C1D	4.10	1.46	1.38
14	a	1107	CLA	CHC-C1C	4.10	1.46	1.38
14	b	1218	CLA	C3C-C2C	4.10	1.45	1.36
14	b	1206	CLA	C1D-ND	-4.10	1.32	1.37
14	A	1130	CLA	CHD-C1D	4.10	1.46	1.38
14	H	1225	CLA	C1B-NB	-4.10	1.32	1.37
14	G	1123	CLA	C3C-C2C	4.10	1.45	1.36
14	A	1103	CLA	CHC-C1C	4.10	1.46	1.38
14	a	1115	CLA	C3C-C2C	4.10	1.45	1.36
18	B	4012	BCR	C10-C9	-4.10	1.26	1.35
14	a	1101	CLA	CHD-C1D	4.10	1.46	1.38
14	G	1115	CLA	C3C-C2C	4.10	1.45	1.36
14	a	1130	CLA	CHD-C1D	4.10	1.46	1.38
14	H	1224	CLA	C1D-ND	-4.10	1.32	1.37
14	A	1101	CLA	CHD-C1D	4.09	1.46	1.38
14	B	1022	CLA	C1D-ND	-4.09	1.32	1.37
14	A	1140	CLA	C3C-C2C	4.09	1.45	1.36
14	A	1107	CLA	CHD-C1D	4.09	1.46	1.38
14	B	1206	CLA	C1D-ND	-4.09	1.32	1.37
14	G	1131	CLA	CHC-C1C	4.09	1.46	1.38
14	G	1125	CLA	C3C-C2C	4.09	1.45	1.36
14	b	1022	CLA	C1D-ND	-4.09	1.32	1.37
14	a	1127	CLA	C3C-C2C	4.09	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1131	CLA	CHC-C1C	4.09	1.46	1.38
14	B	1215	CLA	CHD-C1D	4.08	1.46	1.38
14	H	1216	CLA	CHC-C1C	4.08	1.46	1.38
14	H	1204	CLA	C3C-C2C	4.08	1.45	1.36
16	G	2001	PQN	C10-C5	4.08	1.47	1.40
14	G	1123	CLA	CHD-C1D	4.08	1.46	1.38
20	i	5006	LMG	O7-C10	4.08	1.45	1.34
14	G	1127	CLA	C3C-C2C	4.08	1.45	1.36
14	B	1202	CLA	C3C-C2C	4.08	1.45	1.36
14	b	1023	CLA	C3C-C2C	4.08	1.45	1.36
14	G	1107	CLA	CHD-C1D	4.08	1.46	1.38
14	A	1012	CLA	CHD-C1D	4.08	1.46	1.38
14	A	1104	CLA	C3C-C2C	4.07	1.45	1.36
14	H	1218	CLA	CHD-C1D	4.07	1.46	1.38
14	b	1207	CLA	CHD-C1D	4.07	1.46	1.38
14	L	1502	CLA	CHC-C1C	4.07	1.46	1.38
18	b	4012	BCR	C10-C9	-4.07	1.26	1.35
14	b	1215	CLA	CHD-C1D	4.07	1.46	1.38
14	a	1012	CLA	C3C-C2C	4.07	1.45	1.36
14	H	1207	CLA	CHD-C1D	4.07	1.46	1.38
14	A	1012	CLA	C3C-C2C	4.07	1.45	1.36
14	B	1207	CLA	CHD-C1D	4.07	1.46	1.38
14	a	1125	CLA	C3C-C2C	4.07	1.45	1.36
14	a	1107	CLA	CHD-C1D	4.07	1.46	1.38
20	I	5006	LMG	O7-C10	4.07	1.45	1.34
14	b	1218	CLA	CHD-C1D	4.06	1.46	1.38
14	G	1129	CLA	C3C-C2C	4.06	1.45	1.36
14	b	1215	CLA	C3C-C2C	4.06	1.45	1.36
14	A	1135	CLA	CHD-C1D	4.06	1.46	1.38
20	R	5006	LMG	O7-C10	4.06	1.45	1.34
14	G	1012	CLA	C3C-C2C	4.06	1.45	1.36
14	G	1012	CLA	CHD-C1D	4.06	1.46	1.38
14	a	1012	CLA	CHD-C1D	4.06	1.46	1.38
14	H	1202	CLA	C3C-C2C	4.06	1.45	1.36
14	a	1123	CLA	C3C-C2C	4.06	1.45	1.36
14	a	1124	CLA	CHD-C1D	4.05	1.46	1.38
14	b	1202	CLA	C3C-C2C	4.05	1.45	1.36
14	H	1215	CLA	CHD-C1D	4.05	1.46	1.38
14	A	1129	CLA	C3C-C2C	4.05	1.45	1.36
14	H	1023	CLA	C3C-C2C	4.05	1.45	1.36
14	b	1220	CLA	CHD-C1D	4.05	1.46	1.38
14	G	1124	CLA	CHD-C1D	4.05	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1117	CLA	C3C-C2C	4.05	1.45	1.36
14	a	1123	CLA	CHD-C1D	4.05	1.46	1.38
14	B	1023	CLA	C3C-C2C	4.05	1.45	1.36
14	a	1114	CLA	CHD-C4C	4.05	1.48	1.39
14	a	1104	CLA	C3C-C2C	4.05	1.45	1.36
14	G	1103	CLA	CHC-C1C	4.05	1.46	1.38
14	A	1101	CLA	C3C-C2C	4.05	1.45	1.36
14	G	1101	CLA	CHD-C1D	4.05	1.46	1.38
14	a	1103	CLA	CHC-C1C	4.05	1.46	1.38
14	A	1136	CLA	C3C-C2C	4.05	1.45	1.36
14	A	1124	CLA	CHD-C1D	4.04	1.46	1.38
14	B	1205	CLA	C3C-C2C	4.04	1.45	1.36
14	A	1114	CLA	CHD-C4C	4.04	1.48	1.39
14	a	1107	CLA	C3C-C2C	4.04	1.45	1.36
14	B	1215	CLA	C3C-C2C	4.04	1.45	1.36
14	H	1215	CLA	C3C-C2C	4.04	1.45	1.36
16	A	2001	PQN	C10-C5	4.04	1.47	1.40
14	a	1129	CLA	C3C-C2C	4.04	1.45	1.36
14	G	1136	CLA	C3C-C2C	4.03	1.45	1.36
14	G	1135	CLA	CHD-C1D	4.03	1.46	1.38
14	B	1228	CLA	CHD-C4C	4.03	1.48	1.39
14	A	1117	CLA	CHD-C4C	4.03	1.48	1.39
14	B	1204	CLA	C3C-C2C	4.03	1.45	1.36
14	H	1205	CLA	C3C-C2C	4.03	1.45	1.36
16	a	2001	PQN	C10-C5	4.03	1.47	1.40
14	B	1220	CLA	CHD-C1D	4.03	1.46	1.38
14	H	1225	CLA	C3C-C2C	4.03	1.45	1.36
14	U	1502	CLA	CHC-C1C	4.03	1.46	1.38
14	U	1502	CLA	C1D-ND	-4.03	1.32	1.37
14	G	1114	CLA	CHD-C4C	4.03	1.48	1.39
14	a	1136	CLA	C3C-C2C	4.03	1.45	1.36
14	H	1206	CLA	C1D-ND	-4.03	1.32	1.37
14	G	1101	CLA	C3C-C2C	4.02	1.45	1.36
13	a	1011	CL0	CHD-C4C	4.02	1.47	1.39
14	H	1224	CLA	C3C-C2C	4.02	1.45	1.36
14	b	1228	CLA	CHD-C4C	4.02	1.48	1.39
14	G	1104	CLA	C3C-C2C	4.02	1.45	1.36
14	A	1125	CLA	C3C-C2C	4.02	1.45	1.36
14	B	1220	CLA	C3C-C2C	4.02	1.45	1.36
14	B	1023	CLA	CHC-C1C	4.02	1.46	1.38
14	B	1224	CLA	C3C-C2C	4.02	1.45	1.36
14	G	1013	CLA	C3C-C2C	4.02	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1107	CLA	C3C-C2C	4.02	1.45	1.36
14	H	1021	CLA	CHC-C1C	4.02	1.46	1.38
14	a	1013	CLA	C3C-C2C	4.02	1.45	1.36
14	G	1117	CLA	CHD-C4C	4.02	1.48	1.39
14	H	1228	CLA	CHD-C4C	4.01	1.48	1.39
14	a	1117	CLA	CHD-C4C	4.01	1.48	1.39
14	G	1117	CLA	C3C-C2C	4.01	1.45	1.36
14	B	1225	CLA	C3C-C2C	4.01	1.45	1.36
14	A	1140	CLA	CHD-C1D	4.01	1.46	1.38
14	G	1107	CLA	C3C-C2C	4.01	1.45	1.36
14	A	1137	CLA	CHC-C1C	4.01	1.46	1.38
14	A	1013	CLA	C3C-C2C	4.01	1.45	1.36
14	l	1502	CLA	C1D-ND	-4.01	1.32	1.37
14	b	1205	CLA	C3C-C2C	4.01	1.45	1.36
14	b	1224	CLA	C3C-C2C	4.01	1.45	1.36
14	H	1220	CLA	C3C-C2C	4.01	1.45	1.36
14	l	1502	CLA	CHC-C1C	4.01	1.46	1.38
14	a	1101	CLA	C3C-C2C	4.01	1.45	1.36
14	L	1502	CLA	C1D-ND	-4.01	1.32	1.37
14	a	1135	CLA	CHD-C1D	4.00	1.46	1.38
14	A	1117	CLA	C3C-C2C	4.00	1.45	1.36
14	H	1023	CLA	CHC-C1C	4.00	1.46	1.38
13	G	1011	CL0	CHD-C4C	4.00	1.47	1.39
14	B	1021	CLA	CHC-C1C	4.00	1.46	1.38
14	B	1234	CLA	O2D-CGD	4.00	1.43	1.33
14	H	1220	CLA	CHD-C1D	4.00	1.46	1.38
15	b	1237	F6C	C3D-C4D	-4.00	1.33	1.44
14	b	1023	CLA	CHC-C1C	4.00	1.46	1.38
14	a	1137	CLA	CHC-C1C	4.00	1.46	1.38
14	A	1139	CLA	CHD-C1D	4.00	1.46	1.38
14	A	1116	CLA	C3C-C2C	4.00	1.45	1.36
14	H	1234	CLA	O2D-CGD	4.00	1.43	1.33
14	G	1129	CLA	CHD-C1D	3.99	1.46	1.38
14	b	1220	CLA	C3C-C2C	3.99	1.45	1.36
15	H	1237	F6C	C3D-C4D	-3.99	1.33	1.44
14	G	1137	CLA	CHC-C1C	3.99	1.46	1.38
14	b	1234	CLA	O2D-CGD	3.99	1.43	1.33
14	G	1139	CLA	CHD-C1D	3.99	1.46	1.38
14	b	1225	CLA	C3C-C2C	3.99	1.45	1.36
18	G	4008	BCR	C11-C12	-3.98	1.24	1.34
18	A	4008	BCR	C11-C12	-3.98	1.24	1.34
14	G	1116	CLA	C3C-C2C	3.98	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1204	CLA	CHD-C4C	3.98	1.48	1.39
14	b	1021	CLA	CHC-C1C	3.98	1.46	1.38
13	A	1011	CL0	CHD-C4C	3.98	1.47	1.39
15	B	1237	F6C	C3D-C4D	-3.98	1.33	1.44
14	a	1129	CLA	CHD-C1D	3.98	1.46	1.38
18	a	4008	BCR	C11-C12	-3.98	1.24	1.34
14	a	1127	CLA	CHD-C1D	3.98	1.46	1.38
14	B	1221	CLA	CHD-C1D	3.97	1.46	1.38
14	A	1012	CLA	O2D-CGD	3.97	1.43	1.33
14	b	1222	CLA	C1D-ND	-3.97	1.32	1.37
15	H	1237	F6C	C1C-NC	-3.97	1.32	1.37
14	G	1140	CLA	CHD-C1D	3.97	1.46	1.38
14	a	1116	CLA	C3C-C2C	3.97	1.45	1.36
14	G	1110	CLA	CHD-C1D	3.97	1.46	1.38
14	H	1204	CLA	CHD-C4C	3.97	1.48	1.39
14	B	1204	CLA	CHD-C4C	3.97	1.48	1.39
14	a	1110	CLA	CHD-C1D	3.97	1.46	1.38
14	A	1137	CLA	CHD-C1D	3.97	1.46	1.38
14	A	1126	CLA	C1D-ND	-3.96	1.32	1.37
14	B	1222	CLA	C1D-ND	-3.96	1.32	1.37
14	A	1110	CLA	CHD-C1D	3.96	1.46	1.38
14	W	1701	CLA	CHD-C1D	3.96	1.46	1.38
19	a	5001	LHG	O7-C7	3.96	1.45	1.34
14	X	1701	CLA	CHD-C1D	3.96	1.46	1.38
14	H	1206	CLA	CHC-C1C	3.96	1.46	1.38
14	a	1103	CLA	CHD-C1D	3.96	1.46	1.38
19	b	5004	LHG	O7-C7	3.96	1.45	1.34
14	B	1206	CLA	C3C-C2C	3.96	1.45	1.36
14	a	1137	CLA	CHD-C1D	3.96	1.46	1.38
19	H	5004	LHG	O7-C7	3.96	1.45	1.34
14	G	1127	CLA	CHD-C1D	3.96	1.46	1.38
15	B	1237	F6C	C1C-NC	-3.95	1.32	1.37
14	x	1701	CLA	CHD-C1D	3.95	1.46	1.38
14	a	1126	CLA	C1D-ND	-3.95	1.32	1.37
14	G	1137	CLA	CHD-C1D	3.95	1.46	1.38
14	a	1140	CLA	CHD-C1D	3.95	1.46	1.38
14	A	1129	CLA	CHD-C1D	3.95	1.46	1.38
14	b	1226	CLA	CHC-C1C	3.95	1.46	1.38
14	a	1139	CLA	CHD-C1D	3.95	1.46	1.38
14	B	1236	CLA	C1D-ND	-3.94	1.32	1.37
14	a	1012	CLA	O2D-CGD	3.94	1.42	1.33
19	A	5001	LHG	O7-C7	3.94	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1202	CLA	C1D-ND	-3.94	1.32	1.37
14	b	1202	CLA	C1D-ND	-3.94	1.32	1.37
14	a	1128	CLA	CHC-C1C	3.94	1.46	1.38
14	b	1206	CLA	CHD-C1D	3.94	1.46	1.38
14	b	1231	CLA	CHC-C4B	3.94	1.48	1.39
13	a	1011	CL0	C3D-C2D	3.93	1.46	1.39
14	b	1206	CLA	C3C-C2C	3.93	1.45	1.36
14	H	1231	CLA	CHC-C4B	3.93	1.48	1.39
14	H	1222	CLA	C1D-ND	-3.93	1.32	1.37
14	G	1012	CLA	O2D-CGD	3.93	1.42	1.33
19	G	5001	LHG	O7-C7	3.93	1.45	1.34
14	H	1221	CLA	CHD-C1D	3.93	1.46	1.38
13	A	1011	CL0	C3D-C2D	3.93	1.46	1.39
14	G	1128	CLA	CHC-C1C	3.93	1.46	1.38
14	b	1206	CLA	CHC-C1C	3.92	1.46	1.38
14	A	1127	CLA	CHD-C1D	3.92	1.46	1.38
14	G	1103	CLA	CHD-C1D	3.92	1.46	1.38
14	a	1105	CLA	CHD-C4C	3.92	1.48	1.39
14	H	1206	CLA	CHD-C1D	3.92	1.46	1.38
14	b	1221	CLA	CHD-C1D	3.92	1.46	1.38
14	b	1222	CLA	CHD-C1D	3.92	1.46	1.38
19	B	5004	LHG	O7-C7	3.92	1.45	1.34
14	A	1013	CLA	CHC-C4B	3.92	1.48	1.39
14	B	1226	CLA	CHC-C1C	3.92	1.46	1.38
15	a	1121	F6C	C3D-C4D	-3.92	1.33	1.44
14	H	1206	CLA	C3C-C2C	3.92	1.45	1.36
14	H	1204	CLA	CHD-C1D	3.92	1.46	1.38
14	H	1223	CLA	CHD-C1D	3.91	1.46	1.38
14	H	1214	CLA	CHD-C4C	3.91	1.48	1.39
14	A	1103	CLA	CHD-C1D	3.91	1.46	1.38
15	b	1237	F6C	C1C-NC	-3.91	1.32	1.37
14	b	1221	CLA	C3C-C2C	3.91	1.45	1.36
14	H	1226	CLA	CHC-C1C	3.91	1.46	1.38
14	B	1223	CLA	CHD-C1D	3.91	1.46	1.38
14	A	1105	CLA	CHD-C4C	3.91	1.48	1.39
14	B	1222	CLA	CHD-C1D	3.91	1.46	1.38
15	A	1121	F6C	C3D-C4D	-3.91	1.33	1.44
14	B	1204	CLA	CHD-C1D	3.91	1.46	1.38
14	a	1013	CLA	CHC-C4B	3.90	1.48	1.39
14	B	1215	CLA	C1D-ND	-3.90	1.32	1.37
14	H	1236	CLA	C1D-ND	-3.90	1.32	1.37
14	G	1140	CLA	CHC-C4B	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1011	CL0	C3D-C2D	3.90	1.46	1.39
14	L	1501	CLA	CHD-C1D	3.90	1.46	1.38
14	A	1128	CLA	CHC-C1C	3.90	1.46	1.38
14	G	1107	CLA	C1D-ND	-3.90	1.32	1.37
14	B	1206	CLA	CHC-C1C	3.90	1.46	1.38
14	H	1202	CLA	C1D-ND	-3.90	1.32	1.37
14	B	1206	CLA	CHD-C1D	3.90	1.46	1.38
14	B	1214	CLA	CHD-C4C	3.90	1.48	1.39
14	B	1221	CLA	C3C-C2C	3.90	1.45	1.36
14	H	1212	CLA	CHD-C1D	3.89	1.46	1.38
14	B	1231	CLA	CHC-C4B	3.89	1.48	1.39
14	H	1221	CLA	C3C-C2C	3.89	1.45	1.36
14	B	1212	CLA	CHD-C1D	3.89	1.46	1.38
15	G	1121	F6C	C3D-C4D	-3.89	1.33	1.44
14	A	1139	CLA	C3C-C2C	3.89	1.45	1.36
14	a	1107	CLA	C1D-ND	-3.89	1.32	1.37
14	A	1140	CLA	CHC-C4B	3.89	1.48	1.39
15	b	1230	F6C	CHC-C1C	3.89	1.48	1.39
14	A	1131	CLA	C1D-ND	-3.89	1.32	1.37
14	G	1126	CLA	C1D-ND	-3.89	1.32	1.37
14	G	1013	CLA	CHC-C4B	3.89	1.48	1.39
15	B	1230	F6C	CHC-C1C	3.88	1.48	1.39
14	U	1501	CLA	CHD-C1D	3.88	1.46	1.38
14	A	1139	CLA	CHC-C4B	3.88	1.48	1.39
13	G	1011	CL0	CHD-C1D	3.88	1.45	1.39
14	G	1125	CLA	C1C-NC	-3.88	1.31	1.37
14	H	1216	CLA	CHD-C4C	3.88	1.48	1.39
14	B	1232	CLA	CHD-C4C	3.88	1.48	1.39
14	a	1140	CLA	CHC-C4B	3.88	1.48	1.39
14	b	1236	CLA	C1D-ND	-3.88	1.32	1.37
14	B	1216	CLA	CHD-C4C	3.88	1.48	1.39
14	b	1214	CLA	CHD-C4C	3.88	1.48	1.39
14	G	1139	CLA	C3C-C2C	3.88	1.45	1.36
14	A	1125	CLA	C1C-NC	-3.88	1.31	1.37
14	A	1107	CLA	C1D-ND	-3.88	1.32	1.37
14	b	1234	CLA	C1D-ND	-3.88	1.32	1.37
14	H	1222	CLA	CHD-C1D	3.87	1.46	1.38
14	G	1111	CLA	C3C-C2C	3.87	1.45	1.36
14	A	1117	CLA	C1D-ND	-3.87	1.32	1.37
14	G	1138	CLA	CHD-C4C	3.87	1.48	1.39
14	G	1139	CLA	CHC-C4B	3.87	1.48	1.39
14	B	1234	CLA	C1D-ND	-3.87	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1106	CLA	CHD-C1D	3.87	1.46	1.38
14	U	1501	CLA	C1D-ND	-3.86	1.32	1.37
14	G	1105	CLA	CHD-C4C	3.86	1.48	1.39
14	a	1102	CLA	CHD-C4C	3.86	1.48	1.39
14	A	1111	CLA	C3C-C2C	3.86	1.45	1.36
14	a	1139	CLA	C3C-C2C	3.86	1.45	1.36
14	G	1109	CLA	CHD-C4C	3.86	1.48	1.39
14	b	1223	CLA	CHD-C1D	3.86	1.45	1.38
14	b	1216	CLA	CHD-C4C	3.86	1.48	1.39
14	A	1136	CLA	CHD-C1D	3.86	1.45	1.38
14	H	1226	CLA	CHD-C4C	3.86	1.48	1.39
14	B	1236	CLA	CHC-C4B	3.86	1.48	1.39
14	H	1234	CLA	C1D-ND	-3.85	1.32	1.37
14	H	1229	CLA	CHD-C4C	3.85	1.48	1.39
14	a	1125	CLA	C1C-NC	-3.85	1.31	1.37
13	A	1011	CL0	CHD-C1D	3.85	1.45	1.39
14	b	1204	CLA	CHD-C1D	3.85	1.45	1.38
13	a	1011	CL0	CHD-C1D	3.85	1.45	1.39
14	B	1227	CLA	CHD-C4C	3.85	1.48	1.39
14	A	1106	CLA	CHD-C1D	3.85	1.45	1.38
14	G	1117	CLA	C1D-ND	-3.85	1.32	1.37
14	B	1226	CLA	CHD-C4C	3.85	1.48	1.39
15	b	1230	F6C	CHB-C1B	3.85	1.48	1.39
14	l	1501	CLA	CHD-C1D	3.85	1.45	1.38
14	a	1109	CLA	CHD-C4C	3.85	1.48	1.39
14	b	1215	CLA	C1D-ND	-3.85	1.32	1.37
14	b	1215	CLA	C1B-NB	-3.85	1.32	1.37
15	H	1230	F6C	CHC-C1C	3.85	1.48	1.39
14	H	1236	CLA	CHC-C4B	3.84	1.48	1.39
14	H	1232	CLA	CHD-C4C	3.84	1.48	1.39
14	A	1109	CLA	CHD-C4C	3.84	1.47	1.39
14	A	1137	CLA	C1D-ND	-3.84	1.32	1.37
14	b	1212	CLA	CHD-C1D	3.84	1.45	1.38
14	b	1236	CLA	CHC-C4B	3.84	1.48	1.39
13	a	1011	CL0	CHC-C4B	3.84	1.45	1.39
14	G	1106	CLA	CHD-C1D	3.84	1.45	1.38
14	G	1136	CLA	CHD-C1D	3.84	1.45	1.38
14	T	1401	CLA	CHD-C4C	3.84	1.47	1.39
14	B	1215	CLA	C1B-NB	-3.84	1.32	1.37
14	B	1236	CLA	CHD-C1D	3.84	1.45	1.38
14	b	1226	CLA	CHD-C4C	3.84	1.47	1.39
14	L	1501	CLA	C1D-ND	-3.84	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1111	CLA	C3C-C2C	3.84	1.45	1.36
14	a	1122	CLA	C3C-C2C	3.84	1.45	1.36
13	A	1011	CL0	CHC-C4B	3.84	1.45	1.39
14	B	1205	CLA	C1B-NB	-3.84	1.32	1.37
14	l	1501	CLA	C1D-ND	-3.83	1.32	1.37
14	b	1229	CLA	CHD-C4C	3.83	1.47	1.39
14	b	1202	CLA	CHD-C1D	3.83	1.45	1.38
14	G	1122	CLA	C3C-C2C	3.83	1.45	1.36
15	H	1230	F6C	CHB-C1B	3.83	1.47	1.39
14	G	1102	CLA	CHD-C4C	3.83	1.47	1.39
14	A	1128	CLA	MG-ND	-3.83	1.98	2.05
14	k	1401	CLA	CHD-C4C	3.83	1.47	1.39
15	B	1230	F6C	CHB-C1B	3.83	1.47	1.39
14	H	1215	CLA	C1D-ND	-3.83	1.32	1.37
14	H	1238	CLA	C1B-NB	-3.83	1.32	1.37
14	H	1202	CLA	CHD-C1D	3.83	1.45	1.38
14	a	1139	CLA	CHC-C4B	3.83	1.48	1.39
13	G	1011	CL0	CHC-C4B	3.83	1.45	1.39
14	H	1227	CLA	CHD-C4C	3.83	1.47	1.39
15	H	1230	F6C	C3D-C4D	-3.83	1.34	1.44
14	A	1138	CLA	CHD-C4C	3.83	1.47	1.39
18	i	4020	BCR	C11-C12	-3.83	1.24	1.34
20	l	5007	LMG	C19-C18	-3.83	1.32	1.51
14	B	1202	CLA	CHD-C1D	3.83	1.45	1.38
14	b	1232	CLA	CHD-C4C	3.82	1.47	1.39
15	A	1121	F6C	CHD-C4C	3.82	1.48	1.39
14	l	1502	CLA	CHD-C1D	3.82	1.45	1.38
15	B	1237	F6C	CHD-C1D	3.82	1.46	1.38
20	U	5007	LMG	C19-C18	-3.82	1.32	1.51
20	L	5007	LMG	C19-C18	-3.82	1.32	1.51
14	A	1102	CLA	CHD-C4C	3.82	1.47	1.39
14	B	1238	CLA	C1B-NB	-3.82	1.32	1.37
14	A	1112	CLA	CHD-C4C	3.82	1.47	1.39
14	b	1227	CLA	CHD-C4C	3.82	1.47	1.39
14	a	1112	CLA	CHD-C4C	3.82	1.47	1.39
14	b	1205	CLA	C1B-NB	-3.82	1.32	1.37
14	G	1137	CLA	C1D-ND	-3.82	1.32	1.37
14	b	1206	CLA	C1B-NB	-3.82	1.32	1.37
15	a	1121	F6C	CHD-C4C	3.82	1.48	1.39
14	K	1401	CLA	CHD-C4C	3.82	1.47	1.39
14	G	1131	CLA	C1D-ND	-3.82	1.32	1.37
14	H	1213	CLA	CHD-C4C	3.81	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1138	CLA	CHD-C4C	3.81	1.47	1.39
14	B	1022	CLA	CHC-C4B	3.81	1.48	1.39
14	H	1204	CLA	C1B-NB	-3.81	1.32	1.37
14	G	1104	CLA	CHD-C1D	3.81	1.45	1.38
14	b	1203	CLA	C3C-C2C	3.81	1.45	1.36
14	B	1206	CLA	C1B-NB	-3.81	1.32	1.37
14	H	1206	CLA	C1B-NB	-3.81	1.32	1.37
14	b	1022	CLA	CHC-C4B	3.81	1.48	1.39
14	G	1115	CLA	CHD-C4C	3.81	1.47	1.39
14	H	1203	CLA	C3C-C2C	3.81	1.45	1.36
15	B	1230	F6C	CHD-C4C	3.81	1.48	1.39
14	B	1229	CLA	CHD-C4C	3.81	1.47	1.39
15	b	1237	F6C	CHD-C1D	3.81	1.46	1.38
14	A	1108	CLA	CHD-C4C	3.81	1.47	1.39
14	b	1210	CLA	CHD-C4C	3.81	1.47	1.39
14	B	1231	CLA	CHD-C4C	3.81	1.47	1.39
14	a	1104	CLA	CHD-C1D	3.81	1.45	1.38
15	G	1121	F6C	CHD-C4C	3.81	1.48	1.39
15	b	1230	F6C	CHD-C4C	3.81	1.48	1.39
14	B	1203	CLA	C3C-C2C	3.80	1.45	1.36
14	G	1116	CLA	CHD-C4C	3.80	1.47	1.39
20	B	5002	LMG	O7-C10	3.80	1.45	1.34
20	H	5002	LMG	O7-C10	3.80	1.45	1.34
14	H	1222	CLA	CHD-C4C	3.80	1.47	1.39
15	H	1237	F6C	CHD-C1D	3.80	1.46	1.38
14	a	1012	CLA	C1D-ND	-3.80	1.32	1.37
14	B	1222	CLA	CHD-C4C	3.80	1.47	1.39
14	H	1207	CLA	C3C-C2C	3.80	1.45	1.36
14	b	1222	CLA	CHD-C4C	3.80	1.47	1.39
14	b	1210	CLA	C3C-C2C	3.80	1.45	1.36
18	R	4020	BCR	C11-C12	-3.80	1.24	1.34
14	b	1213	CLA	CHD-C4C	3.80	1.47	1.39
14	b	1236	CLA	CHD-C1D	3.80	1.45	1.38
14	a	1136	CLA	CHD-C1D	3.80	1.45	1.38
14	H	1012	CLA	CHC-C4B	3.80	1.47	1.39
14	b	1225	CLA	MG-ND	-3.80	1.98	2.05
18	I	4020	BCR	C11-C12	-3.80	1.24	1.34
14	H	1236	CLA	CHD-C1D	3.80	1.45	1.38
14	A	1135	CLA	C1D-ND	-3.80	1.32	1.37
15	B	1230	F6C	C3D-C4D	-3.79	1.34	1.44
14	B	1204	CLA	C1B-NB	-3.79	1.32	1.37
14	G	1108	CLA	CHD-C4C	3.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1207	CLA	C3C-C2C	3.79	1.44	1.36
14	B	1213	CLA	CHD-C4C	3.79	1.47	1.39
14	G	1112	CLA	CHD-C4C	3.79	1.47	1.39
14	a	1135	CLA	CHD-C4C	3.79	1.47	1.39
14	a	1117	CLA	C1D-ND	-3.79	1.32	1.37
14	b	1238	CLA	C1B-NB	-3.79	1.32	1.37
14	A	1116	CLA	CHD-C4C	3.79	1.47	1.39
14	A	1115	CLA	CHD-C4C	3.78	1.47	1.39
14	B	1221	CLA	C1D-ND	-3.78	1.32	1.37
14	A	1122	CLA	C3C-C2C	3.78	1.44	1.36
14	B	1225	CLA	MG-ND	-3.78	1.98	2.05
14	G	1113	CLA	CHD-C4C	3.78	1.47	1.39
14	A	1114	CLA	C1B-NB	-3.78	1.32	1.37
14	G	1012	CLA	C1D-ND	-3.78	1.32	1.37
14	B	1238	CLA	CHC-C4B	3.78	1.47	1.39
14	b	1207	CLA	C3C-C2C	3.78	1.44	1.36
14	H	1233	CLA	CHD-C4C	3.78	1.47	1.39
20	U	5007	LMG	C40-C39	-3.78	1.33	1.51
14	A	1113	CLA	CHD-C4C	3.78	1.47	1.39
14	H	1225	CLA	MG-ND	-3.78	1.98	2.05
14	H	1231	CLA	CHD-C4C	3.78	1.47	1.39
14	a	1131	CLA	C1D-ND	-3.78	1.32	1.37
14	U	1502	CLA	CHD-C1D	3.78	1.45	1.38
20	L	5007	LMG	C40-C39	-3.77	1.33	1.51
14	B	1209	CLA	CHD-C4C	3.77	1.47	1.39
14	H	1210	CLA	CHD-C4C	3.77	1.47	1.39
14	a	1108	CLA	CHD-C4C	3.77	1.47	1.39
15	H	1230	F6C	MG-NC	3.77	2.13	2.05
15	b	1230	F6C	C3D-C4D	-3.77	1.34	1.44
14	B	1233	CLA	CHD-C4C	3.77	1.47	1.39
14	G	1128	CLA	MG-ND	-3.77	1.98	2.05
14	B	1210	CLA	C3C-C2C	3.77	1.44	1.36
14	b	1231	CLA	CHD-C4C	3.77	1.47	1.39
14	b	1239	CLA	CHD-C4C	3.77	1.47	1.39
15	B	1230	F6C	MG-NC	3.77	2.13	2.05
14	H	1205	CLA	C1B-NB	-3.77	1.32	1.37
14	L	1502	CLA	CHD-C1D	3.77	1.45	1.38
14	a	1127	CLA	C1B-NB	-3.77	1.32	1.37
20	l	5007	LMG	C40-C39	-3.77	1.33	1.51
14	H	1218	CLA	CHD-C4C	3.77	1.47	1.39
14	a	1113	CLA	CHD-C4C	3.77	1.47	1.39
14	a	1115	CLA	CHD-C4C	3.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1221	CLA	C1D-ND	-3.77	1.32	1.37
14	a	1118	CLA	CHD-C4C	3.77	1.47	1.39
14	b	1238	CLA	CHC-C4B	3.76	1.47	1.39
14	b	1226	CLA	MG-ND	-3.76	1.98	2.05
14	l	1503	CLA	CHD-C4C	3.76	1.47	1.39
14	a	1116	CLA	CHD-C4C	3.76	1.47	1.39
14	b	1233	CLA	CHD-C4C	3.76	1.47	1.39
14	B	1210	CLA	CHD-C4C	3.76	1.47	1.39
14	B	1218	CLA	CHD-C4C	3.76	1.47	1.39
14	a	1114	CLA	C1B-NB	-3.76	1.32	1.37
14	B	1227	CLA	C1D-ND	-3.76	1.32	1.37
20	H	5002	LMG	C22-C21	-3.76	1.33	1.51
20	b	5002	LMG	O7-C10	3.76	1.44	1.34
14	G	1119	CLA	CHD-C4C	3.76	1.47	1.39
14	a	1119	CLA	CHD-C4C	3.76	1.47	1.39
15	H	1230	F6C	CHD-C4C	3.76	1.47	1.39
14	G	1114	CLA	C1B-NB	-3.76	1.32	1.37
14	B	1235	CLA	CHD-C4C	3.76	1.47	1.39
14	G	1135	CLA	CHD-C4C	3.76	1.47	1.39
14	L	1503	CLA	CHD-C4C	3.76	1.47	1.39
14	b	1209	CLA	CHD-C4C	3.76	1.47	1.39
14	A	1104	CLA	CHD-C1D	3.75	1.45	1.38
14	H	1215	CLA	C1B-NB	-3.75	1.32	1.37
20	H	5002	LMG	C37-C36	-3.75	1.33	1.51
14	H	1209	CLA	CHD-C4C	3.75	1.47	1.39
14	H	1235	CLA	CHD-C4C	3.75	1.47	1.39
14	b	1218	CLA	CHD-C4C	3.75	1.47	1.39
20	B	5002	LMG	C22-C21	-3.75	1.33	1.51
20	b	5002	LMG	C22-C21	-3.75	1.33	1.51
18	L	4022	BCR	C11-C12	-3.75	1.24	1.34
14	a	1137	CLA	C1D-ND	-3.75	1.32	1.37
14	b	1204	CLA	C1B-NB	-3.75	1.32	1.37
15	b	1230	F6C	MG-NC	3.75	2.13	2.05
14	b	1233	CLA	CHB-C1B	3.75	1.47	1.39
20	B	5002	LMG	C37-C36	-3.75	1.33	1.51
14	H	1226	CLA	MG-ND	-3.75	1.98	2.05
14	A	1124	CLA	CHC-C4B	3.75	1.47	1.39
14	W	1701	CLA	CHC-C4B	3.75	1.47	1.39
14	H	1210	CLA	C1D-ND	-3.75	1.32	1.37
14	A	1135	CLA	CHD-C4C	3.74	1.47	1.39
14	B	1234	CLA	CHC-C4B	3.74	1.47	1.39
14	b	1210	CLA	C1D-ND	-3.74	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1238	CLA	CHC-C4B	3.74	1.47	1.39
14	A	1133	CLA	CHD-C4C	3.74	1.47	1.39
14	b	1208	CLA	CHD-C4C	3.74	1.47	1.39
14	G	1125	CLA	C1B-NB	-3.74	1.32	1.37
14	a	1128	CLA	MG-ND	-3.74	1.98	2.05
18	l	4022	BCR	C11-C12	-3.74	1.24	1.34
20	b	5002	LMG	C37-C36	-3.74	1.33	1.51
14	b	1234	CLA	CHC-C4B	3.74	1.47	1.39
14	G	1108	CLA	CHC-C4B	3.74	1.47	1.39
14	A	1118	CLA	CHD-C4C	3.74	1.47	1.39
14	a	1124	CLA	CHC-C4B	3.74	1.47	1.39
14	A	1127	CLA	C1B-NB	-3.74	1.33	1.37
14	A	1119	CLA	CHD-C4C	3.74	1.47	1.39
14	B	1021	CLA	C3C-C2C	3.74	1.44	1.36
14	H	1210	CLA	C3C-C2C	3.74	1.44	1.36
14	A	1126	CLA	CHD-C4C	3.73	1.47	1.39
14	H	1021	CLA	C3C-C2C	3.73	1.44	1.36
14	H	1234	CLA	CHC-C4B	3.73	1.47	1.39
14	b	1235	CLA	CHD-C4C	3.73	1.47	1.39
14	B	1225	CLA	CHD-C1D	3.73	1.45	1.38
14	G	1117	CLA	CHC-C1C	3.73	1.46	1.38
14	G	1124	CLA	CHC-C4B	3.73	1.47	1.39
14	A	1012	CLA	C1D-ND	-3.73	1.33	1.37
14	B	1210	CLA	C1D-ND	-3.73	1.33	1.37
14	b	1227	CLA	C1D-ND	-3.73	1.33	1.37
14	a	1101	CLA	CHC-C4B	3.73	1.47	1.39
14	B	1239	CLA	CHC-C1C	3.73	1.46	1.38
14	B	1226	CLA	MG-ND	-3.73	1.98	2.05
14	A	1131	CLA	CHD-C4C	3.73	1.47	1.39
14	b	1239	CLA	CHC-C1C	3.73	1.45	1.38
14	a	1103	CLA	C3C-C2C	3.73	1.44	1.36
14	B	1239	CLA	CHD-C4C	3.72	1.47	1.39
14	a	1108	CLA	CHC-C4B	3.72	1.47	1.39
14	U	1503	CLA	CHD-C4C	3.72	1.47	1.39
18	A	4007	BCR	C11-C12	-3.72	1.25	1.34
14	H	1208	CLA	CHD-C4C	3.72	1.47	1.39
14	G	1118	CLA	CHD-C4C	3.72	1.47	1.39
16	H	2002	PQN	C10-C5	3.72	1.46	1.40
14	A	1125	CLA	C1B-NB	-3.72	1.33	1.37
14	B	1238	CLA	CHD-C1D	3.72	1.45	1.38
14	H	1225	CLA	CHD-C1D	3.72	1.45	1.38
14	H	1217	CLA	CHD-C4C	3.72	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	2002	PQN	C10-C5	3.72	1.46	1.40
14	B	1208	CLA	CHD-C4C	3.72	1.47	1.39
14	G	1127	CLA	C1B-NB	-3.72	1.33	1.37
14	H	1239	CLA	CHC-C1C	3.72	1.45	1.38
16	b	2002	PQN	C10-C5	3.72	1.46	1.40
20	a	5005	LMG	C40-C39	-3.72	1.33	1.51
20	G	5005	LMG	C40-C39	-3.72	1.33	1.51
14	H	1239	CLA	CHD-C4C	3.72	1.47	1.39
14	A	1103	CLA	C3C-C2C	3.71	1.44	1.36
14	B	1211	CLA	CHD-C4C	3.71	1.47	1.39
14	H	1238	CLA	CHD-C1D	3.71	1.45	1.38
14	b	1021	CLA	C3C-C2C	3.71	1.44	1.36
14	A	1117	CLA	CHC-C1C	3.71	1.45	1.38
20	a	5005	LMG	C43-C42	-3.71	1.33	1.51
18	a	4001	BCR	C11-C12	-3.71	1.25	1.34
14	G	1133	CLA	CHD-C4C	3.71	1.47	1.39
14	b	1211	CLA	CHD-C4C	3.71	1.47	1.39
14	A	1108	CLA	CHC-C4B	3.71	1.47	1.39
14	B	1233	CLA	CHB-C1B	3.71	1.47	1.39
14	b	1225	CLA	CHD-C1D	3.70	1.45	1.38
14	A	1136	CLA	C1D-ND	-3.70	1.33	1.37
18	G	4007	BCR	C11-C12	-3.70	1.25	1.34
14	G	1135	CLA	C1D-ND	-3.70	1.33	1.37
14	H	1227	CLA	C1D-ND	-3.70	1.33	1.37
14	X	1701	CLA	CHC-C4B	3.70	1.47	1.39
20	H	5002	LMG	C19-C18	-3.70	1.33	1.51
18	B	4017	BCR	C11-C12	-3.70	1.25	1.34
14	a	1126	CLA	CHD-C4C	3.70	1.47	1.39
14	a	1125	CLA	C1B-NB	-3.70	1.33	1.37
18	b	4017	BCR	C11-C12	-3.70	1.25	1.34
20	A	5005	LMG	C43-C42	-3.70	1.33	1.51
14	B	1222	CLA	CHC-C4B	3.70	1.47	1.39
20	A	5005	LMG	C40-C39	-3.70	1.33	1.51
20	b	5002	LMG	C19-C18	-3.70	1.33	1.51
18	U	4022	BCR	C11-C12	-3.70	1.25	1.34
14	G	1101	CLA	CHC-C4B	3.69	1.47	1.39
14	b	1223	CLA	CHC-C4B	3.69	1.47	1.39
14	a	1122	CLA	C1D-ND	-3.69	1.33	1.37
14	a	1133	CLA	CHD-C4C	3.69	1.47	1.39
14	b	1222	CLA	CHC-C4B	3.69	1.47	1.39
14	G	1103	CLA	C3C-C2C	3.69	1.44	1.36
14	A	1114	CLA	OBD-CAD	3.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1212	CLA	CHC-C4B	3.69	1.47	1.39
14	H	1207	CLA	C1C-NC	-3.69	1.32	1.37
14	a	1117	CLA	CHC-C1C	3.69	1.45	1.38
14	H	1211	CLA	CHD-C4C	3.69	1.47	1.39
14	H	1212	CLA	CHC-C4B	3.69	1.47	1.39
14	G	1126	CLA	CHD-C4C	3.69	1.47	1.39
14	B	1235	CLA	C1D-ND	-3.69	1.33	1.37
20	B	5002	LMG	C19-C18	-3.69	1.33	1.51
18	G	4001	BCR	C11-C12	-3.69	1.25	1.34
18	A	4001	BCR	C11-C12	-3.69	1.25	1.34
14	a	1135	CLA	C1D-ND	-3.69	1.33	1.37
14	b	1207	CLA	C1C-NC	-3.69	1.32	1.37
14	B	1219	CLA	CHD-C4C	3.69	1.47	1.39
14	G	1111	CLA	CHD-C4C	3.68	1.47	1.39
18	a	4007	BCR	C11-C12	-3.68	1.25	1.34
14	G	1136	CLA	C1D-ND	-3.68	1.33	1.37
14	k	1401	CLA	OBD-CAD	3.68	1.28	1.22
18	H	4017	BCR	C11-C12	-3.68	1.25	1.34
14	T	1401	CLA	OBD-CAD	3.68	1.28	1.22
14	b	1208	CLA	CHC-C4B	3.68	1.47	1.39
14	A	1140	CLA	C1D-ND	-3.68	1.33	1.37
14	B	1223	CLA	CHC-C4B	3.68	1.47	1.39
20	G	5005	LMG	C43-C42	-3.68	1.33	1.51
14	b	1217	CLA	CHD-C4C	3.68	1.47	1.39
14	b	1219	CLA	CHD-C4C	3.68	1.47	1.39
20	l	5007	LMG	C37-C36	-3.68	1.33	1.51
14	a	1131	CLA	CHD-C4C	3.68	1.47	1.39
14	x	1701	CLA	CHC-C4B	3.68	1.47	1.39
14	b	1207	CLA	CHC-C1C	3.68	1.45	1.38
14	G	1140	CLA	C1D-ND	-3.67	1.33	1.37
14	H	1221	CLA	C1D-ND	-3.67	1.33	1.37
14	H	1233	CLA	CHB-C1B	3.67	1.47	1.39
14	b	1212	CLA	CHC-C4B	3.67	1.47	1.39
14	G	1131	CLA	CHD-C4C	3.67	1.47	1.39
14	G	1110	CLA	CHC-C4B	3.67	1.47	1.39
14	H	1021	CLA	CHB-C1B	3.67	1.47	1.39
14	G	1122	CLA	C1D-ND	-3.67	1.33	1.37
14	A	1132	CLA	CHD-C4C	3.67	1.47	1.39
14	A	1111	CLA	CHD-C4C	3.67	1.47	1.39
14	B	1213	CLA	OBD-CAD	3.67	1.28	1.22
14	B	1233	CLA	OBD-CAD	3.67	1.28	1.22
14	a	1136	CLA	C1D-ND	-3.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1217	CLA	CHD-C4C	3.67	1.47	1.39
14	G	1124	CLA	CHD-C4C	3.67	1.47	1.39
14	H	1235	CLA	CHC-C4B	3.67	1.47	1.39
14	A	1101	CLA	CHC-C4B	3.67	1.47	1.39
14	H	1021	CLA	C1B-NB	-3.67	1.33	1.37
14	H	1223	CLA	CHC-C4B	3.67	1.47	1.39
14	A	1110	CLA	CHC-C4B	3.67	1.47	1.39
14	a	1105	CLA	CHC-C4B	3.66	1.47	1.39
14	a	1110	CLA	CHC-C4B	3.66	1.47	1.39
14	H	1222	CLA	CHC-C4B	3.66	1.47	1.39
14	b	1235	CLA	CHC-C4B	3.66	1.47	1.39
14	B	1021	CLA	C1B-NB	-3.66	1.33	1.37
14	H	1207	CLA	CHC-C1C	3.66	1.45	1.38
14	b	1235	CLA	C1D-ND	-3.66	1.33	1.37
14	b	1238	CLA	CHD-C1D	3.66	1.45	1.38
14	H	1201	CLA	CHD-C4C	3.66	1.47	1.39
18	a	4011	BCR	C11-C12	-3.66	1.25	1.34
14	H	1219	CLA	CHD-C4C	3.66	1.47	1.39
20	L	5007	LMG	C37-C36	-3.66	1.33	1.51
14	b	1021	CLA	CHB-C1B	3.66	1.47	1.39
20	U	5007	LMG	C37-C36	-3.66	1.33	1.51
14	B	1238	CLA	CHD-C4C	3.66	1.47	1.39
14	a	1132	CLA	CHD-C4C	3.65	1.47	1.39
14	a	1102	CLA	C1D-ND	-3.65	1.33	1.37
14	G	1012	CLA	CHD-C4C	3.65	1.47	1.39
14	b	1021	CLA	C1B-NB	-3.65	1.33	1.37
14	a	1125	CLA	CHD-C1D	3.65	1.45	1.38
14	a	1104	CLA	C1D-ND	-3.65	1.33	1.37
14	G	1117	CLA	C1B-NB	-3.65	1.33	1.37
14	B	1229	CLA	CHC-C4B	3.65	1.47	1.39
14	A	1125	CLA	CHD-C1D	3.65	1.45	1.38
14	A	1124	CLA	CHD-C4C	3.65	1.47	1.39
14	H	1233	CLA	OBD-CAD	3.65	1.28	1.22
14	G	1105	CLA	CHC-C4B	3.65	1.47	1.39
14	B	1023	CLA	C1B-NB	-3.65	1.33	1.37
14	B	1207	CLA	C1C-NC	-3.65	1.32	1.37
14	B	1235	CLA	CHC-C4B	3.65	1.47	1.39
14	H	1235	CLA	C1D-ND	-3.65	1.33	1.37
14	B	1208	CLA	CHC-C4B	3.65	1.47	1.39
14	b	1233	CLA	OBD-CAD	3.65	1.28	1.22
14	G	1116	CLA	C1D-ND	-3.65	1.33	1.37
14	G	1125	CLA	CHD-C1D	3.65	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1114	CLA	OBD-CAD	3.65	1.28	1.22
14	K	1401	CLA	OBD-CAD	3.65	1.28	1.22
14	H	1021	CLA	MG-ND	-3.64	1.98	2.05
14	G	1104	CLA	C1D-ND	-3.64	1.33	1.37
20	a	5005	LMG	C37-C36	-3.64	1.33	1.51
14	B	1022	CLA	CHD-C1D	3.64	1.45	1.38
14	a	1111	CLA	CHD-C4C	3.64	1.47	1.39
14	A	1122	CLA	C1D-ND	-3.64	1.33	1.37
14	a	1012	CLA	CHD-C4C	3.64	1.47	1.39
14	H	1208	CLA	CHC-C4B	3.64	1.47	1.39
14	H	1210	CLA	C1C-NC	-3.64	1.32	1.37
14	H	1229	CLA	CHC-C4B	3.64	1.47	1.39
14	A	1105	CLA	CHC-C4B	3.64	1.47	1.39
14	G	1130	CLA	C1D-ND	-3.64	1.33	1.37
14	a	1116	CLA	C1D-ND	-3.64	1.33	1.37
14	a	1140	CLA	C1D-ND	-3.64	1.33	1.37
14	B	1207	CLA	CHC-C1C	3.64	1.45	1.38
18	H	4014	BCR	C11-C12	-3.64	1.25	1.34
14	A	1012	CLA	CHD-C4C	3.63	1.47	1.39
14	k	1401	CLA	CHB-C1B	3.63	1.47	1.39
14	A	1129	CLA	CHC-C4B	3.63	1.47	1.39
14	A	1117	CLA	C1B-NB	-3.63	1.33	1.37
14	K	1401	CLA	CHB-C1B	3.63	1.47	1.39
14	a	1129	CLA	CHC-C4B	3.63	1.47	1.39
14	G	1132	CLA	CHD-C4C	3.63	1.47	1.39
15	G	1120	F6C	C3D-C4D	-3.63	1.34	1.44
20	G	5005	LMG	C37-C36	-3.63	1.33	1.51
14	A	1130	CLA	C1D-ND	-3.63	1.33	1.37
14	a	1114	CLA	OBD-CAD	3.63	1.28	1.22
14	H	1238	CLA	CHD-C4C	3.63	1.47	1.39
15	a	1120	F6C	C3D-C4D	-3.63	1.34	1.44
14	H	1218	CLA	CHC-C4B	3.63	1.47	1.39
14	b	1218	CLA	CHB-C1B	3.63	1.47	1.39
14	B	1201	CLA	CHD-C4C	3.63	1.47	1.39
14	H	1205	CLA	CHD-C1D	3.63	1.45	1.38
14	G	1102	CLA	C1D-ND	-3.63	1.33	1.37
14	b	1238	CLA	CHD-C4C	3.63	1.47	1.39
15	a	1120	F6C	CHC-C1C	3.63	1.47	1.39
20	A	5005	LMG	C37-C36	-3.63	1.33	1.51
14	B	1224	CLA	CHD-C1D	3.63	1.45	1.38
14	b	1224	CLA	CHD-C1D	3.63	1.45	1.38
15	B	1230	F6C	OBD-CAD	3.62	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1106	CLA	CHD-C4C	3.62	1.47	1.39
18	B	4014	BCR	C11-C12	-3.62	1.25	1.34
14	H	1224	CLA	CHD-C1D	3.62	1.45	1.38
14	B	1021	CLA	CHB-C1B	3.62	1.47	1.39
14	a	1124	CLA	CHD-C4C	3.62	1.47	1.39
14	b	1236	CLA	CHD-C4C	3.62	1.47	1.39
14	a	1117	CLA	C1B-NB	-3.62	1.33	1.37
14	A	1133	CLA	CHB-C1B	3.62	1.47	1.39
14	B	1211	CLA	CHC-C4B	3.62	1.47	1.39
14	b	1201	CLA	CHD-C4C	3.62	1.47	1.39
14	a	1133	CLA	CHB-C1B	3.62	1.47	1.39
14	A	1112	CLA	OBD-CAD	3.62	1.28	1.22
14	H	1213	CLA	OBD-CAD	3.62	1.28	1.22
14	H	1236	CLA	CHD-C4C	3.62	1.47	1.39
14	A	1130	CLA	CHD-C4C	3.62	1.47	1.39
14	B	1236	CLA	CHD-C4C	3.62	1.47	1.39
14	b	1210	CLA	C1C-NC	-3.62	1.32	1.37
14	A	1128	CLA	CHD-C4C	3.62	1.47	1.39
18	G	4011	BCR	C11-C12	-3.62	1.25	1.34
18	b	4014	BCR	C11-C12	-3.62	1.25	1.34
14	b	1205	CLA	CHD-C1D	3.62	1.45	1.38
15	A	1120	F6C	C3D-C4D	-3.62	1.34	1.44
14	B	1218	CLA	CHC-C4B	3.62	1.47	1.39
14	B	1223	CLA	C1D-ND	-3.62	1.33	1.37
14	B	1215	CLA	CHD-C4C	3.62	1.47	1.39
14	G	1112	CLA	OBD-CAD	3.62	1.28	1.22
14	G	1129	CLA	CHC-C4B	3.61	1.47	1.39
14	H	1223	CLA	C1D-ND	-3.61	1.33	1.37
14	L	1502	CLA	CHD-C4C	3.61	1.47	1.39
14	B	1218	CLA	CHB-C1B	3.61	1.47	1.39
14	H	1213	CLA	CHC-C4B	3.61	1.47	1.39
14	B	1218	CLA	OBD-CAD	3.61	1.28	1.22
14	G	1130	CLA	CHD-C4C	3.61	1.47	1.39
14	H	1215	CLA	CHD-C4C	3.61	1.47	1.39
14	H	1218	CLA	CHB-C1B	3.61	1.47	1.39
14	T	1401	CLA	CHB-C1B	3.61	1.47	1.39
14	B	1222	CLA	C1B-NB	-3.61	1.33	1.37
14	G	1115	CLA	C1D-ND	-3.61	1.33	1.37
14	a	1115	CLA	C1D-ND	-3.61	1.33	1.37
14	W	1701	CLA	CHB-C1B	3.61	1.47	1.39
14	b	1022	CLA	CHD-C1D	3.61	1.45	1.38
14	G	1123	CLA	C1D-ND	-3.61	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1124	CLA	C1D-ND	-3.61	1.33	1.37
18	H	4010	BCR	C11-C12	-3.61	1.25	1.34
14	B	1205	CLA	CHD-C1D	3.61	1.45	1.38
14	B	1233	CLA	CHC-C4B	3.61	1.47	1.39
14	A	1102	CLA	CHC-C4B	3.61	1.47	1.39
14	H	1023	CLA	C1B-NB	-3.61	1.33	1.37
14	U	1501	CLA	CHC-C4B	3.61	1.47	1.39
18	A	4011	BCR	C11-C12	-3.60	1.25	1.34
14	b	1229	CLA	CHC-C4B	3.60	1.47	1.39
18	b	4010	BCR	C11-C12	-3.60	1.25	1.34
14	A	1116	CLA	C1D-ND	-3.60	1.33	1.37
14	b	1239	CLA	C1D-ND	-3.60	1.33	1.37
14	H	1221	CLA	CHC-C4B	3.60	1.47	1.39
14	a	1112	CLA	OBD-CAD	3.60	1.28	1.22
14	B	1021	CLA	MG-ND	-3.60	1.98	2.05
14	A	1104	CLA	C1D-ND	-3.60	1.33	1.37
14	b	1023	CLA	C4B-NB	-3.60	1.33	1.37
14	b	1213	CLA	OBD-CAD	3.60	1.28	1.22
14	b	1218	CLA	CHC-C4B	3.60	1.47	1.39
14	U	1502	CLA	CHD-C4C	3.60	1.47	1.39
14	a	1130	CLA	CHD-C4C	3.60	1.47	1.39
14	A	1102	CLA	C1D-ND	-3.60	1.33	1.37
14	k	1401	CLA	CHC-C4B	3.60	1.47	1.39
14	B	1209	CLA	CHC-C4B	3.60	1.47	1.39
14	a	1115	CLA	CHC-C4B	3.60	1.47	1.39
14	b	1023	CLA	C1B-NB	-3.60	1.33	1.37
14	G	1133	CLA	CHB-C1B	3.60	1.47	1.39
14	H	1211	CLA	CHC-C4B	3.60	1.47	1.39
14	H	1233	CLA	CHC-C4B	3.60	1.47	1.39
14	G	1106	CLA	CHD-C4C	3.60	1.47	1.39
14	B	1210	CLA	C1C-NC	-3.60	1.32	1.37
14	G	1128	CLA	CHD-C4C	3.60	1.47	1.39
14	l	1502	CLA	CHD-C4C	3.60	1.47	1.39
14	b	1021	CLA	MG-ND	-3.60	1.98	2.05
14	x	1701	CLA	CHB-C1B	3.60	1.47	1.39
14	a	1013	CLA	MG-ND	-3.59	1.98	2.05
14	b	1211	CLA	CHC-C4B	3.59	1.47	1.39
14	b	1215	CLA	CHD-C4C	3.59	1.47	1.39
14	B	1224	CLA	C1B-NB	-3.59	1.33	1.37
14	a	1128	CLA	CHD-C4C	3.59	1.47	1.39
14	A	1115	CLA	CHC-C4B	3.59	1.47	1.39
14	A	1123	CLA	CHB-C1B	3.59	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	4010	BCR	C11-C12	-3.59	1.25	1.34
14	H	1012	CLA	CHD-C1D	3.59	1.45	1.38
14	l	1501	CLA	CHC-C4B	3.59	1.47	1.39
14	b	1228	CLA	C1D-ND	-3.59	1.33	1.37
15	G	1120	F6C	CHD-C4C	3.59	1.47	1.39
14	b	1231	CLA	OBD-CAD	3.59	1.28	1.22
14	A	1106	CLA	C1D-ND	-3.59	1.33	1.37
14	A	1115	CLA	C1D-ND	-3.59	1.33	1.37
14	H	1220	CLA	CHD-C4C	3.59	1.47	1.39
14	H	1224	CLA	C1B-NB	-3.59	1.33	1.37
14	b	1212	CLA	C1D-ND	-3.59	1.33	1.37
14	L	1501	CLA	CHC-C4B	3.59	1.47	1.39
14	A	1123	CLA	C1D-ND	-3.59	1.33	1.37
14	a	1102	CLA	CHC-C4B	3.59	1.47	1.39
14	A	1104	CLA	CHD-C4C	3.58	1.47	1.39
14	b	1221	CLA	CHC-C4B	3.58	1.47	1.39
14	b	1233	CLA	CHC-C4B	3.58	1.47	1.39
15	A	1120	F6C	CHC-C1C	3.58	1.47	1.39
14	A	1013	CLA	MG-ND	-3.58	1.98	2.05
14	B	1224	CLA	CHC-C4B	3.58	1.47	1.39
14	b	1217	CLA	CHC-C4B	3.58	1.47	1.39
14	B	1203	CLA	C1D-ND	-3.58	1.33	1.37
14	L	1503	CLA	C1D-ND	-3.58	1.33	1.37
14	B	1221	CLA	CHC-C4B	3.58	1.47	1.39
15	a	1120	F6C	CHD-C4C	3.58	1.47	1.39
14	b	1224	CLA	C1B-NB	-3.58	1.33	1.37
14	G	1104	CLA	CHD-C4C	3.58	1.47	1.39
15	H	1230	F6C	OBD-CAD	3.58	1.28	1.22
14	G	1123	CLA	CHB-C1B	3.58	1.47	1.39
14	L	1501	CLA	C1B-NB	-3.58	1.33	1.37
14	B	1213	CLA	CHC-C4B	3.58	1.47	1.39
14	b	1224	CLA	CHC-C4B	3.58	1.47	1.39
14	B	1220	CLA	CHD-C4C	3.58	1.47	1.39
14	b	1212	CLA	CHB-C1B	3.58	1.47	1.39
14	H	1228	CLA	C1D-ND	-3.58	1.33	1.37
14	G	1102	CLA	CHC-C4B	3.58	1.47	1.39
14	H	1217	CLA	CHB-C1B	3.58	1.47	1.39
14	A	1012	CLA	MG-ND	-3.58	1.98	2.05
14	B	1231	CLA	OBD-CAD	3.58	1.28	1.22
14	A	1139	CLA	CHD-C4C	3.58	1.47	1.39
14	H	1224	CLA	CHC-C4B	3.58	1.47	1.39
14	a	1106	CLA	CHD-C4C	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1223	CLA	C1D-ND	-3.58	1.33	1.37
14	b	1219	CLA	CHC-C4B	3.58	1.47	1.39
14	H	1218	CLA	OBD-CAD	3.58	1.28	1.22
14	a	1124	CLA	C1D-ND	-3.57	1.33	1.37
14	a	1132	CLA	C4B-NB	-3.57	1.33	1.37
14	A	1138	CLA	CHC-C4B	3.57	1.47	1.39
14	B	1219	CLA	CHC-C4B	3.57	1.47	1.39
14	b	1213	CLA	CHC-C4B	3.57	1.47	1.39
14	U	1503	CLA	C1D-ND	-3.57	1.33	1.37
14	a	1123	CLA	CHB-C1B	3.57	1.47	1.39
14	B	1217	CLA	CHC-C4B	3.57	1.47	1.39
14	A	1119	CLA	CHC-C4B	3.57	1.47	1.39
14	B	1212	CLA	CHB-C1B	3.57	1.47	1.39
15	A	1120	F6C	CHD-C4C	3.57	1.47	1.39
14	b	1203	CLA	C1D-ND	-3.57	1.33	1.37
14	l	1501	CLA	C1B-NB	-3.57	1.33	1.37
14	b	1207	CLA	CHD-C4C	3.57	1.47	1.39
14	B	1203	CLA	CHD-C1D	3.57	1.45	1.38
14	H	1209	CLA	CHC-C4B	3.57	1.47	1.39
14	G	1101	CLA	CHD-C4C	3.57	1.47	1.39
14	X	1701	CLA	CHB-C1B	3.57	1.47	1.39
14	B	1217	CLA	CHB-C1B	3.57	1.47	1.39
14	K	1401	CLA	CHC-C4B	3.57	1.47	1.39
14	H	1239	CLA	C1D-ND	-3.57	1.33	1.37
14	b	1212	CLA	OBD-CAD	3.57	1.28	1.22
14	A	1137	CLA	CHD-C4C	3.57	1.47	1.39
14	G	1138	CLA	CHC-C4B	3.57	1.47	1.39
15	G	1120	F6C	CHC-C1C	3.57	1.47	1.39
14	a	1106	CLA	C1D-ND	-3.57	1.33	1.37
14	a	1123	CLA	C1D-ND	-3.57	1.33	1.37
14	G	1115	CLA	CHC-C4B	3.57	1.47	1.39
14	H	1214	CLA	C1D-ND	-3.57	1.33	1.37
14	b	1217	CLA	CHB-C1B	3.56	1.47	1.39
14	B	1228	CLA	C1D-ND	-3.56	1.33	1.37
14	B	1239	CLA	C1D-ND	-3.56	1.33	1.37
14	A	1124	CLA	C1D-ND	-3.56	1.33	1.37
14	l	1503	CLA	C1D-ND	-3.56	1.33	1.37
14	B	1212	CLA	CHD-C4C	3.56	1.47	1.39
14	a	1137	CLA	CHD-C4C	3.56	1.47	1.39
14	H	1212	CLA	C1D-ND	-3.56	1.33	1.37
14	a	1130	CLA	C1D-ND	-3.56	1.33	1.37
14	B	1212	CLA	C1D-ND	-3.56	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1203	CLA	C1B-NB	-3.56	1.33	1.37
14	a	1104	CLA	C1B-NB	-3.56	1.33	1.37
14	H	1231	CLA	OBD-CAD	3.56	1.28	1.22
14	G	1013	CLA	MG-ND	-3.56	1.98	2.05
14	T	1401	CLA	CHC-C4B	3.56	1.47	1.39
14	H	1203	CLA	CHD-C1D	3.56	1.45	1.38
14	G	1139	CLA	C1D-ND	-3.56	1.33	1.37
14	b	1212	CLA	CHD-C4C	3.56	1.47	1.39
18	b	4009	BCR	C11-C12	-3.56	1.25	1.34
14	H	1212	CLA	OBD-CAD	3.56	1.28	1.22
14	H	1207	CLA	CHD-C4C	3.56	1.47	1.39
14	a	1139	CLA	CHD-C4C	3.56	1.47	1.39
14	a	1104	CLA	CHD-C4C	3.56	1.47	1.39
14	b	1218	CLA	OBD-CAD	3.56	1.28	1.22
14	b	1209	CLA	CHC-C4B	3.56	1.47	1.39
14	a	1101	CLA	CHD-C4C	3.56	1.47	1.39
14	H	1219	CLA	CHC-C4B	3.55	1.47	1.39
14	a	1116	CLA	CHC-C4B	3.55	1.47	1.39
14	H	1217	CLA	CHC-C4B	3.55	1.47	1.39
14	b	1220	CLA	C1D-ND	-3.55	1.33	1.37
14	a	1138	CLA	CHC-C4B	3.55	1.47	1.39
14	B	1220	CLA	C1D-ND	-3.55	1.33	1.37
14	B	1220	CLA	CHB-C1B	3.55	1.47	1.39
14	A	1136	CLA	CHC-C4B	3.55	1.47	1.39
14	G	1139	CLA	CHD-C4C	3.55	1.47	1.39
14	H	1203	CLA	C1B-NB	-3.55	1.33	1.37
14	a	1136	CLA	CHC-C4B	3.55	1.47	1.39
14	B	1212	CLA	OBD-CAD	3.55	1.28	1.22
14	G	1012	CLA	MG-ND	-3.55	1.98	2.05
14	G	1116	CLA	CHC-C4B	3.55	1.47	1.39
14	A	1103	CLA	CHD-C4C	3.55	1.47	1.39
14	A	1130	CLA	C1B-NB	-3.55	1.33	1.37
14	G	1108	CLA	OBD-CAD	3.54	1.28	1.22
14	G	1137	CLA	CHB-C1B	3.54	1.47	1.39
14	B	1207	CLA	CHD-C4C	3.54	1.47	1.39
15	b	1230	F6C	OBD-CAD	3.54	1.28	1.22
14	A	1130	CLA	CHC-C4B	3.54	1.47	1.39
14	b	1222	CLA	C1B-NB	-3.54	1.33	1.37
14	A	1132	CLA	C4B-NB	-3.54	1.33	1.37
14	G	1119	CLA	CHC-C4B	3.54	1.47	1.39
14	A	1101	CLA	CHD-C4C	3.54	1.47	1.39
14	H	1228	CLA	OBD-CAD	3.54	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1106	CLA	CHB-C1B	3.54	1.47	1.39
14	B	1227	CLA	C1B-NB	-3.54	1.33	1.37
14	H	1239	CLA	CHB-C1B	3.54	1.47	1.39
18	B	4016	BCR	C11-C12	-3.54	1.25	1.34
18	H	4009	BCR	C11-C12	-3.54	1.25	1.34
14	A	1116	CLA	CHC-C4B	3.54	1.47	1.39
14	b	1239	CLA	CHB-C1B	3.54	1.47	1.39
14	U	1501	CLA	C1B-NB	-3.54	1.33	1.37
14	a	1108	CLA	OBD-CAD	3.54	1.28	1.22
14	a	1129	CLA	CHD-C4C	3.54	1.47	1.39
14	A	1104	CLA	C1B-NB	-3.54	1.33	1.37
14	b	1220	CLA	CHD-C4C	3.54	1.47	1.39
14	G	1130	CLA	CHC-C4B	3.54	1.47	1.39
14	G	1136	CLA	CHC-C4B	3.54	1.47	1.39
14	a	1116	CLA	CHB-C1B	3.53	1.47	1.39
14	A	1137	CLA	CHB-C1B	3.53	1.47	1.39
14	G	1110	CLA	CHB-C1B	3.53	1.47	1.39
18	B	4009	BCR	C11-C12	-3.53	1.25	1.34
14	G	1137	CLA	CHD-C4C	3.53	1.47	1.39
14	a	1110	CLA	CHB-C1B	3.53	1.47	1.39
14	A	1110	CLA	CHB-C1B	3.53	1.47	1.39
14	H	1212	CLA	CHB-C1B	3.53	1.47	1.39
14	H	1203	CLA	C1D-ND	-3.53	1.33	1.37
14	H	1224	CLA	MG-ND	-3.53	1.98	2.05
14	G	1136	CLA	C1B-NB	-3.53	1.33	1.37
14	G	1106	CLA	C1D-ND	-3.53	1.33	1.37
14	G	1103	CLA	CHD-C4C	3.53	1.47	1.39
14	B	1228	CLA	OBD-CAD	3.53	1.28	1.22
14	B	1203	CLA	C1B-NB	-3.53	1.33	1.37
14	b	1208	CLA	OBD-CAD	3.53	1.28	1.22
14	a	1130	CLA	C1B-NB	-3.53	1.33	1.37
18	V	4021	BCR	C11-C12	-3.53	1.25	1.34
18	m	4021	BCR	C11-C12	-3.53	1.25	1.34
14	B	1227	CLA	OBD-CAD	3.53	1.28	1.22
14	H	1212	CLA	CHD-C4C	3.53	1.47	1.39
14	G	1115	CLA	OBD-CAD	3.53	1.28	1.22
14	B	1224	CLA	MG-ND	-3.53	1.98	2.05
14	b	1220	CLA	CHB-C1B	3.53	1.47	1.39
14	G	1130	CLA	C1B-NB	-3.53	1.33	1.37
14	H	1220	CLA	CHB-C1B	3.52	1.47	1.39
14	a	1012	CLA	MG-ND	-3.52	1.98	2.05
14	B	1208	CLA	CHB-C1B	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1203	CLA	CHD-C1D	3.52	1.45	1.38
14	B	1239	CLA	CHB-C1B	3.52	1.47	1.39
13	G	1011	CL0	CHC-C1C	3.52	1.46	1.39
14	G	1126	CLA	MG-ND	-3.52	1.98	2.05
14	G	1108	CLA	CHB-C1B	3.52	1.47	1.39
14	H	1206	CLA	CHB-C1B	3.52	1.47	1.39
14	A	1139	CLA	C1D-ND	-3.52	1.33	1.37
14	A	1110	CLA	CHD-C4C	3.52	1.47	1.39
14	G	1102	CLA	OBD-CAD	3.52	1.28	1.22
14	H	1227	CLA	OBD-CAD	3.52	1.28	1.22
14	G	1104	CLA	C1B-NB	-3.52	1.33	1.37
14	b	1228	CLA	OBD-CAD	3.52	1.28	1.22
14	a	1126	CLA	MG-ND	-3.52	1.98	2.05
14	A	1115	CLA	OBD-CAD	3.52	1.28	1.22
14	B	1202	CLA	OBD-CAD	3.52	1.28	1.22
14	a	1130	CLA	CHC-C4B	3.52	1.47	1.39
14	A	1119	CLA	C1B-NB	-3.52	1.33	1.37
14	a	1108	CLA	CHB-C1B	3.52	1.47	1.39
18	H	4016	BCR	C11-C12	-3.52	1.25	1.34
14	G	1116	CLA	CHB-C1B	3.52	1.47	1.39
14	a	1103	CLA	CHD-C4C	3.52	1.47	1.39
14	G	1119	CLA	C1B-NB	-3.52	1.33	1.37
14	a	1105	CLA	C1D-ND	-3.52	1.33	1.37
14	a	1137	CLA	CHB-C1B	3.52	1.47	1.39
14	G	1106	CLA	CHB-C1B	3.51	1.47	1.39
14	a	1119	CLA	CHC-C4B	3.51	1.47	1.39
14	A	1105	CLA	C1D-ND	-3.51	1.33	1.37
14	A	1108	CLA	OBD-CAD	3.51	1.28	1.22
14	a	1140	CLA	CHB-C1B	3.51	1.47	1.39
15	G	1121	F6C	MG-NC	3.51	2.12	2.05
14	l	1501	CLA	CHD-C4C	3.51	1.47	1.39
15	A	1121	F6C	MG-NC	3.51	2.12	2.05
18	b	4016	BCR	C11-C12	-3.51	1.25	1.34
14	G	1105	CLA	C1D-ND	-3.51	1.33	1.37
14	G	1110	CLA	CHD-C4C	3.51	1.47	1.39
14	b	1205	CLA	CHC-C4B	3.51	1.47	1.39
14	b	1208	CLA	CHB-C1B	3.51	1.47	1.39
14	b	1022	CLA	MG-ND	-3.51	1.98	2.05
14	b	1204	CLA	MG-ND	-3.51	1.98	2.05
14	A	1101	CLA	C1D-ND	-3.51	1.33	1.37
14	G	1129	CLA	CHD-C4C	3.51	1.47	1.39
14	H	1214	CLA	MG-ND	-3.51	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1136	CLA	C1B-NB	-3.51	1.33	1.37
14	G	1132	CLA	C4B-NB	-3.51	1.33	1.37
14	a	1135	CLA	C1B-NB	-3.51	1.33	1.37
14	a	1138	CLA	C1D-ND	-3.51	1.33	1.37
14	A	1102	CLA	OBD-CAD	3.51	1.28	1.22
14	b	1227	CLA	CHC-C4B	3.51	1.47	1.39
14	A	1138	CLA	C1D-ND	-3.51	1.33	1.37
14	a	1127	CLA	CHD-C4C	3.51	1.47	1.39
14	b	1224	CLA	MG-ND	-3.51	1.98	2.05
14	A	1108	CLA	CHB-C1B	3.51	1.47	1.39
14	G	1127	CLA	CHD-C4C	3.51	1.47	1.39
14	a	1106	CLA	CHB-C1B	3.51	1.47	1.39
14	A	1123	CLA	C1B-NB	-3.51	1.33	1.37
14	H	1222	CLA	C1B-NB	-3.51	1.33	1.37
14	A	1127	CLA	CHD-C4C	3.51	1.47	1.39
14	A	1133	CLA	C1D-ND	-3.51	1.33	1.37
14	b	1202	CLA	CHD-C4C	3.50	1.47	1.39
15	A	1120	F6C	CHD-C1D	3.50	1.45	1.38
14	a	1102	CLA	OBD-CAD	3.50	1.28	1.22
14	H	1227	CLA	CHC-C4B	3.50	1.47	1.39
14	H	1204	CLA	MG-ND	-3.50	1.98	2.05
14	B	1023	CLA	C4B-NB	-3.50	1.33	1.37
14	b	1206	CLA	CHB-C1B	3.50	1.47	1.39
14	a	1115	CLA	OBD-CAD	3.50	1.28	1.22
14	B	1238	CLA	MG-ND	-3.50	1.98	2.05
14	b	1238	CLA	MG-ND	-3.50	1.98	2.05
14	a	1118	CLA	CHB-C1B	3.50	1.47	1.39
13	a	1011	CL0	CHC-C1C	3.50	1.46	1.39
14	a	1133	CLA	OBD-CAD	3.50	1.28	1.22
14	a	1131	CLA	CHC-C4B	3.50	1.47	1.39
14	a	1115	CLA	CHB-C1B	3.50	1.47	1.39
14	A	1140	CLA	CHB-C1B	3.50	1.47	1.39
18	M	4021	BCR	C11-C12	-3.50	1.25	1.34
14	a	1119	CLA	C1B-NB	-3.50	1.33	1.37
14	a	1139	CLA	C1D-ND	-3.50	1.33	1.37
14	a	1136	CLA	C1B-NB	-3.50	1.33	1.37
13	A	1011	CL0	CHC-C1C	3.50	1.46	1.39
14	G	1131	CLA	CHC-C4B	3.50	1.47	1.39
14	a	1122	CLA	CHD-C4C	3.50	1.47	1.39
14	G	1138	CLA	C1D-ND	-3.50	1.33	1.37
14	A	1129	CLA	CHD-C4C	3.50	1.47	1.39
14	B	1208	CLA	OBD-CAD	3.50	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1210	CLA	C4B-NB	-3.50	1.33	1.37
14	U	1501	CLA	CHD-C4C	3.50	1.47	1.39
14	G	1129	CLA	C1B-NB	-3.50	1.33	1.37
14	a	1125	CLA	MG-ND	-3.50	1.98	2.05
15	a	1121	F6C	MG-NC	3.49	2.12	2.05
14	G	1132	CLA	C1D-ND	-3.49	1.33	1.37
14	A	1126	CLA	MG-ND	-3.49	1.98	2.05
14	a	1109	CLA	CHB-C1B	3.49	1.47	1.39
14	H	1205	CLA	CHC-C4B	3.49	1.47	1.39
14	H	1012	CLA	MG-ND	-3.49	1.98	2.05
14	H	1238	CLA	MG-ND	-3.49	1.98	2.05
14	b	1201	CLA	OBD-CAD	3.49	1.28	1.22
14	H	1208	CLA	OBD-CAD	3.49	1.28	1.22
14	A	1113	CLA	C4B-NB	-3.49	1.33	1.37
14	G	1106	CLA	CHC-C4B	3.49	1.47	1.39
14	B	1214	CLA	C1D-ND	-3.49	1.33	1.37
14	G	1135	CLA	C1B-NB	-3.49	1.33	1.37
14	a	1132	CLA	C1D-ND	-3.49	1.33	1.37
14	b	1227	CLA	C1B-NB	-3.49	1.33	1.37
14	A	1116	CLA	CHB-C1B	3.49	1.47	1.39
14	G	1118	CLA	CHB-C1B	3.49	1.47	1.39
14	A	1122	CLA	CHD-C4C	3.49	1.47	1.39
14	G	1140	CLA	CHB-C1B	3.49	1.47	1.39
14	B	1204	CLA	MG-ND	-3.49	1.98	2.05
14	A	1118	CLA	CHB-C1B	3.49	1.47	1.39
14	B	1205	CLA	CHC-C4B	3.49	1.47	1.39
14	B	1022	CLA	MG-ND	-3.49	1.98	2.05
14	B	1220	CLA	C1B-NB	-3.49	1.33	1.37
14	b	1227	CLA	OBD-CAD	3.49	1.28	1.22
14	a	1112	CLA	CHC-C4B	3.48	1.47	1.39
14	A	1130	CLA	MG-ND	-3.48	1.98	2.05
14	a	1124	CLA	C1B-NB	-3.48	1.33	1.37
14	B	1214	CLA	MG-ND	-3.48	1.98	2.05
14	G	1133	CLA	C1D-ND	-3.48	1.33	1.37
14	H	1023	CLA	C4B-NB	-3.48	1.33	1.37
14	H	1201	CLA	OBD-CAD	3.48	1.28	1.22
14	B	1202	CLA	CHD-C4C	3.48	1.47	1.39
14	G	1109	CLA	OBD-CAD	3.48	1.28	1.22
14	b	1202	CLA	OBD-CAD	3.48	1.28	1.22
14	G	1109	CLA	CHB-C1B	3.48	1.47	1.39
14	a	1135	CLA	CHB-C1B	3.48	1.47	1.39
14	B	1227	CLA	CHC-C4B	3.48	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1232	CLA	OBD-CAD	3.48	1.28	1.22
14	X	1701	CLA	CHD-C4C	3.48	1.47	1.39
14	G	1124	CLA	C1B-NB	-3.48	1.33	1.37
14	x	1701	CLA	CHD-C4C	3.48	1.47	1.39
14	H	1208	CLA	CHB-C1B	3.48	1.47	1.39
14	A	1135	CLA	CHB-C1B	3.48	1.47	1.39
14	A	1129	CLA	C1B-NB	-3.48	1.33	1.37
14	B	1232	CLA	OBD-CAD	3.48	1.28	1.22
14	G	1132	CLA	CHC-C4B	3.48	1.47	1.39
14	a	1110	CLA	CHD-C4C	3.48	1.47	1.39
14	A	1119	CLA	C1D-ND	-3.48	1.33	1.37
14	H	1202	CLA	CHC-C4B	3.48	1.47	1.39
14	A	1133	CLA	OBD-CAD	3.48	1.28	1.22
14	H	1202	CLA	MG-ND	-3.48	1.98	2.05
14	A	1105	CLA	OBD-CAD	3.47	1.28	1.22
14	A	1102	CLA	C1B-NB	-3.47	1.33	1.37
14	b	1214	CLA	C1D-ND	-3.47	1.33	1.37
15	H	1237	F6C	CHD-C4C	3.47	1.47	1.39
14	b	1223	CLA	CHB-C1B	3.47	1.47	1.39
14	a	1103	CLA	C1D-ND	-3.47	1.33	1.37
14	b	1202	CLA	CHC-C4B	3.47	1.47	1.39
14	b	1214	CLA	MG-ND	-3.47	1.98	2.05
14	H	1202	CLA	CHD-C4C	3.47	1.47	1.39
14	G	1126	CLA	CHC-C4B	3.47	1.47	1.39
14	b	1201	CLA	CHC-C4B	3.47	1.47	1.39
14	H	1207	CLA	C1D-ND	-3.47	1.33	1.37
14	b	1220	CLA	C1B-NB	-3.47	1.33	1.37
14	G	1115	CLA	CHB-C1B	3.47	1.47	1.39
14	G	1135	CLA	CHB-C1B	3.47	1.47	1.39
14	H	1214	CLA	C1B-NB	-3.47	1.33	1.37
14	A	1126	CLA	CHC-C4B	3.47	1.47	1.39
14	b	1216	CLA	OBD-CAD	3.47	1.28	1.22
14	A	1106	CLA	CHC-C4B	3.47	1.47	1.39
14	a	1129	CLA	C1B-NB	-3.47	1.33	1.37
15	G	1120	F6C	CHD-C1D	3.47	1.45	1.38
14	b	1210	CLA	C4B-NB	-3.47	1.33	1.37
14	A	1109	CLA	CHB-C1B	3.47	1.47	1.39
14	H	1216	CLA	OBD-CAD	3.47	1.28	1.22
14	B	1206	CLA	CHD-C4C	3.47	1.47	1.39
14	A	1132	CLA	OBD-CAD	3.47	1.28	1.22
14	B	1210	CLA	C1B-NB	-3.47	1.33	1.37
14	B	1214	CLA	C1B-NB	-3.47	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1220	CLA	C1D-ND	-3.47	1.33	1.37
14	A	1107	CLA	CHB-C1B	3.47	1.47	1.39
14	A	1112	CLA	CHC-C4B	3.47	1.47	1.39
14	H	1210	CLA	C4B-NB	-3.47	1.33	1.37
14	a	1136	CLA	CHD-C4C	3.47	1.47	1.39
14	a	1119	CLA	C1D-ND	-3.47	1.33	1.37
14	B	1206	CLA	CHB-C1B	3.47	1.47	1.39
14	G	1125	CLA	MG-ND	-3.47	1.98	2.05
14	G	1107	CLA	CHB-C1B	3.47	1.47	1.39
14	a	1127	CLA	CHB-C1B	3.47	1.47	1.39
14	G	1132	CLA	OBD-CAD	3.46	1.28	1.22
14	A	1115	CLA	CHB-C1B	3.46	1.47	1.39
14	b	1214	CLA	C1B-NB	-3.46	1.33	1.37
14	L	1501	CLA	CHD-C4C	3.46	1.47	1.39
14	G	1123	CLA	CHC-C4B	3.46	1.47	1.39
14	A	1136	CLA	CHD-C4C	3.46	1.47	1.39
14	a	1109	CLA	OBD-CAD	3.46	1.28	1.22
14	A	1132	CLA	CHC-C4B	3.46	1.47	1.39
14	a	1111	CLA	CHC-C4B	3.46	1.47	1.39
18	L	4019	BCR	C11-C12	-3.46	1.25	1.34
14	A	1103	CLA	C1D-ND	-3.46	1.33	1.37
13	G	1011	CL0	MG-ND	-3.46	1.98	2.05
13	A	1011	CL0	MG-ND	-3.46	1.98	2.05
14	A	1135	CLA	C1B-NB	-3.46	1.33	1.37
14	b	1231	CLA	C1B-NB	-3.46	1.33	1.37
14	a	1126	CLA	CHC-C4B	3.46	1.47	1.39
14	H	1220	CLA	OBD-CAD	3.46	1.28	1.22
14	G	1105	CLA	OBD-CAD	3.46	1.28	1.22
14	b	1203	CLA	CHC-C4B	3.46	1.47	1.39
14	b	1232	CLA	OBD-CAD	3.46	1.28	1.22
14	G	1130	CLA	MG-ND	-3.46	1.98	2.05
14	L	1503	CLA	CHB-C1B	3.46	1.47	1.39
14	a	1133	CLA	C1D-ND	-3.46	1.33	1.37
14	G	1133	CLA	OBD-CAD	3.46	1.28	1.22
14	a	1106	CLA	CHC-C4B	3.46	1.47	1.39
14	G	1122	CLA	CHD-C4C	3.46	1.47	1.39
14	B	1201	CLA	OBD-CAD	3.46	1.28	1.22
14	A	1107	CLA	MG-ND	-3.45	1.98	2.05
14	H	1231	CLA	C1B-NB	-3.45	1.33	1.37
14	H	1206	CLA	CHD-C4C	3.45	1.47	1.39
14	a	1107	CLA	CHD-C4C	3.45	1.47	1.39
14	G	1117	CLA	OBD-CAD	3.45	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1107	CLA	CHD-C4C	3.45	1.47	1.39
14	b	1201	CLA	C1D-ND	-3.45	1.33	1.37
14	b	1221	CLA	CHD-C4C	3.45	1.47	1.39
14	B	1202	CLA	CHC-C4B	3.45	1.47	1.39
14	W	1701	CLA	CHD-C4C	3.45	1.47	1.39
14	A	1132	CLA	C1D-ND	-3.45	1.33	1.37
14	G	1101	CLA	C1D-ND	-3.45	1.33	1.37
14	a	1107	CLA	CHB-C1B	3.45	1.47	1.39
14	a	1122	CLA	CHC-C4B	3.45	1.47	1.39
14	H	1202	CLA	OBD-CAD	3.45	1.28	1.22
14	B	1207	CLA	CHB-C1B	3.45	1.47	1.39
14	H	1227	CLA	CHB-C1B	3.45	1.47	1.39
14	l	1503	CLA	C1B-NB	-3.45	1.33	1.37
14	A	1125	CLA	MG-ND	-3.45	1.98	2.05
14	A	1109	CLA	OBD-CAD	3.45	1.28	1.22
14	G	1119	CLA	C1D-ND	-3.45	1.33	1.37
14	A	1127	CLA	CHB-C1B	3.45	1.47	1.39
15	B	1237	F6C	CHD-C4C	3.45	1.47	1.39
14	G	1111	CLA	CHC-C4B	3.45	1.47	1.39
14	G	1135	CLA	C4B-NB	-3.45	1.33	1.37
14	G	1139	CLA	OBD-CAD	3.45	1.28	1.22
14	U	1503	CLA	CHB-C1B	3.45	1.47	1.39
14	A	1133	CLA	CHC-C4B	3.45	1.47	1.39
15	G	1120	F6C	CHB-C1B	3.45	1.47	1.39
15	a	1120	F6C	CHD-C1D	3.45	1.45	1.38
14	H	1203	CLA	CHC-C4B	3.45	1.47	1.39
14	a	1123	CLA	CHC-C4B	3.45	1.47	1.39
14	H	1219	CLA	C1D-ND	-3.44	1.33	1.37
14	b	1207	CLA	C1D-ND	-3.44	1.33	1.37
14	a	1123	CLA	CHD-C4C	3.44	1.47	1.39
14	a	1105	CLA	OBD-CAD	3.44	1.28	1.22
14	A	1123	CLA	CHC-C4B	3.44	1.47	1.39
14	H	1227	CLA	C1B-NB	-3.44	1.33	1.37
13	a	1011	CL0	MG-ND	-3.44	1.99	2.05
14	A	1127	CLA	MG-ND	-3.44	1.99	2.05
14	b	1202	CLA	MG-ND	-3.44	1.99	2.05
14	B	1203	CLA	CHC-C4B	3.44	1.47	1.39
18	a	4003	BCR	C11-C12	-3.44	1.25	1.34
14	G	1102	CLA	C1B-NB	-3.44	1.33	1.37
14	H	1201	CLA	C1D-ND	-3.44	1.33	1.37
14	B	1227	CLA	CHB-C1B	3.44	1.47	1.39
14	a	1118	CLA	CHC-C4B	3.44	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1139	CLA	OBD-CAD	3.44	1.28	1.22
14	B	1229	CLA	C1D-ND	-3.44	1.33	1.37
14	H	1229	CLA	OBD-CAD	3.44	1.28	1.22
14	A	1012	CLA	C1B-NB	-3.44	1.33	1.37
14	G	1110	CLA	C1D-ND	-3.44	1.33	1.37
14	A	1122	CLA	CHC-C4B	3.44	1.47	1.39
14	B	1211	CLA	C1D-ND	-3.44	1.33	1.37
14	U	1502	CLA	C1B-NB	-3.44	1.33	1.37
14	a	1132	CLA	CHC-C4B	3.44	1.47	1.39
14	A	1139	CLA	OBD-CAD	3.44	1.28	1.22
14	a	1117	CLA	OBD-CAD	3.44	1.28	1.22
14	G	1112	CLA	CHC-C4B	3.44	1.47	1.39
14	A	1124	CLA	C1B-NB	-3.44	1.33	1.37
14	B	1207	CLA	C1D-ND	-3.44	1.33	1.37
14	L	1503	CLA	C1B-NB	-3.44	1.33	1.37
14	l	1502	CLA	C1B-NB	-3.44	1.33	1.37
14	B	1216	CLA	OBD-CAD	3.44	1.28	1.22
14	B	1201	CLA	CHC-C4B	3.44	1.47	1.39
14	B	1223	CLA	CHB-C1B	3.44	1.47	1.39
18	G	4003	BCR	C11-C12	-3.44	1.25	1.34
14	b	1206	CLA	CHD-C4C	3.44	1.47	1.39
14	G	1122	CLA	CHC-C4B	3.44	1.47	1.39
14	B	1231	CLA	C1B-NB	-3.43	1.33	1.37
14	H	1223	CLA	CHB-C1B	3.43	1.47	1.39
14	L	1502	CLA	C1B-NB	-3.43	1.33	1.37
14	a	1123	CLA	C1B-NB	-3.43	1.33	1.37
14	A	1107	CLA	CHC-C4B	3.43	1.47	1.39
14	A	1131	CLA	CHC-C4B	3.43	1.47	1.39
14	G	1136	CLA	CHD-C4C	3.43	1.47	1.39
14	a	1132	CLA	OBD-CAD	3.43	1.28	1.22
14	b	1239	CLA	C1C-NC	-3.43	1.32	1.37
14	l	1503	CLA	CHB-C1B	3.43	1.47	1.39
14	H	1201	CLA	CHC-C4B	3.43	1.47	1.39
14	A	1101	CLA	CHB-C1B	3.43	1.47	1.39
18	U	4019	BCR	C11-C12	-3.43	1.25	1.34
18	b	4005	BCR	C11-C12	-3.43	1.25	1.34
14	a	1130	CLA	MG-ND	-3.43	1.99	2.05
14	B	1229	CLA	OBD-CAD	3.43	1.28	1.22
14	G	1133	CLA	CHC-C4B	3.43	1.47	1.39
14	B	1232	CLA	CHC-C4B	3.43	1.47	1.39
14	G	1123	CLA	C1B-NB	-3.43	1.33	1.37
14	a	1107	CLA	CHC-C4B	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1117	CLA	OBD-CAD	3.43	1.28	1.22
14	a	1113	CLA	C1B-NB	-3.43	1.33	1.37
15	b	1237	F6C	CHD-C4C	3.43	1.47	1.39
14	a	1102	CLA	C1B-NB	-3.43	1.33	1.37
14	b	1211	CLA	C1D-ND	-3.43	1.33	1.37
14	a	1127	CLA	MG-ND	-3.43	1.99	2.05
14	G	1107	CLA	CHC-C4B	3.43	1.47	1.39
14	b	1211	CLA	CHB-C1B	3.42	1.47	1.39
14	H	1220	CLA	C1B-NB	-3.42	1.33	1.37
18	b	4013	BCR	C11-C12	-3.42	1.25	1.34
14	G	1123	CLA	CHD-C4C	3.42	1.47	1.39
14	b	1227	CLA	CHB-C1B	3.42	1.47	1.39
18	l	4019	BCR	C11-C12	-3.42	1.25	1.34
14	A	1110	CLA	C1D-ND	-3.42	1.33	1.37
14	A	1118	CLA	CHC-C4B	3.42	1.47	1.39
15	A	1120	F6C	CHB-C1B	3.42	1.47	1.39
14	H	1207	CLA	CHB-C1B	3.42	1.47	1.39
14	B	1202	CLA	MG-ND	-3.42	1.99	2.05
14	B	1231	CLA	C1D-ND	-3.42	1.33	1.37
15	a	1120	F6C	CHB-C1B	3.42	1.47	1.39
14	G	1107	CLA	MG-ND	-3.42	1.99	2.05
14	U	1502	CLA	CHC-C4B	3.42	1.47	1.39
14	a	1110	CLA	C1D-ND	-3.42	1.33	1.37
14	B	1211	CLA	C1B-NB	-3.42	1.33	1.37
14	H	1202	CLA	C1B-NB	-3.42	1.33	1.37
14	A	1111	CLA	CHC-C4B	3.42	1.47	1.39
14	B	1221	CLA	CHD-C4C	3.42	1.47	1.39
14	L	1502	CLA	CHB-C1B	3.42	1.47	1.39
14	G	1127	CLA	CHB-C1B	3.42	1.47	1.39
14	H	1229	CLA	C1D-ND	-3.42	1.33	1.37
14	a	1110	CLA	OBD-CAD	3.42	1.28	1.22
14	A	1140	CLA	CHD-C4C	3.42	1.47	1.39
14	G	1140	CLA	CHD-C4C	3.42	1.47	1.39
14	B	1239	CLA	C1C-NC	-3.42	1.32	1.37
14	G	1109	CLA	C1D-ND	-3.42	1.33	1.37
18	B	4005	BCR	C11-C12	-3.42	1.25	1.34
14	G	1129	CLA	CHB-C1B	3.42	1.47	1.39
14	b	1203	CLA	CHB-C1B	3.42	1.47	1.39
14	a	1113	CLA	C4B-NB	-3.42	1.33	1.37
14	b	1223	CLA	C1B-NB	-3.42	1.33	1.37
14	a	1107	CLA	MG-ND	-3.42	1.99	2.05
14	a	1109	CLA	C1D-ND	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1123	CLA	CHD-C4C	3.41	1.47	1.39
14	H	1221	CLA	CHD-C4C	3.41	1.47	1.39
14	B	1223	CLA	C1B-NB	-3.41	1.33	1.37
14	a	1101	CLA	C1D-ND	-3.41	1.33	1.37
14	b	1207	CLA	CHB-C1B	3.41	1.47	1.39
14	H	1229	CLA	C1B-NB	-3.41	1.33	1.37
14	B	1213	CLA	CHB-C1B	3.41	1.47	1.39
14	B	1225	CLA	C1C-NC	-3.41	1.32	1.37
14	A	1110	CLA	OBD-CAD	3.41	1.28	1.22
14	A	1107	CLA	CHD-C4C	3.41	1.47	1.39
14	H	1023	CLA	MG-ND	-3.41	1.99	2.05
14	B	1215	CLA	OBD-CAD	3.41	1.28	1.22
18	A	4003	BCR	C11-C12	-3.41	1.25	1.34
18	a	4002	BCR	C11-C12	-3.41	1.25	1.34
14	A	1109	CLA	CHC-C4B	3.41	1.47	1.39
14	H	1211	CLA	C1B-NB	-3.41	1.33	1.37
14	H	1239	CLA	C1C-NC	-3.41	1.32	1.37
14	G	1118	CLA	CHC-C4B	3.41	1.47	1.39
14	B	1232	CLA	CHB-C1B	3.41	1.47	1.39
14	H	1213	CLA	CHB-C1B	3.41	1.47	1.39
14	H	1210	CLA	C1B-NB	-3.41	1.33	1.37
14	b	1219	CLA	C1D-ND	-3.41	1.33	1.37
18	b	4004	BCR	C11-C12	-3.41	1.25	1.34
14	B	1210	CLA	OBD-CAD	3.41	1.28	1.22
14	b	1232	CLA	CHC-C4B	3.41	1.47	1.39
14	b	1220	CLA	OBD-CAD	3.41	1.28	1.22
14	b	1215	CLA	CHC-C4B	3.40	1.47	1.39
18	G	4002	BCR	C11-C12	-3.40	1.25	1.34
14	H	1203	CLA	CHB-C1B	3.40	1.47	1.39
14	H	1208	CLA	C1D-ND	-3.40	1.33	1.37
14	B	1023	CLA	MG-ND	-3.40	1.99	2.05
14	G	1126	CLA	C1B-NB	-3.40	1.33	1.37
14	b	1021	CLA	CHD-C1D	3.40	1.45	1.38
14	b	1210	CLA	C1B-NB	-3.40	1.33	1.37
15	a	1120	F6C	C3B-C2B	3.40	1.47	1.39
14	a	1129	CLA	CHB-C1B	3.40	1.47	1.39
14	B	1232	CLA	C1B-NB	-3.40	1.33	1.37
14	B	1203	CLA	CHB-C1B	3.40	1.47	1.39
14	a	1109	CLA	CHC-C4B	3.40	1.47	1.39
14	A	1129	CLA	MG-ND	-3.40	1.99	2.05
14	a	1101	CLA	CHB-C1B	3.40	1.47	1.39
14	l	1502	CLA	CHB-C1B	3.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4013	BCR	C11-C12	-3.40	1.25	1.34
14	G	1127	CLA	CHC-C4B	3.40	1.47	1.39
14	b	1224	CLA	OBD-CAD	3.40	1.28	1.22
18	B	4013	BCR	C11-C12	-3.40	1.25	1.34
14	G	1103	CLA	C1D-ND	-3.40	1.33	1.37
14	a	1133	CLA	CHC-C4B	3.40	1.47	1.39
14	B	1221	CLA	C1B-NB	-3.40	1.33	1.37
15	A	1121	F6C	C1C-NC	-3.40	1.33	1.37
14	H	1215	CLA	CHC-C4B	3.40	1.47	1.39
14	G	1122	CLA	C1C-NC	-3.39	1.32	1.37
14	G	1113	CLA	C4B-NB	-3.39	1.33	1.37
14	A	1123	CLA	MG-ND	-3.39	1.99	2.05
14	b	1023	CLA	MG-ND	-3.39	1.99	2.05
14	A	1111	CLA	C1D-ND	-3.39	1.33	1.37
15	G	1121	F6C	C1C-NC	-3.39	1.33	1.37
14	H	1224	CLA	OBD-CAD	3.39	1.28	1.22
18	B	4004	BCR	C11-C12	-3.39	1.25	1.34
14	b	1232	CLA	CHB-C1B	3.39	1.47	1.39
14	B	1219	CLA	C1D-ND	-3.39	1.33	1.37
14	G	1135	CLA	CHC-C4B	3.39	1.47	1.39
14	B	1224	CLA	OBD-CAD	3.39	1.28	1.22
14	H	1204	CLA	CHC-C4B	3.39	1.47	1.39
14	a	1135	CLA	CHC-C4B	3.39	1.47	1.39
14	l	1502	CLA	CHC-C4B	3.39	1.47	1.39
14	G	1111	CLA	C1D-ND	-3.39	1.33	1.37
14	H	1211	CLA	C1D-ND	-3.39	1.33	1.37
14	G	1131	CLA	MG-ND	-3.39	1.99	2.05
18	H	4004	BCR	C11-C12	-3.39	1.25	1.34
14	A	1129	CLA	CHB-C1B	3.39	1.47	1.39
14	a	1111	CLA	C1D-ND	-3.39	1.33	1.37
14	b	1211	CLA	C1B-NB	-3.39	1.33	1.37
14	A	1127	CLA	CHC-C4B	3.39	1.47	1.39
14	G	1109	CLA	CHC-C4B	3.39	1.47	1.39
14	G	1127	CLA	MG-ND	-3.39	1.99	2.05
14	H	1021	CLA	CHD-C1D	3.39	1.45	1.38
14	G	1101	CLA	CHB-C1B	3.38	1.47	1.39
14	U	1502	CLA	CHB-C1B	3.38	1.47	1.39
14	G	1129	CLA	MG-ND	-3.38	1.99	2.05
14	b	1231	CLA	C1D-ND	-3.38	1.33	1.37
14	b	1213	CLA	CHB-C1B	3.38	1.47	1.39
14	b	1215	CLA	OBD-CAD	3.38	1.28	1.22
14	H	1223	CLA	MG-ND	-3.38	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1211	CLA	CHB-C1B	3.38	1.47	1.39
14	b	1225	CLA	C1C-NC	-3.38	1.32	1.37
14	B	1205	CLA	CHD-C4C	3.38	1.46	1.39
14	H	1232	CLA	CHC-C4B	3.38	1.47	1.39
14	a	1140	CLA	CHD-C4C	3.38	1.46	1.39
14	a	1012	CLA	C1B-NB	-3.38	1.33	1.37
14	b	1232	CLA	C1B-NB	-3.38	1.33	1.37
14	a	1139	CLA	CHB-C1B	3.38	1.47	1.39
14	b	1234	CLA	CHB-C1B	3.38	1.47	1.39
14	B	1023	CLA	CHD-C4C	3.38	1.46	1.39
14	A	1104	CLA	CHC-C4B	3.38	1.47	1.39
14	H	1232	CLA	CHB-C1B	3.38	1.47	1.39
14	B	1219	CLA	OBD-CAD	3.38	1.28	1.22
14	B	1215	CLA	CHC-C4B	3.38	1.47	1.39
14	H	1210	CLA	CHC-C4B	3.38	1.47	1.39
14	H	1235	CLA	C1B-NB	-3.38	1.33	1.37
14	b	1208	CLA	C1D-ND	-3.38	1.33	1.37
14	b	1236	CLA	CHB-C1B	3.38	1.47	1.39
14	H	1211	CLA	CHB-C1B	3.38	1.47	1.39
14	b	1229	CLA	OBD-CAD	3.38	1.28	1.22
14	a	1114	CLA	CHC-C4B	3.38	1.47	1.39
14	a	1135	CLA	C4B-NB	-3.38	1.33	1.37
14	A	1012	CLA	CHC-C4B	3.38	1.47	1.39
14	a	1012	CLA	CHC-C4B	3.38	1.47	1.39
14	H	1215	CLA	OBD-CAD	3.37	1.28	1.22
18	H	4005	BCR	C11-C12	-3.37	1.25	1.34
14	a	1131	CLA	MG-ND	-3.37	1.99	2.05
14	a	1127	CLA	CHC-C4B	3.37	1.47	1.39
14	b	1219	CLA	OBD-CAD	3.37	1.28	1.22
18	A	4002	BCR	C11-C12	-3.37	1.25	1.34
14	H	1221	CLA	C1B-NB	-3.37	1.33	1.37
15	a	1121	F6C	C1C-NC	-3.37	1.33	1.37
14	G	1012	CLA	CHC-C4B	3.37	1.47	1.39
14	B	1220	CLA	OBD-CAD	3.37	1.28	1.22
14	H	1228	CLA	CHC-C4B	3.37	1.47	1.39
14	H	1207	CLA	CHC-C4B	3.37	1.47	1.39
14	A	1125	CLA	C4B-NB	-3.37	1.33	1.37
14	B	1208	CLA	C1D-ND	-3.37	1.33	1.37
14	b	1235	CLA	C1B-NB	-3.37	1.33	1.37
14	B	1021	CLA	CHD-C1D	3.37	1.45	1.38
14	H	1224	CLA	CHD-C4C	3.37	1.46	1.39
14	B	1210	CLA	CHC-C4B	3.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1201	CLA	C1D-ND	-3.37	1.33	1.37
14	H	1205	CLA	CHD-C4C	3.37	1.46	1.39
14	G	1112	CLA	CHB-C1B	3.37	1.47	1.39
14	A	1135	CLA	OBD-CAD	3.37	1.28	1.22
14	H	1231	CLA	C1D-ND	-3.37	1.33	1.37
14	a	1123	CLA	MG-ND	-3.37	1.99	2.05
14	U	1503	CLA	C1B-NB	-3.37	1.33	1.37
14	A	1131	CLA	MG-ND	-3.37	1.99	2.05
14	H	1225	CLA	C1C-NC	-3.37	1.32	1.37
15	G	1120	F6C	C3B-C2B	3.37	1.47	1.39
14	H	1206	CLA	MG-ND	-3.37	1.99	2.05
14	b	1223	CLA	MG-ND	-3.37	1.99	2.05
14	A	1013	CLA	OBD-CAD	3.36	1.28	1.22
14	a	1127	CLA	OBD-CAD	3.36	1.28	1.22
14	b	1205	CLA	CHD-C4C	3.36	1.46	1.39
14	A	1109	CLA	C1D-ND	-3.36	1.33	1.37
14	L	1502	CLA	CHC-C4B	3.36	1.47	1.39
14	a	1129	CLA	MG-ND	-3.36	1.99	2.05
14	H	1226	CLA	OBD-CAD	3.36	1.28	1.22
14	B	1204	CLA	CHC-C4B	3.36	1.47	1.39
14	b	1228	CLA	CHC-C4B	3.36	1.47	1.39
14	b	1205	CLA	MG-ND	-3.36	1.99	2.05
14	A	1111	CLA	C1B-NB	-3.36	1.33	1.37
14	G	1012	CLA	C1B-NB	-3.36	1.33	1.37
14	b	1023	CLA	CHD-C4C	3.36	1.46	1.39
14	B	1207	CLA	CHC-C4B	3.36	1.47	1.39
14	G	1113	CLA	C1B-NB	-3.36	1.33	1.37
14	H	1234	CLA	CHB-C1B	3.36	1.47	1.39
14	G	1104	CLA	CHC-C4B	3.36	1.47	1.39
14	G	1119	CLA	OBD-CAD	3.36	1.28	1.22
14	b	1204	CLA	C4B-NB	-3.36	1.33	1.37
14	b	1210	CLA	CHC-C4B	3.36	1.47	1.39
14	H	1023	CLA	CHD-C4C	3.36	1.46	1.39
14	G	1103	CLA	C1B-NB	-3.36	1.33	1.37
14	a	1104	CLA	CHB-C1B	3.36	1.46	1.39
14	H	1232	CLA	C1B-NB	-3.36	1.33	1.37
14	G	1110	CLA	OBD-CAD	3.36	1.28	1.22
15	A	1120	F6C	C3B-C2B	3.36	1.47	1.39
14	a	1126	CLA	OBD-CAD	3.36	1.28	1.22
14	A	1125	CLA	CHC-C4B	3.36	1.46	1.39
14	b	1207	CLA	CHC-C4B	3.36	1.46	1.39
14	G	1013	CLA	OBD-CAD	3.36	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1125	CLA	CHB-C1B	3.35	1.46	1.39
14	G	1139	CLA	CHB-C1B	3.35	1.46	1.39
14	b	1206	CLA	C1C-NC	-3.35	1.32	1.37
14	H	1221	CLA	MG-ND	-3.35	1.99	2.05
14	b	1224	CLA	CHD-C4C	3.35	1.46	1.39
14	A	1135	CLA	CHC-C4B	3.35	1.46	1.39
14	b	1221	CLA	MG-ND	-3.35	1.99	2.05
14	G	1111	CLA	C1B-NB	-3.35	1.33	1.37
14	b	1022	CLA	CHD-C4C	3.35	1.46	1.39
14	b	1202	CLA	C1B-NB	-3.35	1.33	1.37
14	B	1236	CLA	CHB-C1B	3.35	1.46	1.39
14	H	1206	CLA	C1C-NC	-3.35	1.32	1.37
14	a	1122	CLA	C1C-NC	-3.35	1.32	1.37
14	B	1228	CLA	CHC-C4B	3.35	1.46	1.39
14	a	1104	CLA	CHC-C4B	3.35	1.46	1.39
14	b	1206	CLA	MG-ND	-3.35	1.99	2.05
14	B	1234	CLA	CHB-C1B	3.35	1.46	1.39
14	a	1125	CLA	CHB-C1B	3.35	1.46	1.39
14	b	1220	CLA	CHC-C4B	3.35	1.46	1.39
14	L	1503	CLA	CHC-C4B	3.35	1.46	1.39
14	H	1209	CLA	OBD-CAD	3.35	1.28	1.22
14	a	1013	CLA	OBD-CAD	3.35	1.28	1.22
15	B	1237	F6C	CHB-C1B	3.35	1.46	1.39
14	G	1125	CLA	CHC-C4B	3.35	1.46	1.39
14	B	1213	CLA	C1D-ND	-3.35	1.33	1.37
14	a	1111	CLA	C1B-NB	-3.35	1.33	1.37
14	b	1229	CLA	C1D-ND	-3.35	1.33	1.37
15	H	1237	F6C	CHB-C1B	3.35	1.46	1.39
14	H	1219	CLA	OBD-CAD	3.35	1.28	1.22
14	B	1221	CLA	MG-ND	-3.34	1.99	2.05
14	l	1503	CLA	CHC-C4B	3.34	1.46	1.39
15	a	1121	F6C	CHB-C1B	3.34	1.46	1.39
14	B	1209	CLA	OBD-CAD	3.34	1.28	1.22
14	B	1206	CLA	MG-ND	-3.34	1.99	2.05
14	A	1125	CLA	CHB-C1B	3.34	1.46	1.39
14	H	1210	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1229	CLA	C1B-NB	-3.34	1.33	1.37
14	A	1135	CLA	C4B-NB	-3.34	1.33	1.37
14	H	1218	CLA	C1D-ND	-3.34	1.33	1.37
14	b	1209	CLA	C1D-ND	-3.34	1.33	1.37
14	A	1139	CLA	CHB-C1B	3.34	1.46	1.39
14	A	1122	CLA	OBD-CAD	3.34	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1226	CLA	OBD-CAD	3.34	1.28	1.22
15	a	1120	F6C	C1D-ND	-3.34	1.32	1.37
14	G	1123	CLA	MG-ND	-3.34	1.99	2.05
14	a	1122	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1210	CLA	OBD-CAD	3.34	1.28	1.22
14	U	1503	CLA	CHC-C4B	3.34	1.46	1.39
14	b	1204	CLA	CHC-C4B	3.34	1.46	1.39
14	H	1203	CLA	CHD-C4C	3.34	1.46	1.39
14	B	1235	CLA	C1B-NB	-3.34	1.33	1.37
14	G	1114	CLA	CHC-C4B	3.34	1.46	1.39
14	H	1205	CLA	MG-ND	-3.34	1.99	2.05
14	b	1201	CLA	C4B-NB	-3.34	1.33	1.37
14	G	1135	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1226	CLA	OBD-CAD	3.34	1.28	1.22
14	H	1236	CLA	CHB-C1B	3.34	1.46	1.39
14	A	1112	CLA	CHB-C1B	3.34	1.46	1.39
14	b	1221	CLA	C1B-NB	-3.34	1.33	1.37
14	a	1128	CLA	C1C-NC	-3.34	1.32	1.37
14	A	1127	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1223	CLA	CHD-C4C	3.34	1.46	1.39
14	a	1112	CLA	CHB-C1B	3.34	1.46	1.39
14	G	1128	CLA	C1C-NC	-3.34	1.32	1.37
14	G	1105	CLA	CHB-C1B	3.33	1.46	1.39
14	A	1103	CLA	C1B-NB	-3.33	1.33	1.37
14	G	1104	CLA	OBD-CAD	3.33	1.28	1.22
14	a	1125	CLA	CHC-C4B	3.33	1.46	1.39
14	A	1122	CLA	C1C-NC	-3.33	1.32	1.37
14	G	1125	CLA	C4B-NB	-3.33	1.33	1.37
14	B	1223	CLA	CHD-C4C	3.33	1.46	1.39
14	B	1204	CLA	C4B-NB	-3.33	1.33	1.37
14	G	1125	CLA	C1D-ND	-3.33	1.33	1.37
14	H	1201	CLA	C4B-NB	-3.33	1.33	1.37
14	a	1103	CLA	C1B-NB	-3.33	1.33	1.37
14	B	1236	CLA	OBD-CAD	3.33	1.28	1.22
14	b	1236	CLA	OBD-CAD	3.33	1.28	1.22
14	B	1220	CLA	CHC-C4B	3.33	1.46	1.39
14	b	1226	CLA	C1C-NC	-3.33	1.32	1.37
14	a	1126	CLA	C1B-NB	-3.33	1.33	1.37
14	A	1104	CLA	CHB-C1B	3.33	1.46	1.39
14	A	1113	CLA	CHC-C4B	3.33	1.46	1.39
14	a	1139	CLA	C1B-NB	-3.33	1.33	1.37
14	G	1126	CLA	OBD-CAD	3.33	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1201	CLA	C4B-NB	-3.33	1.33	1.37
15	G	1121	F6C	CHB-C1B	3.33	1.46	1.39
15	A	1121	F6C	CHB-C1B	3.33	1.46	1.39
14	B	1224	CLA	CHD-C4C	3.33	1.46	1.39
14	A	1119	CLA	OBD-CAD	3.33	1.28	1.22
14	B	1223	CLA	MG-ND	-3.33	1.99	2.05
14	H	1222	CLA	OBD-CAD	3.33	1.28	1.22
14	B	1218	CLA	C1D-ND	-3.33	1.33	1.37
14	H	1209	CLA	C1D-ND	-3.33	1.33	1.37
14	a	1113	CLA	CHB-C1B	3.33	1.46	1.39
14	H	1204	CLA	C4B-NB	-3.33	1.33	1.37
14	G	1137	CLA	MG-ND	-3.33	1.99	2.05
14	A	1126	CLA	OBD-CAD	3.32	1.28	1.22
14	a	1135	CLA	OBD-CAD	3.32	1.28	1.22
14	H	1012	CLA	CHD-C4C	3.32	1.46	1.39
14	B	1205	CLA	MG-ND	-3.32	1.99	2.05
14	a	1137	CLA	MG-ND	-3.32	1.99	2.05
15	A	1121	F6C	CHC-C1C	3.32	1.46	1.39
14	B	1202	CLA	C1B-NB	-3.32	1.33	1.37
14	G	1113	CLA	CHC-C4B	3.32	1.46	1.39
15	A	1120	F6C	C1D-ND	-3.32	1.32	1.37
14	A	1113	CLA	CHB-C1B	3.32	1.46	1.39
14	H	1229	CLA	CHB-C1B	3.32	1.46	1.39
14	H	1223	CLA	CHD-C4C	3.32	1.46	1.39
14	b	1239	CLA	OBD-CAD	3.32	1.28	1.22
14	A	1126	CLA	C1B-NB	-3.32	1.33	1.37
14	H	1223	CLA	C1B-NB	-3.32	1.33	1.37
14	b	1229	CLA	CHB-C1B	3.32	1.46	1.39
14	b	1222	CLA	OBD-CAD	3.32	1.28	1.22
14	A	1108	CLA	C1D-ND	-3.32	1.33	1.37
14	B	1227	CLA	MG-ND	-3.32	1.99	2.05
15	b	1237	F6C	CHB-C1B	3.32	1.46	1.39
14	H	1220	CLA	CHC-C4B	3.32	1.46	1.39
14	G	1127	CLA	OBD-CAD	3.32	1.28	1.22
14	H	1239	CLA	OBD-CAD	3.32	1.28	1.22
14	G	1104	CLA	CHB-C1B	3.32	1.46	1.39
14	A	1114	CLA	CHC-C4B	3.32	1.46	1.39
14	a	1125	CLA	C1D-ND	-3.32	1.33	1.37
14	H	1236	CLA	OBD-CAD	3.32	1.28	1.22
14	b	1234	CLA	CHD-C1D	3.32	1.44	1.38
15	G	1121	F6C	CHC-C1C	3.32	1.46	1.39
14	H	1225	CLA	CHB-C1B	3.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	1120	F6C	C1D-ND	-3.32	1.32	1.37
14	L	1501	CLA	CHB-C1B	3.31	1.46	1.39
14	G	1137	CLA	C4B-NB	-3.31	1.33	1.37
14	a	1113	CLA	CHC-C4B	3.31	1.46	1.39
15	B	1237	F6C	MG-NC	3.31	2.12	2.05
14	G	1122	CLA	OBD-CAD	3.31	1.28	1.22
14	G	1122	CLA	C1B-NB	-3.31	1.33	1.37
14	A	1136	CLA	CHB-C1B	3.31	1.46	1.39
14	b	1214	CLA	CHC-C4B	3.31	1.46	1.39
14	B	1229	CLA	CHB-C1B	3.31	1.46	1.39
14	B	1234	CLA	C1B-NB	-3.31	1.33	1.37
14	B	1021	CLA	CHC-C4B	3.31	1.46	1.39
14	B	1225	CLA	CHC-C4B	3.31	1.46	1.39
14	b	1234	CLA	C1B-NB	-3.31	1.33	1.37
14	A	1105	CLA	CHB-C1B	3.31	1.46	1.39
14	H	1021	CLA	CHC-C4B	3.31	1.46	1.39
14	a	1136	CLA	CHB-C1B	3.31	1.46	1.39
14	B	1222	CLA	OBD-CAD	3.31	1.28	1.22
14	A	1126	CLA	C4B-NB	-3.31	1.33	1.37
14	H	1227	CLA	MG-ND	-3.31	1.99	2.05
14	b	1225	CLA	CHB-C1B	3.31	1.46	1.39
15	G	1120	F6C	MG-NC	3.31	2.12	2.05
14	A	1122	CLA	C1B-NB	-3.30	1.33	1.37
14	b	1218	CLA	C1D-ND	-3.30	1.33	1.37
14	b	1209	CLA	OBD-CAD	3.30	1.28	1.22
14	G	1103	CLA	CHB-C1B	3.30	1.46	1.39
14	a	1105	CLA	CHB-C1B	3.30	1.46	1.39
15	a	1121	F6C	CHC-C1C	3.30	1.46	1.39
14	b	1213	CLA	C1D-ND	-3.30	1.33	1.37
14	B	1206	CLA	C1C-NC	-3.30	1.32	1.37
14	A	1013	CLA	CHD-C4C	3.30	1.46	1.39
14	B	1203	CLA	CHD-C4C	3.30	1.46	1.39
15	A	1120	F6C	MG-NC	3.30	2.12	2.05
14	a	1119	CLA	OBD-CAD	3.30	1.28	1.22
14	b	1021	CLA	CHC-C4B	3.30	1.46	1.39
14	B	1225	CLA	OBD-CAD	3.30	1.28	1.22
14	a	1124	CLA	OBD-CAD	3.30	1.28	1.22
14	A	1128	CLA	C1C-NC	-3.30	1.32	1.37
14	G	1013	CLA	CHD-C4C	3.30	1.46	1.39
14	H	1234	CLA	C1B-NB	-3.30	1.33	1.37
14	H	1225	CLA	CHC-C4B	3.30	1.46	1.39
14	A	1113	CLA	C1B-NB	-3.30	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1137	CLA	MG-ND	-3.30	1.99	2.05
14	A	1103	CLA	CHB-C1B	3.30	1.46	1.39
14	b	1205	CLA	C1C-NC	-3.30	1.32	1.37
14	H	1226	CLA	C1C-NC	-3.30	1.32	1.37
14	G	1136	CLA	CHB-C1B	3.29	1.46	1.39
14	B	1022	CLA	CHD-C4C	3.29	1.46	1.39
14	B	1229	CLA	C1B-NB	-3.29	1.33	1.37
14	B	1234	CLA	CHD-C1D	3.29	1.44	1.38
15	H	1237	F6C	MG-NC	3.29	2.12	2.05
14	G	1138	CLA	OBD-CAD	3.29	1.28	1.22
14	a	1104	CLA	OBD-CAD	3.29	1.28	1.22
14	a	1103	CLA	CHB-C1B	3.29	1.46	1.39
14	G	1124	CLA	OBD-CAD	3.29	1.28	1.22
14	b	1225	CLA	OBD-CAD	3.29	1.28	1.22
14	b	1203	CLA	CHD-C4C	3.29	1.46	1.39
14	b	1225	CLA	CHC-C4B	3.29	1.46	1.39
14	b	1219	CLA	C1B-NB	-3.29	1.33	1.37
14	b	1234	CLA	C1C-NC	-3.29	1.32	1.37
14	B	1209	CLA	C1D-ND	-3.29	1.33	1.37
14	H	1236	CLA	C1B-NB	-3.29	1.33	1.37
14	X	1701	CLA	C1D-ND	-3.29	1.33	1.37
14	B	1226	CLA	C1C-NC	-3.29	1.32	1.37
14	A	1125	CLA	C1D-ND	-3.29	1.33	1.37
14	H	1211	CLA	OBD-CAD	3.28	1.28	1.22
14	U	1501	CLA	CHB-C1B	3.28	1.46	1.39
14	H	1234	CLA	CHD-C1D	3.28	1.44	1.38
14	B	1225	CLA	CHB-C1B	3.28	1.46	1.39
14	a	1013	CLA	CHD-C4C	3.28	1.46	1.39
14	A	1124	CLA	OBD-CAD	3.28	1.28	1.22
15	a	1120	F6C	MG-NC	3.28	2.12	2.05
14	a	1106	CLA	OBD-CAD	3.28	1.28	1.22
14	a	1116	CLA	C1B-NB	-3.28	1.33	1.37
18	b	4006	BCR	C11-C12	-3.28	1.26	1.34
14	G	1139	CLA	C1B-NB	-3.28	1.33	1.37
14	G	1102	CLA	MG-ND	-3.28	1.99	2.05
14	A	1116	CLA	MG-ND	-3.28	1.99	2.05
15	b	1237	F6C	MG-NC	3.28	2.12	2.05
14	b	1221	CLA	CHB-C1B	3.28	1.46	1.39
14	H	1213	CLA	C1D-ND	-3.28	1.33	1.37
14	B	1214	CLA	CHC-C4B	3.28	1.46	1.39
14	A	1128	CLA	OBD-CAD	3.28	1.28	1.22
14	B	1234	CLA	C1C-NC	-3.27	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1216	CLA	CHC-C4B	3.27	1.46	1.39
14	B	1225	CLA	CHD-C4C	3.27	1.46	1.39
18	H	4006	BCR	C11-C12	-3.27	1.26	1.34
14	A	1104	CLA	OBD-CAD	3.27	1.28	1.22
14	a	1122	CLA	C1B-NB	-3.27	1.33	1.37
14	b	1222	CLA	CHB-C1B	3.27	1.46	1.39
14	b	1217	CLA	OBD-CAD	3.27	1.28	1.22
14	a	1108	CLA	C1D-ND	-3.27	1.33	1.37
14	G	1122	CLA	CHB-C1B	3.27	1.46	1.39
14	G	1106	CLA	OBD-CAD	3.27	1.28	1.22
14	H	1214	CLA	CHC-C4B	3.27	1.46	1.39
14	A	1102	CLA	MG-ND	-3.27	1.99	2.05
14	b	1211	CLA	OBD-CAD	3.27	1.28	1.22
14	a	1125	CLA	C4B-NB	-3.27	1.33	1.37
18	B	4006	BCR	C11-C12	-3.27	1.26	1.34
14	B	1211	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1221	CLA	CHB-C1B	3.27	1.46	1.39
14	H	1225	CLA	CHD-C4C	3.27	1.46	1.39
14	B	1205	CLA	C1C-NC	-3.27	1.32	1.37
14	H	1221	CLA	CHB-C1B	3.27	1.46	1.39
14	a	1101	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1021	CLA	OBD-CAD	3.26	1.28	1.22
14	G	1113	CLA	CHB-C1B	3.26	1.46	1.39
14	a	1126	CLA	C4B-NB	-3.26	1.33	1.37
14	A	1137	CLA	CHC-C4B	3.26	1.46	1.39
14	B	1222	CLA	CHB-C1B	3.26	1.46	1.39
14	b	1023	CLA	OBD-CAD	3.26	1.28	1.22
14	G	1140	CLA	OBD-CAD	3.26	1.28	1.22
14	A	1111	CLA	CHB-C1B	3.26	1.46	1.39
14	G	1128	CLA	OBD-CAD	3.26	1.28	1.22
14	b	1216	CLA	C4B-NB	-3.26	1.33	1.37
14	A	1140	CLA	OBD-CAD	3.26	1.28	1.22
14	B	1239	CLA	OBD-CAD	3.26	1.28	1.22
14	a	1138	CLA	OBD-CAD	3.26	1.28	1.22
14	G	1137	CLA	CHC-C4B	3.26	1.46	1.39
15	A	1120	F6C	OBD-CAD	3.26	1.28	1.22
14	l	1501	CLA	CHB-C1B	3.26	1.46	1.39
14	A	1137	CLA	C4B-NB	-3.26	1.33	1.37
14	H	1216	CLA	CHC-C4B	3.26	1.46	1.39
14	a	1102	CLA	MG-ND	-3.26	1.99	2.05
14	G	1101	CLA	OBD-CAD	3.26	1.28	1.22
14	a	1140	CLA	OBD-CAD	3.26	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1137	CLA	CHC-C4B	3.26	1.46	1.39
14	H	1205	CLA	C1C-NC	-3.26	1.32	1.37
14	A	1122	CLA	CHB-C1B	3.26	1.46	1.39
14	H	1225	CLA	OBD-CAD	3.26	1.28	1.22
14	H	1023	CLA	OBD-CAD	3.26	1.28	1.22
14	B	1228	CLA	CHB-C1B	3.25	1.46	1.39
14	a	1137	CLA	C4B-NB	-3.25	1.33	1.37
14	X	1701	CLA	OBD-CAD	3.25	1.28	1.22
14	H	1228	CLA	CHB-C1B	3.25	1.46	1.39
14	H	1239	CLA	CHC-C4B	3.25	1.46	1.39
14	b	1207	CLA	MG-ND	-3.25	1.99	2.05
14	H	1222	CLA	CHB-C1B	3.25	1.46	1.39
14	b	1225	CLA	CHD-C4C	3.25	1.46	1.39
14	A	1139	CLA	C1B-NB	-3.25	1.33	1.37
14	G	1111	CLA	C1C-NC	-3.25	1.32	1.37
14	l	1503	CLA	C1C-NC	-3.25	1.32	1.37
14	b	1239	CLA	CHC-C4B	3.25	1.46	1.39
14	A	1138	CLA	OBD-CAD	3.25	1.28	1.22
14	G	1116	CLA	MG-ND	-3.25	1.99	2.05
14	B	1236	CLA	C1B-NB	-3.25	1.33	1.37
14	H	1217	CLA	OBD-CAD	3.25	1.28	1.22
14	b	1228	CLA	CHB-C1B	3.25	1.46	1.39
14	H	1217	CLA	C1D-ND	-3.25	1.33	1.37
14	B	1217	CLA	OBD-CAD	3.25	1.28	1.22
14	H	1207	CLA	MG-ND	-3.25	1.99	2.05
13	G	1011	CL0	CHB-C4A	-3.25	1.34	1.38
14	B	1234	CLA	MG-ND	-3.25	1.99	2.05
14	b	1216	CLA	C1C-NC	-3.25	1.32	1.37
15	a	1120	F6C	C1C-NC	-3.25	1.33	1.37
14	B	1216	CLA	C1D-ND	-3.24	1.33	1.37
14	B	1219	CLA	C1B-NB	-3.24	1.33	1.37
14	x	1701	CLA	C1D-ND	-3.24	1.33	1.37
14	H	1209	CLA	CHB-C1B	3.24	1.46	1.39
15	A	1120	F6C	C1C-NC	-3.24	1.33	1.37
14	B	1209	CLA	CHB-C1B	3.24	1.46	1.39
14	b	1209	CLA	CHB-C1B	3.24	1.46	1.39
14	B	1219	CLA	CHB-C1B	3.24	1.46	1.39
14	a	1116	CLA	MG-ND	-3.24	1.99	2.05
14	B	1216	CLA	CHC-C4B	3.24	1.46	1.39
14	b	1227	CLA	MG-ND	-3.24	1.99	2.05
14	A	1101	CLA	OBD-CAD	3.24	1.28	1.22
15	B	1237	F6C	CHC-C1C	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1216	CLA	C1D-ND	-3.24	1.33	1.37
15	G	1120	F6C	OBD-CAD	3.24	1.28	1.22
14	b	1219	CLA	CHB-C1B	3.24	1.46	1.39
14	b	1216	CLA	C1D-ND	-3.23	1.33	1.37
14	H	1219	CLA	CHB-C1B	3.23	1.46	1.39
14	H	1219	CLA	C1B-NB	-3.23	1.33	1.37
14	G	1108	CLA	C1D-ND	-3.23	1.33	1.37
14	a	1122	CLA	CHB-C1B	3.23	1.46	1.39
14	H	1234	CLA	C1C-NC	-3.23	1.32	1.37
14	A	1106	CLA	OBD-CAD	3.23	1.28	1.22
14	b	1234	CLA	MG-ND	-3.23	1.99	2.05
14	a	1111	CLA	CHB-C1B	3.23	1.46	1.39
14	B	1023	CLA	OBD-CAD	3.23	1.28	1.22
14	H	1210	CLA	CHB-C1B	3.23	1.46	1.39
14	H	1021	CLA	OBD-CAD	3.23	1.28	1.22
14	B	1239	CLA	CHC-C4B	3.23	1.46	1.39
14	G	1126	CLA	C4B-NB	-3.23	1.33	1.37
14	L	1501	CLA	OBD-CAD	3.23	1.28	1.22
14	H	1234	CLA	MG-ND	-3.23	1.99	2.05
14	H	1216	CLA	C1C-NC	-3.23	1.32	1.37
14	L	1503	CLA	C1C-NC	-3.22	1.32	1.37
13	a	1011	CL0	CHB-C4A	-3.22	1.34	1.38
14	G	1116	CLA	OBD-CAD	3.22	1.28	1.22
14	a	1128	CLA	OBD-CAD	3.22	1.28	1.22
14	G	1118	CLA	C1B-NB	-3.22	1.33	1.37
14	H	1207	CLA	OBD-CAD	3.22	1.28	1.22
14	B	1207	CLA	MG-ND	-3.22	1.99	2.05
14	G	1111	CLA	CHB-C1B	3.22	1.46	1.39
14	H	1021	CLA	C4B-NB	-3.22	1.33	1.37
15	b	1237	F6C	CHC-C1C	3.22	1.46	1.39
15	a	1120	F6C	OBD-CAD	3.22	1.28	1.22
14	A	1118	CLA	C1D-ND	-3.22	1.33	1.37
15	G	1120	F6C	C1C-NC	-3.22	1.33	1.37
14	G	1013	CLA	C1C-NC	-3.22	1.32	1.37
14	G	1135	CLA	MG-ND	-3.22	1.99	2.05
14	B	1210	CLA	CHB-C1B	3.22	1.46	1.39
14	H	1234	CLA	CHD-C4C	3.22	1.46	1.39
14	x	1701	CLA	OBD-CAD	3.21	1.28	1.22
14	a	1118	CLA	C1B-NB	-3.21	1.33	1.37
14	B	1234	CLA	CHD-C4C	3.21	1.46	1.39
14	H	1238	CLA	OBD-CAD	3.21	1.28	1.22
14	b	1232	CLA	C1D-ND	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1116	CLA	C1B-NB	-3.21	1.33	1.37
14	L	1502	CLA	C1C-NC	-3.21	1.32	1.37
15	B	1237	F6C	C1D-ND	-3.21	1.32	1.37
14	a	1111	CLA	C1C-NC	-3.21	1.32	1.37
14	B	1207	CLA	OBD-CAD	3.21	1.28	1.22
14	A	1132	CLA	MG-ND	-3.21	1.99	2.05
14	a	1140	CLA	C1C-NC	-3.21	1.32	1.37
14	B	1021	CLA	C1C-NC	-3.21	1.32	1.37
14	b	1210	CLA	CHB-C1B	3.21	1.46	1.39
14	W	1701	CLA	C1D-ND	-3.21	1.33	1.37
14	b	1021	CLA	C4B-NB	-3.21	1.33	1.37
14	U	1503	CLA	C1C-NC	-3.20	1.32	1.37
14	a	1125	CLA	CHD-C4C	3.20	1.46	1.39
14	b	1234	CLA	CHD-C4C	3.20	1.46	1.39
14	G	1128	CLA	CHB-C1B	3.20	1.46	1.39
14	b	1021	CLA	OBD-CAD	3.20	1.28	1.22
14	A	1118	CLA	C1B-NB	-3.20	1.33	1.37
14	W	1701	CLA	OBD-CAD	3.20	1.28	1.22
14	a	1116	CLA	OBD-CAD	3.20	1.28	1.22
14	l	1503	CLA	OBD-CAD	3.20	1.28	1.22
14	A	1131	CLA	C1B-NB	-3.20	1.33	1.37
14	b	1217	CLA	C1D-ND	-3.20	1.33	1.37
14	a	1128	CLA	CHB-C1B	3.20	1.46	1.39
14	G	1012	CLA	OBD-CAD	3.20	1.28	1.22
14	B	1216	CLA	C1C-NC	-3.20	1.32	1.37
14	A	1103	CLA	C1C-NC	-3.20	1.32	1.37
14	A	1140	CLA	C1C-NC	-3.20	1.32	1.37
14	B	1022	CLA	OBD-CAD	3.20	1.28	1.22
14	b	1215	CLA	CHB-C1B	3.20	1.46	1.39
15	b	1237	F6C	C1D-ND	-3.20	1.32	1.37
13	A	1011	CL0	CHB-C4A	-3.20	1.34	1.38
14	a	1131	CLA	OBD-CAD	3.20	1.28	1.22
14	b	1207	CLA	OBD-CAD	3.20	1.28	1.22
14	H	1231	CLA	CHB-C1B	3.20	1.46	1.39
14	A	1013	CLA	C4B-NB	-3.20	1.33	1.37
15	H	1237	F6C	C1D-ND	-3.19	1.32	1.37
14	A	1127	CLA	C4B-NB	-3.19	1.33	1.37
14	A	1125	CLA	CHD-C4C	3.19	1.46	1.39
14	B	1232	CLA	C1D-ND	-3.19	1.33	1.37
14	B	1231	CLA	CHB-C1B	3.19	1.46	1.39
14	b	1022	CLA	CHB-C1B	3.19	1.46	1.39
14	b	1236	CLA	C1B-NB	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1202	CLA	CHB-C1B	3.19	1.46	1.39
14	G	1118	CLA	OBD-CAD	3.19	1.28	1.22
14	A	1110	CLA	MG-ND	-3.19	1.99	2.05
14	b	1214	CLA	CHB-C1B	3.19	1.46	1.39
14	a	1136	CLA	OBD-CAD	3.19	1.28	1.22
14	A	1103	CLA	C4B-NB	-3.19	1.33	1.37
14	l	1501	CLA	OBD-CAD	3.19	1.28	1.22
14	a	1131	CLA	C1B-NB	-3.19	1.33	1.37
14	A	1135	CLA	MG-ND	-3.19	1.99	2.05
14	B	1021	CLA	C4B-NB	-3.19	1.33	1.37
14	B	1217	CLA	C1D-ND	-3.19	1.33	1.37
14	A	1013	CLA	C1C-NC	-3.19	1.32	1.37
14	a	1111	CLA	C4B-NB	-3.19	1.33	1.37
14	a	1103	CLA	CHC-C4B	3.19	1.46	1.39
14	U	1503	CLA	OBD-CAD	3.19	1.28	1.22
14	A	1116	CLA	OBD-CAD	3.19	1.28	1.22
14	B	1216	CLA	C4B-NB	-3.19	1.33	1.37
14	H	1214	CLA	CHB-C1B	3.19	1.46	1.39
14	B	1216	CLA	MG-ND	-3.18	1.99	2.05
14	a	1133	CLA	MG-ND	-3.18	1.99	2.05
14	G	1116	CLA	C1B-NB	-3.18	1.33	1.37
15	b	1237	F6C	OBD-CAD	3.18	1.28	1.22
14	H	1225	CLA	C4B-NB	-3.18	1.33	1.37
14	A	1131	CLA	OBD-CAD	3.18	1.28	1.22
14	H	1215	CLA	CHB-C1B	3.18	1.46	1.39
14	b	1220	CLA	MG-ND	-3.18	1.99	2.05
15	H	1237	F6C	CHC-C1C	3.18	1.46	1.39
14	H	1021	CLA	C1C-NC	-3.18	1.32	1.37
14	a	1117	CLA	CHB-C1B	3.18	1.46	1.39
14	B	1202	CLA	CHB-C1B	3.18	1.46	1.39
14	U	1501	CLA	MG-ND	-3.18	1.99	2.05
14	a	1135	CLA	MG-ND	-3.18	1.99	2.05
14	H	1216	CLA	C4B-NB	-3.18	1.33	1.37
14	B	1207	CLA	C1B-NB	-3.18	1.33	1.37
14	b	1022	CLA	OBD-CAD	3.18	1.28	1.22
14	A	1128	CLA	CHB-C1B	3.18	1.46	1.39
14	a	1132	CLA	C1B-NB	-3.18	1.33	1.37
14	a	1103	CLA	C1C-NC	-3.18	1.32	1.37
14	G	1125	CLA	CHD-C4C	3.18	1.46	1.39
14	b	1231	CLA	CHB-C1B	3.18	1.46	1.39
14	B	1204	CLA	OBD-CAD	3.18	1.28	1.22
14	a	1132	CLA	MG-ND	-3.17	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1013	CLA	C1C-NC	-3.17	1.32	1.37
15	B	1237	F6C	OBD-CAD	3.17	1.28	1.22
14	b	1214	CLA	OBD-CAD	3.17	1.27	1.22
14	A	1126	CLA	C1C-NC	-3.17	1.32	1.37
14	G	1131	CLA	C1B-NB	-3.17	1.33	1.37
14	U	1501	CLA	OBD-CAD	3.17	1.27	1.22
14	a	1118	CLA	OBD-CAD	3.17	1.27	1.22
15	a	1121	F6C	OBD-CAD	3.17	1.27	1.22
14	G	1132	CLA	MG-ND	-3.17	1.99	2.05
14	B	1215	CLA	CHB-C1B	3.17	1.46	1.39
14	B	1022	CLA	C1B-NB	-3.17	1.33	1.37
14	G	1013	CLA	C4B-NB	-3.17	1.33	1.37
14	A	1137	CLA	C1B-NB	-3.17	1.33	1.37
14	A	1140	CLA	C1B-NB	-3.17	1.33	1.37
14	G	1113	CLA	MG-ND	-3.17	1.99	2.05
14	b	1204	CLA	OBD-CAD	3.17	1.27	1.22
14	A	1103	CLA	CHC-C4B	3.17	1.46	1.39
14	B	1238	CLA	OBD-CAD	3.17	1.27	1.22
14	U	1502	CLA	C1C-NC	-3.17	1.32	1.37
14	G	1131	CLA	OBD-CAD	3.17	1.27	1.22
14	a	1136	CLA	MG-ND	-3.17	1.99	2.05
14	G	1132	CLA	C1B-NB	-3.17	1.33	1.37
14	b	1022	CLA	C1B-NB	-3.17	1.33	1.37
14	a	1137	CLA	C1B-NB	-3.17	1.33	1.37
14	H	1202	CLA	CHB-C1B	3.17	1.46	1.39
14	l	1502	CLA	C1C-NC	-3.17	1.32	1.37
14	G	1140	CLA	C1B-NB	-3.17	1.33	1.37
14	a	1140	CLA	C1B-NB	-3.17	1.33	1.37
14	G	1136	CLA	MG-ND	-3.17	1.99	2.05
14	A	1107	CLA	C1B-NB	-3.17	1.33	1.37
14	G	1118	CLA	C1D-ND	-3.17	1.33	1.37
14	H	1232	CLA	C1D-ND	-3.17	1.33	1.37
14	H	1023	CLA	CHB-C1B	3.16	1.46	1.39
14	H	1012	CLA	OBD-CAD	3.16	1.27	1.22
14	A	1012	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1127	CLA	C4B-NB	-3.16	1.33	1.37
14	B	1220	CLA	MG-ND	-3.16	1.99	2.05
14	G	1103	CLA	C4B-NB	-3.16	1.33	1.37
14	G	1137	CLA	C1B-NB	-3.16	1.33	1.37
14	H	1201	CLA	C1B-NB	-3.16	1.33	1.37
14	A	1111	CLA	OBD-CAD	3.16	1.27	1.22
14	a	1111	CLA	OBD-CAD	3.16	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	1121	F6C	OBD-CAD	3.16	1.27	1.22
14	a	1113	CLA	MG-ND	-3.16	1.99	2.05
14	B	1214	CLA	CHB-C1B	3.16	1.46	1.39
14	L	1501	CLA	MG-ND	-3.16	1.99	2.05
14	B	1022	CLA	CHB-C1B	3.16	1.46	1.39
14	b	1216	CLA	MG-ND	-3.16	1.99	2.05
14	a	1126	CLA	C1C-NC	-3.16	1.32	1.37
14	H	1220	CLA	MG-ND	-3.16	1.99	2.05
14	a	1127	CLA	C4B-NB	-3.16	1.33	1.37
14	H	1012	CLA	CHB-C1B	3.16	1.46	1.39
14	a	1012	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1140	CLA	C1C-NC	-3.16	1.32	1.37
14	H	1203	CLA	C4B-NB	-3.16	1.33	1.37
14	H	1204	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1136	CLA	OBD-CAD	3.16	1.27	1.22
14	A	1132	CLA	C1B-NB	-3.16	1.33	1.37
14	H	1222	CLA	C4B-NB	-3.16	1.33	1.37
14	B	1239	CLA	MG-ND	-3.16	1.99	2.05
14	b	1235	CLA	C4B-NB	-3.16	1.33	1.37
14	A	1140	CLA	MG-ND	-3.16	1.99	2.05
14	a	1118	CLA	C1D-ND	-3.16	1.33	1.37
14	B	1214	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1103	CLA	MG-ND	-3.16	1.99	2.05
14	A	1113	CLA	MG-ND	-3.16	1.99	2.05
14	a	1138	CLA	C1B-NB	-3.15	1.33	1.37
14	A	1133	CLA	MG-ND	-3.15	1.99	2.05
14	A	1136	CLA	OBD-CAD	3.15	1.27	1.22
14	b	1221	CLA	OBD-CAD	3.15	1.27	1.22
14	G	1140	CLA	MG-ND	-3.15	1.99	2.05
14	H	1222	CLA	MG-ND	-3.15	1.99	2.05
14	b	1021	CLA	C1C-NC	-3.15	1.32	1.37
14	G	1110	CLA	MG-ND	-3.15	1.99	2.05
14	a	1140	CLA	MG-ND	-3.15	1.99	2.05
14	A	1111	CLA	C4B-NB	-3.15	1.33	1.37
14	b	1222	CLA	C4B-NB	-3.15	1.33	1.37
14	b	1239	CLA	MG-ND	-3.15	1.99	2.05
14	A	1111	CLA	C1C-NC	-3.15	1.32	1.37
14	A	1118	CLA	OBD-CAD	3.15	1.27	1.22
14	B	1201	CLA	C1B-NB	-3.15	1.33	1.37
14	b	1238	CLA	OBD-CAD	3.15	1.27	1.22
14	a	1110	CLA	MG-ND	-3.15	1.99	2.05
14	b	1203	CLA	MG-ND	-3.15	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1107	CLA	C1B-NB	-3.15	1.33	1.37
14	H	1012	CLA	C1B-NB	-3.15	1.33	1.37
14	b	1203	CLA	C4B-NB	-3.15	1.33	1.37
14	H	1239	CLA	MG-ND	-3.15	1.99	2.05
14	B	1205	CLA	OBD-CAD	3.15	1.27	1.22
14	G	1103	CLA	C1C-NC	-3.15	1.32	1.37
14	G	1103	CLA	CHC-C4B	3.15	1.46	1.39
14	l	1501	CLA	MG-ND	-3.15	1.99	2.05
14	A	1128	CLA	CHC-C4B	3.15	1.46	1.39
14	H	1203	CLA	MG-ND	-3.15	1.99	2.05
14	B	1225	CLA	C4B-NB	-3.15	1.33	1.37
14	b	1225	CLA	C4B-NB	-3.15	1.33	1.37
14	B	1235	CLA	C4B-NB	-3.15	1.33	1.37
14	G	1117	CLA	CHB-C1B	3.15	1.46	1.39
14	G	1128	CLA	CHC-C4B	3.14	1.46	1.39
14	H	1221	CLA	OBD-CAD	3.14	1.27	1.22
14	B	1023	CLA	CHD-C1D	3.14	1.44	1.38
14	B	1236	CLA	C1C-NC	-3.14	1.32	1.37
14	G	1130	CLA	C4B-NB	-3.14	1.33	1.37
14	A	1103	CLA	OBD-CAD	3.14	1.27	1.22
14	H	1201	CLA	CHB-C1B	3.14	1.46	1.39
14	B	1235	CLA	OBD-CAD	3.14	1.27	1.22
14	G	1133	CLA	MG-ND	-3.14	1.99	2.05
14	H	1214	CLA	OBD-CAD	3.14	1.27	1.22
14	G	1126	CLA	C1C-NC	-3.13	1.32	1.37
14	H	1235	CLA	OBD-CAD	3.13	1.27	1.22
14	a	1103	CLA	C4B-NB	-3.13	1.33	1.37
14	G	1118	CLA	MG-ND	-3.13	1.99	2.05
14	b	1207	CLA	C1B-NB	-3.13	1.33	1.37
15	H	1237	F6C	OBD-CAD	3.13	1.27	1.22
14	H	1236	CLA	C1C-NC	-3.13	1.33	1.37
14	a	1013	CLA	C4B-NB	-3.13	1.33	1.37
14	B	1228	CLA	C1C-NC	-3.13	1.33	1.37
14	a	1107	CLA	C1B-NB	-3.13	1.33	1.37
14	G	1111	CLA	OBD-CAD	3.13	1.27	1.22
14	H	1207	CLA	C1B-NB	-3.13	1.33	1.37
14	b	1236	CLA	C1C-NC	-3.13	1.33	1.37
14	H	1235	CLA	CHB-C1B	3.13	1.46	1.39
14	A	1124	CLA	C4B-NB	-3.13	1.33	1.37
14	a	1131	CLA	C1C-NC	-3.13	1.33	1.37
14	b	1201	CLA	CHB-C1B	3.13	1.46	1.39
14	L	1503	CLA	OBD-CAD	3.13	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1215	CLA	C4B-NB	-3.13	1.33	1.37
14	G	1132	CLA	C1C-NC	-3.13	1.33	1.37
14	A	1132	CLA	C1C-NC	-3.13	1.33	1.37
14	b	1205	CLA	OBD-CAD	3.13	1.27	1.22
14	B	1023	CLA	CHB-C1B	3.13	1.46	1.39
14	A	1112	CLA	C1B-NB	-3.13	1.33	1.37
14	a	1138	CLA	MG-ND	-3.12	1.99	2.05
14	H	1023	CLA	CHD-C1D	3.12	1.44	1.38
14	a	1112	CLA	C1B-NB	-3.12	1.33	1.37
14	B	1201	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1201	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1216	CLA	MG-ND	-3.12	1.99	2.05
14	A	1131	CLA	C1C-NC	-3.12	1.33	1.37
14	A	1138	CLA	MG-ND	-3.12	1.99	2.05
14	l	1502	CLA	MG-ND	-3.12	1.99	2.05
14	a	1138	CLA	CHB-C1B	3.12	1.46	1.39
14	A	1117	CLA	CHB-C1B	3.12	1.46	1.39
14	G	1130	CLA	CHB-C1B	3.12	1.46	1.39
14	b	1235	CLA	OBD-CAD	3.12	1.27	1.22
14	b	1222	CLA	MG-ND	-3.12	1.99	2.05
14	a	1113	CLA	C1C-NC	-3.12	1.33	1.37
14	b	1201	CLA	C1C-NC	-3.12	1.33	1.37
14	G	1113	CLA	OBD-CAD	3.12	1.27	1.22
14	b	1235	CLA	CHB-C1B	3.12	1.46	1.39
14	B	1222	CLA	C4B-NB	-3.12	1.33	1.37
14	a	1106	CLA	C4B-NB	-3.12	1.33	1.37
14	b	1209	CLA	C1B-NB	-3.12	1.33	1.37
14	a	1113	CLA	C1D-ND	-3.12	1.33	1.37
14	b	1023	CLA	CHD-C1D	3.12	1.44	1.38
14	G	1129	CLA	OBD-CAD	3.12	1.27	1.22
14	H	1205	CLA	OBD-CAD	3.12	1.27	1.22
14	b	1023	CLA	CHB-C1B	3.12	1.46	1.39
14	a	1118	CLA	MG-ND	-3.12	1.99	2.05
14	a	1119	CLA	MG-ND	-3.12	1.99	2.05
14	A	1113	CLA	C1C-NC	-3.11	1.33	1.37
14	A	1106	CLA	C4B-NB	-3.11	1.33	1.37
14	U	1503	CLA	MG-ND	-3.11	1.99	2.05
14	a	1111	CLA	MG-ND	-3.11	1.99	2.05
14	B	1206	CLA	CHC-C4B	3.11	1.46	1.39
14	H	1212	CLA	C1B-NB	-3.11	1.33	1.37
14	b	1208	CLA	C1B-NB	-3.11	1.33	1.37
14	B	1224	CLA	C4B-NB	-3.11	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1124	CLA	C4B-NB	-3.11	1.33	1.37
14	G	1138	CLA	MG-ND	-3.11	1.99	2.05
14	L	1502	CLA	MG-ND	-3.11	1.99	2.05
14	G	1102	CLA	CHB-C1B	3.11	1.46	1.39
14	b	1216	CLA	CHB-C1B	3.11	1.46	1.39
14	H	1210	CLA	MG-ND	-3.11	1.99	2.05
14	B	1212	CLA	C1B-NB	-3.11	1.33	1.37
14	H	1224	CLA	C4B-NB	-3.11	1.33	1.37
15	G	1120	F6C	C4C-NC	-3.11	1.33	1.37
14	G	1103	CLA	OBD-CAD	3.11	1.27	1.22
14	B	1203	CLA	C4B-NB	-3.11	1.33	1.37
14	a	1128	CLA	CHC-C4B	3.11	1.46	1.39
14	H	1203	CLA	C1C-NC	-3.11	1.33	1.37
14	G	1111	CLA	C4B-NB	-3.11	1.33	1.37
14	H	1235	CLA	C4B-NB	-3.11	1.33	1.37
14	A	1136	CLA	MG-ND	-3.11	1.99	2.05
14	G	1119	CLA	MG-ND	-3.11	1.99	2.05
14	a	1132	CLA	C1C-NC	-3.11	1.33	1.37
14	a	1139	CLA	C1C-NC	-3.11	1.33	1.37
14	a	1012	CLA	C4B-NB	-3.11	1.33	1.37
14	a	1115	CLA	MG-ND	-3.11	1.99	2.05
14	B	1221	CLA	OBD-CAD	3.11	1.27	1.22
14	A	1122	CLA	C4B-NB	-3.11	1.33	1.37
14	b	1239	CLA	C4B-NB	-3.11	1.33	1.37
15	a	1120	F6C	C3D-C2D	3.11	1.47	1.39
14	A	1138	CLA	C1B-NB	-3.10	1.33	1.37
14	B	1228	CLA	C1B-NB	-3.10	1.33	1.37
14	G	1138	CLA	C1B-NB	-3.10	1.33	1.37
14	A	1103	CLA	MG-ND	-3.10	1.99	2.05
14	H	1233	CLA	C1D-ND	-3.10	1.33	1.37
14	H	1239	CLA	C1B-NB	-3.10	1.33	1.37
14	a	1113	CLA	OBD-CAD	3.10	1.27	1.22
14	G	1122	CLA	C4B-NB	-3.10	1.33	1.37
14	H	1228	CLA	C1B-NB	-3.10	1.33	1.37
14	a	1122	CLA	C4B-NB	-3.10	1.33	1.37
14	B	1205	CLA	CHB-C1B	3.10	1.46	1.39
14	B	1235	CLA	CHB-C1B	3.10	1.46	1.39
14	b	1201	CLA	C1B-NB	-3.10	1.33	1.37
18	H	4012	BCR	C11-C12	-3.10	1.26	1.34
14	B	1203	CLA	C1C-NC	-3.10	1.33	1.37
18	b	4012	BCR	C11-C12	-3.10	1.26	1.34
14	G	1124	CLA	C4B-NB	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1119	CLA	MG-ND	-3.10	1.99	2.05
14	B	1203	CLA	MG-ND	-3.10	1.99	2.05
15	G	1120	F6C	C3D-C2D	3.10	1.47	1.39
14	H	1238	CLA	C4B-NB	-3.10	1.33	1.37
14	A	1138	CLA	CHB-C1B	3.10	1.46	1.39
14	A	1115	CLA	MG-ND	-3.09	1.99	2.05
14	a	1102	CLA	CHB-C1B	3.09	1.46	1.39
14	b	1202	CLA	C1C-NC	-3.09	1.33	1.37
14	A	1118	CLA	MG-ND	-3.09	1.99	2.05
14	b	1205	CLA	CHB-C1B	3.09	1.46	1.39
14	B	1209	CLA	C1B-NB	-3.09	1.33	1.37
14	B	1216	CLA	CHB-C1B	3.09	1.46	1.39
14	A	1012	CLA	C4B-NB	-3.09	1.33	1.37
14	A	1113	CLA	C1D-ND	-3.09	1.33	1.37
14	G	1123	CLA	MG-NC	3.09	2.13	2.06
14	B	1222	CLA	MG-ND	-3.09	1.99	2.05
14	b	1210	CLA	MG-ND	-3.09	1.99	2.05
14	G	1115	CLA	MG-ND	-3.09	1.99	2.05
14	H	1206	CLA	CHC-C4B	3.09	1.46	1.39
14	A	1122	CLA	MG-ND	-3.09	1.99	2.05
14	H	1224	CLA	CHB-C1B	3.09	1.46	1.39
14	A	1112	CLA	C1D-ND	-3.09	1.33	1.37
14	H	1211	CLA	C4B-NB	-3.09	1.33	1.37
14	b	1224	CLA	CHB-C1B	3.09	1.46	1.39
14	A	1102	CLA	CHB-C1B	3.09	1.46	1.39
14	K	1401	CLA	MG-NC	3.09	2.13	2.06
14	a	1103	CLA	OBD-CAD	3.09	1.27	1.22
14	k	1401	CLA	MG-NC	3.09	2.13	2.06
14	B	1223	CLA	C1C-NC	-3.09	1.33	1.37
14	W	1701	CLA	MG-ND	-3.09	1.99	2.05
14	a	1103	CLA	MG-ND	-3.09	1.99	2.05
14	A	1133	CLA	C1B-NB	-3.09	1.33	1.37
18	B	4012	BCR	C11-C12	-3.08	1.26	1.34
14	G	1106	CLA	C4B-NB	-3.08	1.33	1.37
14	a	1122	CLA	MG-ND	-3.08	1.99	2.05
14	a	1130	CLA	C1C-NC	-3.08	1.33	1.37
14	b	1203	CLA	C1C-NC	-3.08	1.33	1.37
14	A	1123	CLA	MG-NC	3.08	2.13	2.06
14	H	1228	CLA	C1C-NC	-3.08	1.33	1.37
14	H	1209	CLA	C1B-NB	-3.08	1.33	1.37
14	b	1206	CLA	CHC-C4B	3.08	1.46	1.39
14	G	1112	CLA	C1D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1201	CLA	CHB-C1B	3.08	1.46	1.39
14	T	1401	CLA	MG-NC	3.08	2.13	2.06
14	U	1502	CLA	MG-ND	-3.08	1.99	2.05
14	G	1013	CLA	C3D-C2D	3.08	1.47	1.39
15	A	1120	F6C	C3D-C2D	3.08	1.47	1.39
14	A	1113	CLA	OBD-CAD	3.08	1.27	1.22
15	A	1121	F6C	OBD-CAD	3.08	1.27	1.22
14	H	1216	CLA	CHB-C1B	3.08	1.46	1.39
14	b	1228	CLA	C1B-NB	-3.08	1.33	1.37
14	A	1106	CLA	C1C-NC	-3.08	1.33	1.37
14	G	1106	CLA	C1C-NC	-3.08	1.33	1.37
14	L	1503	CLA	MG-ND	-3.08	1.99	2.05
14	A	1130	CLA	C4B-NB	-3.08	1.33	1.37
14	b	1212	CLA	C1B-NB	-3.08	1.33	1.37
14	A	1110	CLA	C1B-NB	-3.08	1.33	1.37
14	B	1211	CLA	C4B-NB	-3.08	1.33	1.37
14	b	1211	CLA	C4B-NB	-3.08	1.33	1.37
14	G	1112	CLA	C1B-NB	-3.08	1.33	1.37
14	G	1107	CLA	OBD-CAD	3.08	1.27	1.22
14	B	1238	CLA	C4B-NB	-3.08	1.33	1.37
14	B	1224	CLA	CHB-C1B	3.08	1.46	1.39
14	a	1106	CLA	C1C-NC	-3.08	1.33	1.37
14	b	1239	CLA	C1B-NB	-3.08	1.33	1.37
14	b	1207	CLA	C4B-NB	-3.08	1.33	1.37
14	a	1130	CLA	CHB-C1B	3.08	1.46	1.39
14	B	1202	CLA	C1C-NC	-3.07	1.33	1.37
14	A	1013	CLA	C3D-C2D	3.07	1.47	1.39
14	b	1224	CLA	C4B-NB	-3.07	1.33	1.37
14	G	1138	CLA	CHB-C1B	3.07	1.46	1.39
14	l	1503	CLA	MG-ND	-3.07	1.99	2.05
14	A	1130	CLA	CHB-C1B	3.07	1.46	1.39
14	a	1129	CLA	OBD-CAD	3.07	1.27	1.22
14	b	1223	CLA	OBD-CAD	3.07	1.27	1.22
14	B	1229	CLA	C4B-NB	-3.07	1.33	1.37
14	a	1130	CLA	C4B-NB	-3.07	1.33	1.37
14	G	1111	CLA	MG-ND	-3.07	1.99	2.05
14	a	1107	CLA	OBD-CAD	3.07	1.27	1.22
14	a	1123	CLA	MG-NC	3.07	2.13	2.06
14	G	1012	CLA	C4B-NB	-3.07	1.33	1.37
14	b	1215	CLA	C4B-NB	-3.07	1.33	1.37
14	A	1107	CLA	OBD-CAD	3.07	1.27	1.22
14	G	1113	CLA	C1C-NC	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1117	CLA	CHC-C4B	3.07	1.46	1.39
14	G	1139	CLA	C1C-NC	-3.07	1.33	1.37
14	b	1233	CLA	C1D-ND	-3.07	1.33	1.37
14	a	1013	CLA	C3D-C2D	3.06	1.47	1.39
14	H	1205	CLA	CHB-C1B	3.06	1.46	1.39
14	A	1111	CLA	MG-ND	-3.06	1.99	2.05
14	B	1210	CLA	MG-ND	-3.06	1.99	2.05
14	A	1136	CLA	C1C-NC	-3.06	1.33	1.37
14	H	1239	CLA	C4B-NB	-3.06	1.33	1.37
14	L	1503	CLA	C4B-NB	-3.06	1.33	1.37
14	A	1119	CLA	C3D-C2D	3.06	1.47	1.39
14	H	1207	CLA	C3D-C2D	3.06	1.47	1.39
14	G	1131	CLA	C1C-NC	-3.06	1.33	1.37
14	B	1239	CLA	C1B-NB	-3.06	1.33	1.37
14	a	1112	CLA	C1D-ND	-3.06	1.33	1.37
14	G	1114	CLA	CHB-C1B	3.06	1.46	1.39
14	b	1217	CLA	MG-ND	-3.06	1.99	2.05
14	B	1208	CLA	C1B-NB	-3.06	1.33	1.37
14	b	1228	CLA	C1C-NC	-3.06	1.33	1.37
14	H	1208	CLA	C1B-NB	-3.06	1.33	1.37
14	H	1204	CLA	CHB-C1B	3.06	1.46	1.39
14	b	1223	CLA	C1C-NC	-3.05	1.33	1.37
14	U	1503	CLA	C4B-NB	-3.05	1.33	1.37
14	b	1238	CLA	C4B-NB	-3.05	1.33	1.37
14	G	1114	CLA	C1D-ND	-3.05	1.33	1.37
14	H	1231	CLA	MG-ND	-3.05	1.99	2.05
14	x	1701	CLA	MG-ND	-3.05	1.99	2.05
14	B	1204	CLA	CHB-C1B	3.05	1.46	1.39
14	H	1207	CLA	C4B-NB	-3.05	1.33	1.37
14	G	1136	CLA	C1C-NC	-3.05	1.33	1.37
14	a	1136	CLA	C1C-NC	-3.05	1.33	1.37
14	A	1129	CLA	OBD-CAD	3.05	1.27	1.22
14	X	1701	CLA	MG-ND	-3.05	1.99	2.05
14	A	1114	CLA	CHB-C1B	3.05	1.46	1.39
14	B	1228	CLA	MG-ND	-3.05	1.99	2.05
14	l	1503	CLA	C4B-NB	-3.04	1.33	1.37
14	B	1216	CLA	C1B-NB	-3.04	1.33	1.37
14	a	1115	CLA	C1B-NB	-3.04	1.33	1.37
15	A	1120	F6C	C4C-NC	-3.04	1.33	1.37
14	b	1204	CLA	CHB-C1B	3.04	1.46	1.39
14	G	1122	CLA	MG-ND	-3.04	1.99	2.05
14	A	1130	CLA	C1C-NC	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1215	CLA	C4B-NB	-3.04	1.33	1.37
14	B	1207	CLA	C3D-C2D	3.04	1.47	1.39
14	b	1207	CLA	C3D-C2D	3.04	1.47	1.39
14	B	1207	CLA	C4B-NB	-3.04	1.33	1.37
14	a	1114	CLA	CHB-C1B	3.04	1.46	1.39
14	a	1133	CLA	C1B-NB	-3.04	1.33	1.37
14	G	1114	CLA	MG-ND	-3.04	1.99	2.05
14	H	1228	CLA	MG-ND	-3.04	1.99	2.05
14	b	1223	CLA	MG-NC	3.04	2.13	2.06
14	a	1119	CLA	C3D-C2D	3.04	1.47	1.39
14	b	1220	CLA	C1C-NC	-3.04	1.33	1.37
14	H	1223	CLA	C1C-NC	-3.04	1.33	1.37
14	H	1211	CLA	MG-ND	-3.03	1.99	2.05
14	b	1228	CLA	MG-ND	-3.03	1.99	2.05
14	G	1110	CLA	C1B-NB	-3.03	1.33	1.37
14	B	1217	CLA	MG-ND	-3.03	1.99	2.05
14	U	1502	CLA	OBD-CAD	3.03	1.27	1.22
14	A	1105	CLA	C1B-NB	-3.03	1.33	1.37
14	a	1124	CLA	C1C-NC	-3.03	1.33	1.37
14	A	1101	CLA	C1B-NB	-3.03	1.33	1.37
14	B	1219	CLA	MG-ND	-3.03	1.99	2.05
14	H	1217	CLA	C1B-NB	-3.03	1.33	1.37
14	a	1114	CLA	C1D-ND	-3.03	1.33	1.37
14	A	1128	CLA	C3D-C2D	3.03	1.47	1.39
14	H	1202	CLA	C1C-NC	-3.03	1.33	1.37
14	G	1113	CLA	C1D-ND	-3.03	1.33	1.37
14	G	1127	CLA	C1C-NC	-3.03	1.33	1.37
14	L	1502	CLA	OBD-CAD	3.03	1.27	1.22
14	B	1223	CLA	C4B-NB	-3.03	1.33	1.37
14	H	1229	CLA	C4B-NB	-3.03	1.33	1.37
14	b	1217	CLA	C1B-NB	-3.03	1.33	1.37
15	B	1237	F6C	C4C-NC	-3.03	1.33	1.37
14	A	1114	CLA	C1D-ND	-3.03	1.33	1.37
14	a	1117	CLA	CHC-C4B	3.03	1.46	1.39
14	a	1127	CLA	C1C-NC	-3.03	1.33	1.37
14	G	1117	CLA	C3D-C2D	3.03	1.47	1.39
14	b	1220	CLA	C4B-NB	-3.03	1.33	1.37
14	B	1231	CLA	MG-ND	-3.03	1.99	2.05
14	b	1231	CLA	MG-ND	-3.03	1.99	2.05
14	G	1119	CLA	C3D-C2D	3.03	1.47	1.39
14	A	1119	CLA	CHB-C1B	3.02	1.46	1.39
14	A	1124	CLA	C1C-NC	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1127	CLA	C1C-NC	-3.02	1.33	1.37
15	B	1230	F6C	C3B-C2B	3.02	1.46	1.39
14	H	1223	CLA	OBD-CAD	3.02	1.27	1.22
14	H	1231	CLA	C4B-NB	-3.02	1.33	1.37
14	A	1132	CLA	CHB-C1B	3.02	1.46	1.39
14	B	1239	CLA	C4B-NB	-3.02	1.33	1.37
14	G	1117	CLA	CHC-C4B	3.02	1.46	1.39
14	a	1119	CLA	CHB-C1B	3.02	1.46	1.39
14	G	1124	CLA	C1C-NC	-3.02	1.33	1.37
14	a	1132	CLA	CHB-C1B	3.02	1.46	1.39
14	b	1215	CLA	C1C-NC	-3.02	1.33	1.37
14	b	1235	CLA	MG-ND	-3.02	1.99	2.05
15	a	1120	F6C	C4C-NC	-3.02	1.33	1.37
14	A	1104	CLA	C4B-NB	-3.02	1.33	1.37
14	G	1128	CLA	C3D-C2D	3.02	1.47	1.39
15	H	1237	F6C	C4C-NC	-3.02	1.33	1.37
14	L	1501	CLA	C1C-NC	-3.02	1.33	1.37
14	a	1128	CLA	C3D-C2D	3.02	1.47	1.39
14	H	1222	CLA	C1C-NC	-3.02	1.33	1.37
14	A	1114	CLA	MG-ND	-3.02	1.99	2.05
14	a	1123	CLA	OBD-CAD	3.02	1.27	1.22
14	a	1110	CLA	C1B-NB	-3.02	1.33	1.37
14	G	1119	CLA	CHB-C1B	3.02	1.46	1.39
14	H	1212	CLA	MG-ND	-3.01	1.99	2.05
14	B	1223	CLA	OBD-CAD	3.01	1.27	1.22
14	b	1211	CLA	MG-ND	-3.01	1.99	2.05
14	b	1213	CLA	MG-ND	-3.01	1.99	2.05
14	B	1223	CLA	MG-NC	3.01	2.13	2.06
14	B	1216	CLA	C3D-C2D	3.01	1.47	1.39
14	H	1217	CLA	MG-ND	-3.01	1.99	2.05
14	G	1133	CLA	C1B-NB	-3.01	1.33	1.37
14	A	1139	CLA	MG-ND	-3.01	1.99	2.05
14	a	1117	CLA	C3D-C2D	3.01	1.47	1.39
14	U	1501	CLA	C1C-NC	-3.01	1.33	1.37
14	a	1114	CLA	MG-ND	-3.01	1.99	2.05
14	A	1139	CLA	C1C-NC	-3.01	1.33	1.37
14	G	1132	CLA	CHB-C1B	3.01	1.46	1.39
14	k	1401	CLA	C4D-CHA	3.01	1.48	1.38
14	b	1208	CLA	C1C-NC	-3.01	1.33	1.37
14	B	1232	CLA	MG-ND	-3.01	1.99	2.05
14	H	1220	CLA	C3D-C2D	3.01	1.47	1.39
14	B	1217	CLA	C1B-NB	-3.01	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1123	CLA	C4B-NB	-3.01	1.33	1.37
14	a	1123	CLA	C4B-NB	-3.01	1.33	1.37
14	H	1220	CLA	C4B-NB	-3.01	1.33	1.37
14	b	1227	CLA	MG-NC	3.01	2.13	2.06
14	G	1130	CLA	C1C-NC	-3.01	1.33	1.37
14	b	1212	CLA	MG-ND	-3.01	1.99	2.05
14	A	1123	CLA	C4B-NB	-3.00	1.33	1.37
14	B	1212	CLA	MG-ND	-3.00	1.99	2.05
14	B	1220	CLA	C1C-NC	-3.00	1.33	1.37
14	H	1216	CLA	C3D-C2D	3.00	1.47	1.39
14	G	1139	CLA	MG-ND	-3.00	1.99	2.05
14	B	1233	CLA	C1D-ND	-3.00	1.33	1.37
14	G	1108	CLA	C1B-NB	-3.00	1.33	1.37
14	a	1131	CLA	CHB-C1B	3.00	1.46	1.39
14	B	1236	CLA	MG-ND	-3.00	1.99	2.05
14	H	1226	CLA	C3D-C2D	3.00	1.47	1.39
14	H	1223	CLA	MG-NC	3.00	2.13	2.06
14	a	1108	CLA	C1B-NB	-3.00	1.33	1.37
14	G	1117	CLA	C1C-NC	-3.00	1.33	1.37
14	B	1209	CLA	MG-ND	-3.00	1.99	2.05
14	H	1226	CLA	CHC-C4B	3.00	1.46	1.39
14	l	1501	CLA	C1C-NC	-3.00	1.33	1.37
14	T	1401	CLA	C4D-CHA	3.00	1.48	1.38
14	B	1211	CLA	MG-ND	-3.00	1.99	2.05
14	H	1236	CLA	MG-ND	-3.00	1.99	2.05
14	B	1227	CLA	MG-NC	3.00	2.13	2.06
14	B	1217	CLA	MG-NC	3.00	2.13	2.06
14	b	1220	CLA	C3D-C2D	3.00	1.47	1.39
14	H	1233	CLA	MG-NC	3.00	2.13	2.06
14	L	1502	CLA	C4B-NB	-3.00	1.33	1.37
14	b	1222	CLA	C1C-NC	-3.00	1.33	1.37
14	A	1123	CLA	OBD-CAD	3.00	1.27	1.22
14	B	1215	CLA	C1C-NC	-3.00	1.33	1.37
14	H	1220	CLA	C1C-NC	-3.00	1.33	1.37
14	H	1213	CLA	MG-ND	-3.00	1.99	2.05
14	b	1216	CLA	C3D-C2D	3.00	1.47	1.39
14	G	1105	CLA	C1B-NB	-3.00	1.33	1.37
14	A	1131	CLA	CHB-C1B	3.00	1.46	1.39
14	b	1232	CLA	MG-ND	-3.00	1.99	2.05
14	A	1012	CLA	CHB-C1B	2.99	1.46	1.39
14	A	1117	CLA	C3D-C2D	2.99	1.47	1.39
14	B	1222	CLA	C1C-NC	-2.99	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1012	CLA	CHB-C1B	2.99	1.46	1.39
14	G	1101	CLA	C1B-NB	-2.99	1.33	1.37
14	a	1105	CLA	C1B-NB	-2.99	1.33	1.37
14	l	1502	CLA	OBD-CAD	2.99	1.27	1.22
14	B	1220	CLA	C3D-C2D	2.99	1.47	1.39
15	H	1230	F6C	C3B-C2B	2.99	1.46	1.39
14	b	1217	CLA	MG-NC	2.99	2.13	2.06
14	b	1236	CLA	MG-ND	-2.99	1.99	2.05
14	B	1233	CLA	MG-NC	2.99	2.13	2.06
14	K	1401	CLA	C4D-CHA	2.99	1.48	1.38
14	H	1238	CLA	CHB-C1B	2.99	1.46	1.39
14	H	1206	CLA	C3D-C2D	2.99	1.47	1.39
14	A	1117	CLA	C1C-NC	-2.99	1.33	1.37
14	G	1114	CLA	C3D-C2D	2.99	1.47	1.39
14	B	1235	CLA	MG-ND	-2.99	1.99	2.05
15	b	1230	F6C	C3B-C2B	2.99	1.46	1.39
14	b	1201	CLA	MG-ND	-2.99	1.99	2.05
14	B	1226	CLA	CHC-C4B	2.99	1.46	1.39
14	B	1206	CLA	C4B-NB	-2.99	1.33	1.37
14	G	1138	CLA	C1C-NC	-2.99	1.33	1.37
14	b	1226	CLA	C3D-C2D	2.99	1.47	1.39
14	A	1137	CLA	C1C-NC	-2.99	1.33	1.37
14	a	1105	CLA	MG-ND	-2.99	1.99	2.05
14	a	1114	CLA	C3D-C2D	2.99	1.47	1.39
14	a	1129	CLA	C4B-NB	-2.99	1.33	1.37
14	a	1106	CLA	MG-ND	-2.98	1.99	2.05
14	U	1501	CLA	C4B-NB	-2.98	1.33	1.37
15	b	1237	F6C	C4C-NC	-2.98	1.33	1.37
14	G	1131	CLA	CHB-C1B	2.98	1.46	1.39
14	A	1119	CLA	C1C-NC	-2.98	1.33	1.37
14	H	1217	CLA	MG-NC	2.98	2.13	2.06
14	G	1107	CLA	C4B-NB	-2.98	1.33	1.37
14	B	1201	CLA	MG-ND	-2.98	1.99	2.05
14	H	1235	CLA	MG-ND	-2.98	1.99	2.05
14	H	1232	CLA	MG-ND	-2.98	1.99	2.05
14	H	1206	CLA	C4B-NB	-2.98	1.33	1.37
14	a	1138	CLA	C4B-NB	-2.98	1.33	1.37
14	A	1138	CLA	C1C-NC	-2.98	1.33	1.37
14	H	1224	CLA	C1C-NC	-2.98	1.33	1.37
14	a	1137	CLA	C1C-NC	-2.98	1.33	1.37
14	G	1115	CLA	C1B-NB	-2.98	1.33	1.37
15	A	1121	F6C	C3B-C2B	2.98	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1208	CLA	C1C-NC	-2.98	1.33	1.37
14	H	1227	CLA	MG-NC	2.98	2.13	2.06
14	a	1126	CLA	CHB-C1B	2.98	1.46	1.39
14	b	1219	CLA	MG-ND	-2.98	1.99	2.05
14	b	1206	CLA	C4B-NB	-2.98	1.33	1.37
14	G	1137	CLA	C1C-NC	-2.98	1.33	1.37
14	B	1213	CLA	MG-ND	-2.98	1.99	2.05
14	B	1224	CLA	C1C-NC	-2.98	1.33	1.37
14	b	1238	CLA	CHB-C1B	2.98	1.46	1.39
14	a	1104	CLA	C4B-NB	-2.98	1.34	1.37
14	b	1204	CLA	C1C-NC	-2.98	1.33	1.37
14	G	1123	CLA	OBD-CAD	2.98	1.27	1.22
14	H	1219	CLA	MG-ND	-2.98	1.99	2.05
14	b	1023	CLA	CHC-C4B	2.98	1.46	1.39
14	G	1012	CLA	CHB-C1B	2.97	1.46	1.39
14	H	1232	CLA	MG-NC	2.97	2.13	2.06
14	B	1226	CLA	C3D-C2D	2.97	1.47	1.39
20	L	5007	LMG	C43-C42	-2.97	1.33	1.51
14	b	1214	CLA	C3D-C2D	2.97	1.47	1.39
20	l	5007	LMG	C43-C42	-2.97	1.33	1.51
14	A	1126	CLA	CHB-C1B	2.97	1.46	1.39
14	B	1214	CLA	MG-NC	2.97	2.13	2.06
14	b	1232	CLA	MG-NC	2.97	2.13	2.06
14	b	1206	CLA	C3D-C2D	2.97	1.47	1.39
14	a	1117	CLA	C1C-NC	-2.97	1.33	1.37
14	a	1138	CLA	C1C-NC	-2.97	1.33	1.37
14	A	1109	CLA	C1C-NC	-2.97	1.33	1.37
14	G	1109	CLA	C1C-NC	-2.97	1.33	1.37
14	B	1023	CLA	CHC-C4B	2.97	1.46	1.39
14	A	1106	CLA	MG-ND	-2.97	1.99	2.05
14	G	1105	CLA	MG-ND	-2.97	1.99	2.05
14	H	1204	CLA	C1C-NC	-2.97	1.33	1.37
14	A	1106	CLA	C1B-NB	-2.97	1.34	1.37
14	A	1114	CLA	C3D-C2D	2.97	1.47	1.39
14	B	1206	CLA	C3D-C2D	2.97	1.47	1.39
14	G	1126	CLA	CHB-C1B	2.97	1.46	1.39
14	B	1232	CLA	C4D-CHA	2.97	1.48	1.38
14	a	1101	CLA	C1B-NB	-2.97	1.34	1.37
14	b	1216	CLA	C1B-NB	-2.97	1.34	1.37
14	B	1021	CLA	CHD-C4C	2.97	1.46	1.39
14	H	1216	CLA	C1B-NB	-2.97	1.34	1.37
14	L	1501	CLA	C4B-NB	-2.97	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1208	CLA	C1C-NC	-2.97	1.33	1.37
14	B	1214	CLA	C3D-C2D	2.96	1.47	1.39
14	a	1013	CLA	CHD-C1D	2.96	1.44	1.38
14	H	1214	CLA	C3D-C2D	2.96	1.47	1.39
14	a	1109	CLA	C1B-NB	-2.96	1.34	1.37
14	A	1137	CLA	OBD-CAD	2.96	1.27	1.22
14	a	1114	CLA	C4D-CHA	2.96	1.48	1.38
14	B	1238	CLA	CHB-C1B	2.96	1.46	1.39
14	A	1105	CLA	MG-ND	-2.96	1.99	2.05
14	a	1137	CLA	OBD-CAD	2.96	1.27	1.22
14	H	1226	CLA	CHB-C1B	2.96	1.46	1.39
14	H	1201	CLA	MG-ND	-2.96	1.99	2.05
14	H	1023	CLA	CHC-C4B	2.96	1.46	1.39
14	b	1233	CLA	MG-NC	2.96	2.13	2.06
14	b	1205	CLA	C4B-NB	-2.96	1.34	1.37
20	U	5007	LMG	C43-C42	-2.96	1.33	1.51
14	a	1119	CLA	C1C-NC	-2.96	1.33	1.37
14	b	1214	CLA	MG-NC	2.96	2.13	2.06
14	b	1229	CLA	C4B-NB	-2.96	1.34	1.37
14	b	1232	CLA	C4D-CHA	2.96	1.48	1.38
14	b	1231	CLA	C4B-NB	-2.96	1.34	1.37
14	A	1013	CLA	CHD-C1D	2.96	1.44	1.38
14	a	1139	CLA	MG-ND	-2.95	1.99	2.05
14	A	1108	CLA	C1B-NB	-2.95	1.34	1.37
14	b	1226	CLA	CHB-C1B	2.95	1.46	1.39
14	G	1109	CLA	C1B-NB	-2.95	1.34	1.37
14	G	1012	CLA	C1C-NC	-2.95	1.33	1.37
14	G	1129	CLA	C4B-NB	-2.95	1.34	1.37
15	b	1230	F6C	C1C-NC	-2.95	1.34	1.37
14	G	1106	CLA	MG-ND	-2.95	1.99	2.05
14	H	1232	CLA	C4D-CHA	2.95	1.48	1.38
14	b	1238	CLA	C1C-NC	-2.95	1.33	1.37
14	A	1114	CLA	C4D-CHA	2.95	1.48	1.38
14	H	1218	CLA	MG-ND	-2.95	1.99	2.05
14	H	1215	CLA	MG-ND	-2.95	1.99	2.05
14	H	1214	CLA	MG-NC	2.95	2.13	2.06
14	b	1021	CLA	CHD-C4C	2.95	1.45	1.39
14	G	1119	CLA	C1C-NC	-2.95	1.33	1.37
14	B	1219	CLA	C3D-C2D	2.95	1.47	1.39
14	B	1204	CLA	C1C-NC	-2.95	1.33	1.37
15	G	1121	F6C	C3B-C2B	2.95	1.46	1.39
14	A	1115	CLA	C1B-NB	-2.95	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1231	CLA	C4B-NB	-2.95	1.34	1.37
14	b	1218	CLA	C1B-NB	-2.95	1.34	1.37
14	H	1215	CLA	C1C-NC	-2.95	1.33	1.37
15	H	1230	F6C	C3D-C2D	2.94	1.47	1.39
14	a	1012	CLA	C1C-NC	-2.94	1.33	1.37
14	b	1224	CLA	C1C-NC	-2.94	1.33	1.37
14	U	1502	CLA	C4B-NB	-2.94	1.34	1.37
15	a	1121	F6C	C3B-C2B	2.94	1.46	1.39
14	B	1232	CLA	MG-NC	2.94	2.13	2.06
14	B	1234	CLA	OBD-CAD	2.94	1.27	1.22
14	B	1226	CLA	CHB-C1B	2.94	1.46	1.39
14	H	1219	CLA	C3D-C2D	2.94	1.47	1.39
15	b	1230	F6C	C3D-C2D	2.94	1.47	1.39
15	B	1230	F6C	C1C-NC	-2.94	1.34	1.37
14	B	1235	CLA	C1C-NC	-2.94	1.33	1.37
14	G	1110	CLA	C4D-CHA	2.94	1.48	1.38
14	H	1223	CLA	C4B-NB	-2.94	1.34	1.37
14	H	1021	CLA	CHD-C4C	2.94	1.45	1.39
14	H	1212	CLA	C4D-CHA	2.94	1.48	1.38
14	a	1104	CLA	C1C-NC	-2.94	1.33	1.37
14	b	1209	CLA	MG-ND	-2.94	2.00	2.05
14	l	1501	CLA	C4B-NB	-2.94	1.34	1.37
14	A	1110	CLA	C4D-CHA	2.94	1.48	1.38
14	A	1012	CLA	C1C-NC	-2.93	1.33	1.37
14	A	1138	CLA	C4B-NB	-2.93	1.34	1.37
14	G	1124	CLA	MG-ND	-2.93	2.00	2.05
14	b	1223	CLA	C4B-NB	-2.93	1.34	1.37
14	A	1109	CLA	C1B-NB	-2.93	1.34	1.37
14	G	1106	CLA	C1B-NB	-2.93	1.34	1.37
14	G	1137	CLA	OBD-CAD	2.93	1.27	1.22
14	B	1235	CLA	C3D-C2D	2.93	1.47	1.39
14	H	1218	CLA	C3D-C2D	2.93	1.47	1.39
14	k	1401	CLA	C1B-C2B	2.93	1.50	1.43
14	A	1112	CLA	C4D-CHA	2.93	1.48	1.38
14	H	1238	CLA	C1C-NC	-2.93	1.33	1.37
14	b	1226	CLA	CHC-C4B	2.93	1.46	1.39
14	B	1215	CLA	MG-ND	-2.93	2.00	2.05
14	B	1212	CLA	C4D-CHA	2.93	1.48	1.38
14	G	1114	CLA	C4D-CHA	2.93	1.48	1.38
14	G	1101	CLA	MG-ND	-2.93	2.00	2.05
14	B	1022	CLA	C4B-NB	-2.93	1.34	1.37
14	H	1226	CLA	C4D-CHA	2.93	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1106	CLA	C1B-NB	-2.93	1.34	1.37
14	b	1219	CLA	C3D-C2D	2.93	1.47	1.39
14	b	1215	CLA	MG-ND	-2.93	2.00	2.05
14	b	1226	CLA	C4D-CHA	2.93	1.48	1.38
14	G	1104	CLA	C4B-NB	-2.93	1.34	1.37
14	G	1116	CLA	MG-NC	2.93	2.13	2.06
14	A	1116	CLA	MG-NC	2.93	2.13	2.06
14	b	1218	CLA	MG-ND	-2.92	2.00	2.05
14	B	1220	CLA	C4B-NB	-2.92	1.34	1.37
14	B	1226	CLA	C4D-CHA	2.92	1.48	1.38
14	b	1212	CLA	C4D-CHA	2.92	1.48	1.38
14	G	1112	CLA	MG-ND	-2.92	2.00	2.05
14	a	1101	CLA	MG-ND	-2.92	2.00	2.05
14	a	1110	CLA	C4D-CHA	2.92	1.48	1.38
14	k	1401	CLA	C3D-C2D	2.92	1.47	1.39
14	H	1012	CLA	C4B-NB	-2.92	1.34	1.37
14	a	1124	CLA	MG-ND	-2.92	2.00	2.05
14	G	1013	CLA	CHD-C1D	2.92	1.44	1.38
14	l	1502	CLA	C4B-NB	-2.92	1.34	1.37
14	H	1235	CLA	C3D-C2D	2.92	1.46	1.39
20	U	5007	LMG	C22-C21	-2.92	1.33	1.51
14	a	1131	CLA	C4B-NB	-2.92	1.34	1.37
15	B	1230	F6C	C3D-C2D	2.91	1.46	1.39
14	B	1213	CLA	C3D-C2D	2.91	1.46	1.39
14	a	1110	CLA	MG-NC	2.91	2.13	2.06
14	a	1104	CLA	MG-ND	-2.91	2.00	2.05
14	G	1115	CLA	C3D-C2D	2.91	1.46	1.39
14	K	1401	CLA	C1B-C2B	2.91	1.50	1.43
20	l	5007	LMG	C22-C21	-2.91	1.33	1.51
14	B	1208	CLA	MG-ND	-2.91	2.00	2.05
20	L	5007	LMG	C22-C21	-2.91	1.33	1.51
14	a	1107	CLA	C1C-NC	-2.91	1.33	1.37
14	b	1234	CLA	C4B-NB	-2.91	1.34	1.37
14	B	1218	CLA	C1B-NB	-2.91	1.34	1.37
14	A	1115	CLA	C3D-C2D	2.91	1.46	1.39
14	G	1112	CLA	C3D-C2D	2.91	1.46	1.39
14	B	1212	CLA	C3D-C2D	2.91	1.46	1.39
14	b	1209	CLA	C4D-CHA	2.91	1.48	1.38
14	G	1107	CLA	C1C-NC	-2.91	1.33	1.37
14	b	1211	CLA	C1C-NC	-2.91	1.33	1.37
14	A	1112	CLA	MG-ND	-2.91	2.00	2.05
14	H	1209	CLA	MG-ND	-2.91	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1401	CLA	C1B-C2B	2.91	1.50	1.43
14	G	1104	CLA	MG-ND	-2.91	2.00	2.05
14	a	1115	CLA	C3D-C2D	2.91	1.46	1.39
14	B	1218	CLA	C3D-C2D	2.91	1.46	1.39
14	K	1401	CLA	C3D-C2D	2.91	1.46	1.39
14	A	1104	CLA	MG-ND	-2.91	2.00	2.05
14	H	1223	CLA	C4D-CHA	2.91	1.48	1.38
14	b	1213	CLA	C3D-C2D	2.91	1.46	1.39
14	A	1129	CLA	C4B-NB	-2.91	1.34	1.37
14	H	1205	CLA	C4B-NB	-2.91	1.34	1.37
14	A	1101	CLA	MG-ND	-2.91	2.00	2.05
14	A	1107	CLA	C1C-NC	-2.91	1.33	1.37
14	B	1228	CLA	C3D-C2D	2.91	1.46	1.39
14	b	1218	CLA	C3D-C2D	2.91	1.46	1.39
14	a	1107	CLA	C4B-NB	-2.91	1.34	1.37
14	B	1223	CLA	C4D-CHA	2.90	1.48	1.38
14	G	1012	CLA	C3D-C2D	2.90	1.46	1.39
14	A	1107	CLA	C4B-NB	-2.90	1.34	1.37
14	H	1228	CLA	C3D-C2D	2.90	1.46	1.39
14	H	1213	CLA	C3D-C2D	2.90	1.46	1.39
14	H	1208	CLA	MG-ND	-2.90	2.00	2.05
14	a	1112	CLA	MG-ND	-2.90	2.00	2.05
14	B	1213	CLA	C1B-NB	-2.90	1.34	1.37
14	H	1221	CLA	C1C-NC	-2.90	1.33	1.37
14	b	1235	CLA	C1C-NC	-2.90	1.33	1.37
14	W	1701	CLA	C1B-NB	-2.90	1.34	1.37
14	b	1208	CLA	MG-ND	-2.90	2.00	2.05
14	G	1104	CLA	C1C-NC	-2.90	1.33	1.37
14	H	1235	CLA	C1C-NC	-2.90	1.33	1.37
14	a	1109	CLA	C1C-NC	-2.90	1.33	1.37
14	b	1212	CLA	C3D-C2D	2.90	1.46	1.39
14	B	1205	CLA	C4B-NB	-2.90	1.34	1.37
14	A	1133	CLA	MG-NC	2.90	2.13	2.06
15	a	1121	F6C	C1D-ND	-2.90	1.33	1.37
14	A	1111	CLA	C4D-CHA	2.90	1.48	1.38
14	A	1104	CLA	C1C-NC	-2.90	1.33	1.37
14	a	1102	CLA	C3D-C2D	2.90	1.46	1.39
14	A	1112	CLA	C3D-C2D	2.89	1.46	1.39
14	H	1209	CLA	C4D-CHA	2.89	1.48	1.38
14	b	1223	CLA	C4D-CHA	2.89	1.48	1.38
14	b	1214	CLA	C4D-CHA	2.89	1.48	1.38
14	H	1218	CLA	C1B-NB	-2.89	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1228	CLA	C3D-C2D	2.89	1.46	1.39
14	a	1111	CLA	C4D-CHA	2.89	1.48	1.38
14	B	1218	CLA	MG-ND	-2.89	2.00	2.05
14	G	1108	CLA	MG-ND	-2.89	2.00	2.05
14	T	1401	CLA	C3D-C2D	2.89	1.46	1.39
14	A	1124	CLA	MG-ND	-2.89	2.00	2.05
14	B	1209	CLA	C4D-CHA	2.89	1.48	1.38
14	H	1233	CLA	C3D-C2D	2.89	1.46	1.39
14	a	1012	CLA	C3D-C2D	2.89	1.46	1.39
15	a	1121	F6C	C3D-C2D	2.89	1.46	1.39
14	a	1112	CLA	C4D-CHA	2.89	1.48	1.38
14	G	1108	CLA	MG-NC	2.89	2.13	2.06
14	B	1218	CLA	MG-NC	2.89	2.13	2.06
14	b	1022	CLA	C1C-NC	-2.89	1.33	1.37
14	x	1701	CLA	MG-NC	2.89	2.13	2.06
14	a	1112	CLA	C3D-C2D	2.89	1.46	1.39
14	b	1221	CLA	C1C-NC	-2.89	1.33	1.37
14	A	1124	CLA	CHB-C1B	2.88	1.45	1.39
14	B	1219	CLA	C4D-CHA	2.88	1.48	1.38
14	G	1131	CLA	C4B-NB	-2.88	1.34	1.37
14	a	1102	CLA	MG-NC	2.88	2.13	2.06
15	A	1121	F6C	C1D-ND	-2.88	1.33	1.37
14	b	1233	CLA	C3D-C2D	2.88	1.46	1.39
14	b	1235	CLA	C3D-C2D	2.88	1.46	1.39
14	X	1701	CLA	MG-NC	2.88	2.13	2.06
14	A	1140	CLA	MG-NC	2.88	2.13	2.06
14	B	1238	CLA	C1C-NC	-2.88	1.33	1.37
14	B	1211	CLA	C1C-NC	-2.88	1.33	1.37
14	A	1119	CLA	C4B-NB	-2.88	1.34	1.37
14	G	1112	CLA	C4D-CHA	2.88	1.48	1.38
14	H	1218	CLA	C4D-CHA	2.88	1.48	1.38
14	G	1110	CLA	MG-NC	2.88	2.13	2.06
14	X	1701	CLA	C1C-NC	-2.88	1.33	1.37
15	A	1121	F6C	C3D-C2D	2.88	1.46	1.39
14	b	1218	CLA	C4D-CHA	2.88	1.48	1.38
14	A	1012	CLA	C3D-C2D	2.88	1.46	1.39
14	A	1108	CLA	MG-ND	-2.88	2.00	2.05
15	H	1230	F6C	C1C-NC	-2.88	1.34	1.37
14	A	1108	CLA	MG-NC	2.88	2.13	2.06
14	B	1221	CLA	C1C-NC	-2.88	1.33	1.37
14	b	1022	CLA	C4B-NB	-2.88	1.34	1.37
14	B	1218	CLA	C4D-CHA	2.87	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1226	CLA	C4B-NB	-2.87	1.34	1.37
14	G	1111	CLA	C4D-CHA	2.87	1.48	1.38
14	G	1138	CLA	C4B-NB	-2.87	1.34	1.37
14	H	1219	CLA	C4D-CHA	2.87	1.48	1.38
15	G	1121	F6C	C1D-ND	-2.87	1.33	1.37
14	a	1116	CLA	MG-NC	2.87	2.13	2.06
14	H	1211	CLA	C1C-NC	-2.87	1.33	1.37
14	H	1234	CLA	C4B-NB	-2.87	1.34	1.37
14	a	1108	CLA	MG-NC	2.87	2.13	2.06
14	B	1022	CLA	C1C-NC	-2.87	1.33	1.37
14	a	1135	CLA	MG-NC	2.87	2.13	2.06
14	G	1102	CLA	MG-NC	2.87	2.13	2.06
14	a	1133	CLA	MG-NC	2.87	2.13	2.06
14	B	1209	CLA	C3D-C2D	2.87	1.46	1.39
14	A	1110	CLA	MG-NC	2.87	2.13	2.06
14	G	1124	CLA	CHB-C1B	2.87	1.45	1.39
15	G	1121	F6C	C3D-C2D	2.87	1.46	1.39
14	A	1133	CLA	C4D-CHA	2.87	1.48	1.38
14	B	1234	CLA	C4B-NB	-2.87	1.34	1.37
14	B	1022	CLA	MG-NC	2.87	2.13	2.06
14	H	1214	CLA	C4D-CHA	2.87	1.48	1.38
14	B	1214	CLA	C4B-NB	-2.87	1.34	1.37
14	G	1133	CLA	MG-NC	2.87	2.13	2.06
14	b	1212	CLA	C1C-NC	-2.87	1.33	1.37
14	a	1133	CLA	C4D-CHA	2.87	1.48	1.38
14	G	1133	CLA	C4D-CHA	2.87	1.48	1.38
14	G	1119	CLA	C4B-NB	-2.87	1.34	1.37
14	a	1107	CLA	MG-NC	2.87	2.13	2.06
14	a	1124	CLA	CHB-C1B	2.86	1.45	1.39
14	B	1023	CLA	C3D-C2D	2.86	1.46	1.39
14	X	1701	CLA	C4D-CHA	2.86	1.48	1.38
14	H	1213	CLA	C1B-NB	-2.86	1.34	1.37
14	W	1701	CLA	C4D-CHA	2.86	1.48	1.38
14	H	1212	CLA	C3D-C2D	2.86	1.46	1.39
14	G	1102	CLA	C3D-C2D	2.86	1.46	1.39
14	B	1214	CLA	C4D-CHA	2.86	1.48	1.38
14	b	1233	CLA	C4D-CHA	2.86	1.48	1.38
14	G	1140	CLA	MG-NC	2.86	2.13	2.06
14	H	1023	CLA	C3D-C2D	2.86	1.46	1.39
14	b	1219	CLA	C4D-CHA	2.86	1.48	1.38
14	H	1209	CLA	C3D-C2D	2.86	1.46	1.39
14	A	1135	CLA	MG-NC	2.86	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1135	CLA	MG-NC	2.86	2.13	2.06
14	A	1106	CLA	C4D-CHA	2.86	1.48	1.38
14	a	1112	CLA	C1C-NC	-2.86	1.33	1.37
14	b	1022	CLA	MG-NC	2.86	2.13	2.06
14	x	1701	CLA	C1C-NC	-2.86	1.33	1.37
14	a	1138	CLA	C3D-C2D	2.86	1.46	1.39
14	b	1023	CLA	C3D-C2D	2.86	1.46	1.39
14	b	1209	CLA	C3D-C2D	2.86	1.46	1.39
14	G	1132	CLA	MG-NC	2.86	2.13	2.06
15	A	1121	F6C	MG-ND	-2.86	1.99	2.06
14	B	1212	CLA	C1C-NC	-2.85	1.33	1.37
14	A	1102	CLA	MG-NC	2.85	2.13	2.06
14	A	1102	CLA	C3D-C2D	2.85	1.46	1.39
14	H	1232	CLA	C3D-C2D	2.85	1.46	1.39
14	A	1131	CLA	C4B-NB	-2.85	1.34	1.37
14	H	1233	CLA	C1B-NB	-2.85	1.34	1.37
14	G	1135	CLA	C1C-NC	-2.85	1.33	1.37
14	a	1109	CLA	MG-ND	-2.85	2.00	2.05
14	l	1502	CLA	C3D-C2D	2.85	1.46	1.39
14	H	1233	CLA	C4D-CHA	2.85	1.48	1.38
14	b	1231	CLA	C1C-NC	-2.85	1.33	1.37
14	A	1109	CLA	MG-ND	-2.85	2.00	2.05
14	b	1215	CLA	C4D-CHA	2.85	1.48	1.38
14	H	1218	CLA	MG-NC	2.85	2.13	2.06
14	G	1106	CLA	C4D-CHA	2.85	1.48	1.38
14	B	1233	CLA	C4D-CHA	2.85	1.48	1.38
14	x	1701	CLA	C4D-CHA	2.85	1.48	1.38
14	a	1140	CLA	MG-NC	2.85	2.13	2.06
14	a	1106	CLA	C4D-CHA	2.85	1.48	1.38
14	b	1214	CLA	C4B-NB	-2.85	1.34	1.37
15	G	1121	F6C	MG-ND	-2.85	1.99	2.06
14	B	1233	CLA	C3D-C2D	2.85	1.46	1.39
14	x	1701	CLA	C1B-NB	-2.85	1.34	1.37
14	G	1107	CLA	MG-NC	2.85	2.13	2.06
14	b	1217	CLA	C4D-CHA	2.85	1.48	1.38
15	a	1121	F6C	MG-ND	-2.85	1.99	2.06
14	A	1127	CLA	MG-NC	2.85	2.13	2.06
14	A	1132	CLA	MG-NC	2.85	2.13	2.06
14	b	1234	CLA	OBD-CAD	2.85	1.27	1.22
14	W	1701	CLA	C1C-NC	-2.85	1.33	1.37
14	G	1117	CLA	C4D-CHA	2.85	1.48	1.38
14	H	1215	CLA	C4D-CHA	2.85	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1215	CLA	C3D-C2D	2.85	1.46	1.39
14	b	1212	CLA	MG-NC	2.85	2.13	2.06
14	U	1502	CLA	C3D-C2D	2.85	1.46	1.39
14	B	1233	CLA	MG-ND	-2.85	2.00	2.05
14	H	1219	CLA	C4B-NB	-2.84	1.34	1.37
14	b	1233	CLA	C1B-NB	-2.84	1.34	1.37
14	H	1212	CLA	C1C-NC	-2.84	1.33	1.37
14	H	1234	CLA	OBD-CAD	2.84	1.27	1.22
14	a	1102	CLA	C4D-CHA	2.84	1.48	1.38
14	b	1213	CLA	C1B-NB	-2.84	1.34	1.37
14	H	1208	CLA	C3D-C2D	2.84	1.46	1.39
14	G	1109	CLA	MG-ND	-2.84	2.00	2.05
14	H	1012	CLA	C3D-C2D	2.84	1.46	1.39
14	G	1113	CLA	C4D-CHA	2.84	1.48	1.38
14	a	1132	CLA	C3D-C2D	2.84	1.46	1.39
14	a	1127	CLA	MG-NC	2.84	2.13	2.06
14	W	1701	CLA	MG-NC	2.84	2.13	2.06
14	G	1138	CLA	C4D-CHA	2.84	1.48	1.38
14	B	1022	CLA	C3D-C2D	2.84	1.46	1.39
14	a	1138	CLA	C4D-CHA	2.84	1.48	1.38
14	A	1117	CLA	C4D-CHA	2.84	1.48	1.38
14	A	1129	CLA	C1C-NC	-2.84	1.33	1.37
14	G	1112	CLA	C1C-NC	-2.84	1.33	1.37
14	X	1701	CLA	C1B-NB	-2.84	1.34	1.37
14	A	1102	CLA	C4D-CHA	2.84	1.48	1.38
14	A	1138	CLA	C3D-C2D	2.84	1.46	1.39
14	H	1012	CLA	MG-NC	2.83	2.13	2.06
14	A	1113	CLA	C4D-CHA	2.83	1.48	1.38
14	G	1102	CLA	C4D-CHA	2.83	1.48	1.38
14	a	1117	CLA	C4D-CHA	2.83	1.48	1.38
14	b	1215	CLA	C3D-C2D	2.83	1.46	1.39
14	b	1221	CLA	C4B-NB	-2.83	1.34	1.37
14	B	1215	CLA	C3D-C2D	2.83	1.46	1.39
14	B	1208	CLA	C3D-C2D	2.83	1.46	1.39
14	b	1208	CLA	C3D-C2D	2.83	1.46	1.39
14	a	1108	CLA	MG-ND	-2.83	2.00	2.05
14	H	1231	CLA	C1C-NC	-2.83	1.33	1.37
14	A	1108	CLA	C3D-C2D	2.83	1.46	1.39
14	b	1022	CLA	C3D-C2D	2.83	1.46	1.39
14	G	1127	CLA	MG-NC	2.83	2.13	2.06
14	A	1131	CLA	C4D-CHA	2.83	1.48	1.38
14	a	1113	CLA	C4D-CHA	2.83	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1219	CLA	C4B-NB	-2.83	1.34	1.37
14	H	1217	CLA	C4D-CHA	2.83	1.48	1.38
14	B	1231	CLA	C1C-NC	-2.83	1.33	1.37
14	A	1138	CLA	C4D-CHA	2.83	1.48	1.38
15	b	1237	F6C	C3D-C2D	2.83	1.46	1.39
14	G	1131	CLA	C4D-CHA	2.83	1.48	1.38
14	a	1112	CLA	C4B-NB	-2.83	1.34	1.37
14	B	1217	CLA	C4D-CHA	2.83	1.48	1.38
14	A	1112	CLA	C1C-NC	-2.83	1.33	1.37
14	G	1136	CLA	C4D-CHA	2.83	1.48	1.38
14	A	1140	CLA	C4D-CHA	2.82	1.48	1.38
15	B	1237	F6C	C3D-C2D	2.82	1.46	1.39
14	l	1501	CLA	C4D-CHA	2.82	1.48	1.38
14	L	1502	CLA	C3D-C2D	2.82	1.46	1.39
14	A	1115	CLA	C1C-NC	-2.82	1.33	1.37
14	B	1232	CLA	C3D-C2D	2.82	1.46	1.39
14	G	1128	CLA	C4D-CHA	2.82	1.48	1.38
14	a	1115	CLA	C1C-NC	-2.82	1.33	1.37
14	A	1112	CLA	C4B-NB	-2.82	1.34	1.37
14	H	1212	CLA	MG-NC	2.82	2.13	2.06
14	G	1132	CLA	C4D-CHA	2.82	1.48	1.38
14	G	1129	CLA	MG-NC	2.82	2.13	2.06
14	G	1140	CLA	C4D-CHA	2.82	1.48	1.38
14	a	1128	CLA	C4D-CHA	2.82	1.48	1.38
14	B	1212	CLA	MG-NC	2.82	2.13	2.06
14	H	1214	CLA	C4B-NB	-2.82	1.34	1.37
14	a	1119	CLA	C4B-NB	-2.82	1.34	1.37
14	a	1131	CLA	C4D-CHA	2.82	1.48	1.38
14	b	1201	CLA	C4D-CHA	2.82	1.48	1.38
14	G	1115	CLA	C1C-NC	-2.82	1.33	1.37
14	B	1219	CLA	C4B-NB	-2.82	1.34	1.37
14	B	1229	CLA	C1C-NC	-2.82	1.33	1.37
14	H	1012	CLA	C1C-NC	-2.82	1.33	1.37
14	a	1132	CLA	MG-NC	2.82	2.13	2.06
14	a	1113	CLA	C3D-C2D	2.82	1.46	1.39
14	B	1215	CLA	C4D-CHA	2.81	1.48	1.38
14	A	1107	CLA	MG-NC	2.81	2.13	2.06
14	H	1221	CLA	C4B-NB	-2.81	1.34	1.37
14	G	1139	CLA	C4D-CHA	2.81	1.48	1.38
15	a	1120	F6C	MG-ND	-2.81	1.99	2.06
14	G	1138	CLA	C3D-C2D	2.81	1.46	1.39
14	a	1140	CLA	C4D-CHA	2.81	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	C4D-CHA	2.81	1.48	1.38
14	H	1227	CLA	C4D-CHA	2.81	1.48	1.38
14	G	1109	CLA	C3D-C2D	2.81	1.46	1.39
14	a	1132	CLA	C4D-CHA	2.81	1.48	1.38
14	G	1112	CLA	MG-NC	2.81	2.13	2.06
14	A	1112	CLA	MG-NC	2.81	2.12	2.06
14	l	1501	CLA	MG-NC	2.81	2.12	2.06
14	a	1108	CLA	C3D-C2D	2.81	1.46	1.39
14	A	1139	CLA	C4D-CHA	2.81	1.48	1.38
14	a	1109	CLA	C3D-C2D	2.81	1.46	1.39
14	H	1227	CLA	C4B-NB	-2.81	1.34	1.37
14	U	1501	CLA	C4D-CHA	2.81	1.48	1.38
14	H	1229	CLA	C1C-NC	-2.81	1.33	1.37
14	G	1140	CLA	C3D-C2D	2.81	1.46	1.39
14	b	1232	CLA	C3D-C2D	2.81	1.46	1.39
14	A	1128	CLA	C4B-NB	-2.81	1.34	1.37
14	G	1137	CLA	MG-NC	2.81	2.12	2.06
14	G	1133	CLA	C1C-NC	-2.81	1.33	1.37
14	b	1209	CLA	C1C-NC	-2.81	1.33	1.37
14	A	1140	CLA	C3D-C2D	2.81	1.46	1.39
14	G	1132	CLA	C3D-C2D	2.81	1.46	1.39
14	b	1218	CLA	MG-NC	2.81	2.12	2.06
14	b	1227	CLA	C4D-CHA	2.81	1.48	1.38
14	A	1135	CLA	C1C-NC	-2.81	1.33	1.37
14	A	1128	CLA	C4D-CHA	2.80	1.48	1.38
14	H	1233	CLA	MG-ND	-2.80	2.00	2.05
14	a	1129	CLA	MG-NC	2.80	2.12	2.06
14	a	1136	CLA	C4D-CHA	2.80	1.48	1.38
14	G	1129	CLA	C1C-NC	-2.80	1.33	1.37
14	l	1501	CLA	C3D-C2D	2.80	1.46	1.39
14	a	1112	CLA	MG-NC	2.80	2.12	2.06
14	a	1105	CLA	C4B-NB	-2.80	1.34	1.37
14	a	1140	CLA	C3D-C2D	2.80	1.46	1.39
15	G	1120	F6C	MG-ND	-2.80	1.99	2.06
14	G	1111	CLA	MG-NC	2.80	2.12	2.06
14	A	1109	CLA	C3D-C2D	2.80	1.46	1.39
14	A	1113	CLA	C3D-C2D	2.80	1.46	1.39
14	B	1227	CLA	C4D-CHA	2.80	1.48	1.38
14	B	1201	CLA	C4D-CHA	2.80	1.48	1.38
14	b	1233	CLA	MG-ND	-2.80	2.00	2.05
14	a	1139	CLA	C4D-CHA	2.80	1.48	1.38
14	a	1139	CLA	MG-NC	2.80	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1108	CLA	C4D-CHA	2.80	1.48	1.38
14	b	1206	CLA	C4D-CHA	2.80	1.48	1.38
14	A	1118	CLA	C1C-NC	-2.80	1.33	1.37
14	A	1133	CLA	C1C-NC	-2.80	1.33	1.37
14	A	1132	CLA	C4D-CHA	2.80	1.48	1.38
14	A	1137	CLA	MG-NC	2.80	2.12	2.06
14	G	1108	CLA	C4D-CHA	2.80	1.48	1.38
14	T	1401	CLA	C1D-ND	-2.80	1.34	1.37
14	G	1105	CLA	C1C-NC	-2.80	1.33	1.37
14	A	1132	CLA	C3D-C2D	2.80	1.46	1.39
14	a	1105	CLA	C3D-C2D	2.80	1.46	1.39
14	G	1113	CLA	C3D-C2D	2.80	1.46	1.39
14	A	1101	CLA	C4D-CHA	2.80	1.48	1.38
15	A	1120	F6C	MG-ND	-2.80	1.99	2.06
14	B	1226	CLA	C4B-NB	-2.80	1.34	1.37
14	A	1136	CLA	C4D-CHA	2.80	1.48	1.38
14	L	1501	CLA	C4D-CHA	2.80	1.48	1.38
14	K	1401	CLA	C1D-ND	-2.79	1.34	1.37
14	A	1129	CLA	MG-NC	2.79	2.12	2.06
14	a	1111	CLA	MG-NC	2.79	2.12	2.06
14	a	1118	CLA	C1C-NC	-2.79	1.33	1.37
14	H	1220	CLA	C4D-CHA	2.79	1.48	1.38
14	a	1133	CLA	C1C-NC	-2.79	1.33	1.37
14	H	1206	CLA	C4D-CHA	2.79	1.48	1.38
14	G	1128	CLA	C4B-NB	-2.79	1.34	1.37
14	A	1111	CLA	MG-NC	2.79	2.12	2.06
14	H	1201	CLA	C4D-CHA	2.79	1.48	1.38
14	a	1101	CLA	C4D-CHA	2.79	1.48	1.38
14	a	1102	CLA	C4B-NB	-2.79	1.34	1.37
14	H	1239	CLA	C4D-CHA	2.79	1.48	1.38
14	B	1206	CLA	OBD-CAD	2.79	1.27	1.22
15	H	1237	F6C	C3D-C2D	2.79	1.46	1.39
14	a	1128	CLA	C4B-NB	-2.79	1.34	1.37
14	H	1222	CLA	MG-NC	2.79	2.12	2.06
14	B	1239	CLA	C4D-CHA	2.79	1.48	1.38
14	G	1118	CLA	C1C-NC	-2.79	1.33	1.37
14	A	1123	CLA	C4D-CHA	2.79	1.48	1.38
14	b	1226	CLA	C4B-NB	-2.79	1.34	1.37
14	B	1224	CLA	MG-NC	2.79	2.12	2.06
14	G	1123	CLA	C4D-CHA	2.79	1.47	1.38
14	L	1501	CLA	C3D-C2D	2.79	1.46	1.39
14	G	1108	CLA	C3D-C2D	2.79	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1137	CLA	MG-NC	2.79	2.12	2.06
14	b	1231	CLA	MG-NC	2.79	2.12	2.06
14	G	1114	CLA	C4B-NB	-2.79	1.34	1.37
14	L	1501	CLA	MG-NC	2.79	2.12	2.06
14	b	1213	CLA	MG-NC	2.79	2.12	2.06
14	G	1101	CLA	C4D-CHA	2.78	1.47	1.38
14	k	1401	CLA	C1D-ND	-2.78	1.34	1.37
14	U	1501	CLA	C3D-C2D	2.78	1.46	1.39
14	A	1101	CLA	C1C-NC	-2.78	1.33	1.37
14	b	1224	CLA	MG-NC	2.78	2.12	2.06
14	b	1222	CLA	MG-NC	2.78	2.12	2.06
14	b	1220	CLA	C4D-CHA	2.78	1.47	1.38
14	b	1219	CLA	MG-NC	2.78	2.12	2.06
14	A	1105	CLA	C3D-C2D	2.78	1.46	1.39
14	b	1206	CLA	OBD-CAD	2.78	1.27	1.22
14	A	1139	CLA	MG-NC	2.78	2.12	2.06
14	B	1220	CLA	C4D-CHA	2.78	1.47	1.38
14	B	1221	CLA	C4B-NB	-2.78	1.34	1.37
14	b	1221	CLA	C3D-C2D	2.78	1.46	1.39
14	a	1135	CLA	C1C-NC	-2.78	1.33	1.37
14	B	1213	CLA	MG-NC	2.78	2.12	2.06
14	H	1213	CLA	MG-NC	2.78	2.12	2.06
14	H	1224	CLA	MG-NC	2.78	2.12	2.06
14	B	1206	CLA	C4D-CHA	2.78	1.47	1.38
14	b	1239	CLA	C4D-CHA	2.78	1.47	1.38
14	H	1225	CLA	C4D-CHA	2.78	1.47	1.38
14	a	1105	CLA	C1C-NC	-2.78	1.33	1.37
14	b	1225	CLA	C4D-CHA	2.78	1.47	1.38
14	G	1112	CLA	C4B-NB	-2.77	1.34	1.37
14	G	1116	CLA	C4D-CHA	2.77	1.47	1.38
14	B	1221	CLA	C3D-C2D	2.77	1.46	1.39
14	B	1233	CLA	C1B-NB	-2.77	1.34	1.37
14	b	1213	CLA	C4B-NB	-2.77	1.34	1.37
14	B	1231	CLA	MG-NC	2.77	2.12	2.06
14	a	1131	CLA	C3D-C2D	2.77	1.46	1.39
14	A	1131	CLA	C3D-C2D	2.77	1.46	1.39
14	B	1225	CLA	MG-NC	2.77	2.12	2.06
14	A	1107	CLA	C4D-CHA	2.77	1.47	1.38
14	a	1107	CLA	C4D-CHA	2.77	1.47	1.38
14	a	1126	CLA	C3D-C2D	2.77	1.46	1.39
14	A	1116	CLA	C4D-CHA	2.77	1.47	1.38
14	B	1225	CLA	C4D-CHA	2.77	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1123	CLA	C4D-CHA	2.77	1.47	1.38
14	G	1126	CLA	C3D-C2D	2.77	1.46	1.39
14	U	1503	CLA	C3D-C2D	2.77	1.46	1.39
14	A	1105	CLA	C1C-NC	-2.77	1.33	1.37
21	a	6002	LMT	O3'-C3'	-2.77	1.36	1.43
14	a	1101	CLA	C1C-NC	-2.77	1.33	1.37
14	U	1501	CLA	MG-NC	2.77	2.12	2.06
14	A	1108	CLA	C1C-NC	-2.77	1.33	1.37
14	a	1129	CLA	C1C-NC	-2.77	1.33	1.37
14	A	1125	CLA	C4D-CHA	2.77	1.47	1.38
14	B	1221	CLA	C4D-CHA	2.77	1.47	1.38
14	G	1131	CLA	C3D-C2D	2.77	1.46	1.39
14	G	1118	CLA	C3D-C2D	2.77	1.46	1.39
14	A	1117	CLA	C4B-NB	-2.77	1.34	1.37
14	B	1222	CLA	MG-NC	2.76	2.12	2.06
14	a	1109	CLA	C4B-NB	-2.76	1.34	1.37
14	a	1125	CLA	C4D-CHA	2.76	1.47	1.38
21	A	6002	LMT	O3'-C3'	-2.76	1.36	1.43
14	H	1238	CLA	MG-NC	2.76	2.12	2.06
14	H	1208	CLA	C4D-CHA	2.76	1.47	1.38
14	b	1214	CLA	C1C-NC	-2.76	1.33	1.37
14	A	1126	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1118	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1105	CLA	C4D-CHA	2.76	1.47	1.38
14	A	1109	CLA	C4B-NB	-2.76	1.34	1.37
14	b	1231	CLA	C4D-CHA	2.76	1.47	1.38
14	A	1118	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1106	CLA	C3D-C2D	2.76	1.46	1.39
14	G	1122	CLA	C4D-CHA	2.76	1.47	1.38
14	G	1139	CLA	MG-NC	2.76	2.12	2.06
14	G	1139	CLA	C3D-C2D	2.76	1.46	1.39
14	A	1106	CLA	C3D-C2D	2.76	1.46	1.39
14	B	1213	CLA	C4D-CHA	2.76	1.47	1.38
14	H	1212	CLA	C4B-NB	-2.76	1.34	1.37
14	A	1122	CLA	C4D-CHA	2.76	1.47	1.38
14	b	1229	CLA	C1C-NC	-2.76	1.33	1.37
14	G	1105	CLA	C3D-C2D	2.76	1.46	1.39
14	b	1212	CLA	C4B-NB	-2.76	1.34	1.37
14	H	1225	CLA	MG-NC	2.76	2.12	2.06
14	a	1123	CLA	C1C-NC	-2.76	1.33	1.37
14	b	1221	CLA	C4D-CHA	2.76	1.47	1.38
15	b	1230	F6C	C1D-C2D	2.76	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1231	CLA	C4D-CHA	2.76	1.47	1.38
14	H	1221	CLA	C4D-CHA	2.76	1.47	1.38
14	a	1012	CLA	C4D-CHA	2.76	1.47	1.38
14	b	1218	CLA	C1B-C2B	2.76	1.49	1.43
14	H	1216	CLA	C4D-CHA	2.76	1.47	1.38
14	G	1106	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1139	CLA	C3D-C2D	2.76	1.46	1.39
14	B	1216	CLA	C4D-CHA	2.76	1.47	1.38
14	a	1106	CLA	C1B-C2B	2.75	1.49	1.43
14	B	1208	CLA	C4D-CHA	2.75	1.47	1.38
14	H	1213	CLA	C4D-CHA	2.75	1.47	1.38
14	H	1207	CLA	C4D-CHA	2.75	1.47	1.38
14	A	1106	CLA	MG-NC	2.75	2.12	2.06
15	H	1230	F6C	C3C-C2C	2.75	1.46	1.38
14	G	1108	CLA	C1C-NC	-2.75	1.33	1.37
14	G	1122	CLA	C3D-C2D	2.75	1.46	1.39
14	a	1114	CLA	C4B-NB	-2.75	1.34	1.37
14	b	1229	CLA	MG-ND	-2.75	2.00	2.05
14	b	1219	CLA	C1C-NC	-2.75	1.33	1.37
14	H	1219	CLA	MG-NC	2.75	2.12	2.06
14	A	1105	CLA	C4B-NB	-2.75	1.34	1.37
14	G	1124	CLA	C4D-CHA	2.75	1.47	1.38
14	a	1122	CLA	C4D-CHA	2.75	1.47	1.38
14	H	1206	CLA	OBD-CAD	2.75	1.27	1.22
14	a	1110	CLA	C1C-NC	-2.75	1.33	1.37
14	G	1107	CLA	C4D-CHA	2.75	1.47	1.38
14	A	1105	CLA	C4D-CHA	2.75	1.47	1.38
14	G	1125	CLA	C4D-CHA	2.75	1.47	1.38
14	G	1101	CLA	C3D-C2D	2.75	1.46	1.39
14	G	1106	CLA	MG-NC	2.75	2.12	2.06
14	B	1212	CLA	C4B-NB	-2.75	1.34	1.37
14	G	1101	CLA	C1C-NC	-2.75	1.33	1.37
14	G	1105	CLA	C4B-NB	-2.75	1.34	1.37
14	b	1225	CLA	MG-NC	2.75	2.12	2.06
14	L	1503	CLA	C3D-C2D	2.75	1.46	1.39
14	b	1238	CLA	MG-NC	2.75	2.12	2.06
14	B	1209	CLA	C1C-NC	-2.75	1.33	1.37
14	a	1116	CLA	C4D-CHA	2.75	1.47	1.38
14	H	1221	CLA	C3D-C2D	2.75	1.46	1.39
14	l	1503	CLA	C3D-C2D	2.75	1.46	1.39
14	B	1238	CLA	MG-NC	2.75	2.12	2.06
14	B	1222	CLA	C3D-C2D	2.75	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1012	CLA	C4D-CHA	2.75	1.47	1.38
14	B	1214	CLA	C1C-NC	-2.74	1.33	1.37
14	b	1229	CLA	C3D-C2D	2.74	1.46	1.39
14	G	1130	CLA	C4D-CHA	2.74	1.47	1.38
14	A	1130	CLA	C4D-CHA	2.74	1.47	1.38
14	B	1228	CLA	C4D-CHA	2.74	1.47	1.38
14	H	1209	CLA	C1C-NC	-2.74	1.33	1.37
14	B	1219	CLA	MG-NC	2.74	2.12	2.06
14	G	1105	CLA	C4D-CHA	2.74	1.47	1.38
14	H	1214	CLA	C1C-NC	-2.74	1.33	1.37
14	b	1208	CLA	C4D-CHA	2.74	1.47	1.38
14	A	1127	CLA	C4D-CHA	2.74	1.47	1.38
14	A	1114	CLA	C4B-NB	-2.74	1.34	1.37
14	a	1127	CLA	C4D-CHA	2.74	1.47	1.38
14	H	1231	CLA	MG-NC	2.74	2.12	2.06
14	H	1239	CLA	MG-NC	2.74	2.12	2.06
14	B	1229	CLA	C3D-C2D	2.74	1.46	1.39
14	b	1216	CLA	C4D-CHA	2.74	1.47	1.38
14	H	1235	CLA	C4D-CHA	2.74	1.47	1.38
14	G	1123	CLA	C1C-NC	-2.74	1.33	1.37
21	G	6002	LMT	O3'-C3'	-2.74	1.36	1.43
14	G	1127	CLA	C4D-CHA	2.74	1.47	1.38
14	A	1115	CLA	MG-NC	2.74	2.12	2.06
14	b	1239	CLA	MG-NC	2.74	2.12	2.06
14	H	1224	CLA	C3D-C2D	2.74	1.46	1.39
14	B	1239	CLA	MG-NC	2.73	2.12	2.06
14	H	1228	CLA	C4D-CHA	2.73	1.47	1.38
14	H	1217	CLA	C1C-NC	-2.73	1.33	1.37
14	A	1122	CLA	C3D-C2D	2.73	1.46	1.39
14	a	1122	CLA	C3D-C2D	2.73	1.46	1.39
14	H	1217	CLA	C1B-C2B	2.73	1.49	1.43
14	H	1218	CLA	C1B-C2B	2.73	1.49	1.43
14	b	1222	CLA	C3D-C2D	2.73	1.46	1.39
14	G	1104	CLA	C4D-CHA	2.73	1.47	1.38
14	A	1123	CLA	C1C-NC	-2.73	1.33	1.37
14	A	1101	CLA	MG-NC	2.73	2.12	2.06
14	a	1104	CLA	C4D-CHA	2.73	1.47	1.38
14	a	1124	CLA	C4D-CHA	2.73	1.47	1.38
14	H	1229	CLA	C3D-C2D	2.73	1.46	1.39
14	H	1229	CLA	MG-ND	-2.73	2.00	2.05
14	B	1235	CLA	C4D-CHA	2.73	1.47	1.38
14	a	1101	CLA	C3D-C2D	2.73	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1228	CLA	C4B-NB	-2.73	1.34	1.37
15	B	1230	F6C	C3C-C2C	2.73	1.46	1.38
14	H	1228	CLA	C4B-NB	-2.73	1.34	1.37
14	b	1213	CLA	C4D-CHA	2.73	1.47	1.38
14	G	1114	CLA	MG-NC	2.73	2.12	2.06
14	b	1235	CLA	C4D-CHA	2.73	1.47	1.38
14	B	1207	CLA	C4D-CHA	2.73	1.47	1.38
14	H	1229	CLA	C4D-CHA	2.73	1.47	1.38
14	B	1022	CLA	C4D-CHA	2.73	1.47	1.38
14	A	1103	CLA	C3D-C2D	2.73	1.46	1.39
14	G	1106	CLA	C1B-C2B	2.73	1.49	1.43
14	a	1118	CLA	C4B-NB	-2.73	1.34	1.37
14	H	1210	CLA	C4D-CHA	2.73	1.47	1.38
14	G	1101	CLA	MG-NC	2.72	2.12	2.06
14	G	1114	CLA	C1C-NC	-2.72	1.33	1.37
14	a	1115	CLA	MG-NC	2.72	2.12	2.06
14	B	1201	CLA	C3D-C2D	2.72	1.46	1.39
15	b	1230	F6C	C3C-C2C	2.72	1.46	1.38
14	A	1115	CLA	C4D-CHA	2.72	1.47	1.38
14	H	1201	CLA	MG-NC	2.72	2.12	2.06
14	G	1012	CLA	C4D-CHA	2.72	1.47	1.38
14	H	1231	CLA	C4D-CHA	2.72	1.47	1.38
14	b	1217	CLA	C1B-C2B	2.72	1.49	1.43
14	b	1207	CLA	C4D-CHA	2.72	1.47	1.38
14	a	1114	CLA	C1C-NC	-2.72	1.33	1.37
14	A	1118	CLA	C4B-NB	-2.72	1.34	1.37
14	A	1124	CLA	C4D-CHA	2.72	1.47	1.38
14	A	1102	CLA	C4B-NB	-2.72	1.34	1.37
14	b	1227	CLA	C4B-NB	-2.72	1.34	1.37
14	b	1201	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1201	CLA	MG-NC	2.72	2.12	2.06
14	A	1119	CLA	C4D-CHA	2.72	1.47	1.38
14	b	1217	CLA	C1C-NC	-2.72	1.33	1.37
14	G	1105	CLA	MG-NC	2.72	2.12	2.06
14	H	1205	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1205	CLA	C3D-C2D	2.72	1.46	1.39
14	B	1227	CLA	C4B-NB	-2.72	1.34	1.37
14	A	1104	CLA	C4D-CHA	2.72	1.47	1.38
14	H	1012	CLA	C4D-CHA	2.72	1.47	1.38
14	a	1119	CLA	C4D-CHA	2.72	1.47	1.38
14	B	1217	CLA	C1C-NC	-2.72	1.33	1.37
14	A	1101	CLA	C3D-C2D	2.72	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1210	CLA	MG-NC	2.72	2.12	2.06
14	b	1213	CLA	C1C-NC	-2.72	1.33	1.37
14	b	1208	CLA	MG-NC	2.72	2.12	2.06
14	b	1229	CLA	C4D-CHA	2.72	1.47	1.38
14	G	1115	CLA	C4D-CHA	2.72	1.47	1.38
14	a	1130	CLA	C4D-CHA	2.72	1.47	1.38
14	A	1139	CLA	C3D-C2D	2.72	1.46	1.39
14	A	1106	CLA	C1B-C2B	2.72	1.49	1.43
14	B	1227	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1201	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1210	CLA	C3D-C2D	2.71	1.46	1.39
14	G	1119	CLA	C4D-CHA	2.71	1.47	1.38
14	G	1118	CLA	C4B-NB	-2.71	1.34	1.37
21	a	6001	LMT	O3'-C3'	-2.71	1.36	1.43
14	G	1122	CLA	MG-NC	2.71	2.12	2.06
14	B	1218	CLA	C1B-C2B	2.71	1.49	1.43
14	a	1114	CLA	MG-NC	2.71	2.12	2.06
14	b	1022	CLA	C4D-CHA	2.71	1.47	1.38
14	G	1109	CLA	C4D-CHA	2.71	1.47	1.38
14	H	1233	CLA	C1B-C2B	2.71	1.49	1.43
14	G	1115	CLA	MG-NC	2.71	2.12	2.06
14	G	1103	CLA	C4D-CHA	2.71	1.47	1.38
14	B	1210	CLA	C3D-C2D	2.71	1.46	1.39
14	G	1137	CLA	C4D-CHA	2.71	1.47	1.38
14	B	1236	CLA	C3D-C2D	2.71	1.46	1.39
14	A	1103	CLA	C4D-CHA	2.71	1.47	1.38
14	B	1205	CLA	C3D-C2D	2.71	1.46	1.39
14	G	1136	CLA	MG-NC	2.71	2.12	2.06
21	A	6001	LMT	O3'-C3'	-2.71	1.36	1.43
14	a	1101	CLA	MG-NC	2.71	2.12	2.06
21	A	6001	LMT	O2'-C2'	-2.71	1.36	1.43
14	b	1228	CLA	C4D-CHA	2.71	1.47	1.38
14	G	1115	CLA	C4B-NB	-2.71	1.34	1.37
14	a	1115	CLA	C4B-NB	-2.71	1.34	1.37
14	H	1222	CLA	C3D-C2D	2.71	1.46	1.39
14	A	1114	CLA	MG-NC	2.71	2.12	2.06
14	G	1102	CLA	C4B-NB	-2.71	1.34	1.37
14	B	1217	CLA	C1B-C2B	2.71	1.49	1.43
14	B	1220	CLA	MG-NC	2.71	2.12	2.06
14	a	1117	CLA	C4B-NB	-2.71	1.34	1.37
14	b	1224	CLA	C3D-C2D	2.71	1.46	1.39
15	H	1237	F6C	MG-ND	-2.71	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1118	CLA	C4D-CHA	2.71	1.47	1.38
14	B	1224	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1213	CLA	C4B-NB	-2.70	1.34	1.37
14	G	1126	CLA	C4D-CHA	2.70	1.47	1.38
14	a	1103	CLA	C4D-CHA	2.70	1.47	1.38
21	G	6001	LMT	O2'-C2'	-2.70	1.36	1.43
21	a	6001	LMT	O2'-C2'	-2.70	1.36	1.43
14	H	1220	CLA	MG-NC	2.70	2.12	2.06
14	B	1238	CLA	C4D-CHA	2.70	1.47	1.38
14	b	1238	CLA	C4D-CHA	2.70	1.47	1.38
15	b	1237	F6C	MG-ND	-2.70	1.99	2.06
14	a	1126	CLA	C4D-CHA	2.70	1.47	1.38
14	G	1117	CLA	C4B-NB	-2.70	1.34	1.37
14	a	1106	CLA	MG-NC	2.70	2.12	2.06
14	H	1213	CLA	C4B-NB	-2.70	1.34	1.37
14	H	1203	CLA	C4D-CHA	2.70	1.47	1.38
14	H	1213	CLA	C1C-NC	-2.70	1.33	1.37
14	b	1236	CLA	C3D-C2D	2.70	1.46	1.39
14	G	1103	CLA	C3D-C2D	2.70	1.46	1.39
14	b	1227	CLA	C3D-C2D	2.70	1.46	1.39
14	A	1114	CLA	C1C-NC	-2.70	1.33	1.37
14	G	1118	CLA	MG-NC	2.70	2.12	2.06
14	H	1218	CLA	C1C-NC	-2.70	1.33	1.37
14	G	1109	CLA	C4B-NB	-2.70	1.34	1.37
14	b	1210	CLA	C3D-C2D	2.70	1.46	1.39
14	A	1105	CLA	MG-NC	2.70	2.12	2.06
14	a	1137	CLA	C4D-CHA	2.70	1.47	1.38
14	A	1126	CLA	C4D-CHA	2.69	1.47	1.38
14	H	1227	CLA	C3D-C2D	2.69	1.46	1.39
14	a	1115	CLA	C4D-CHA	2.69	1.47	1.38
14	B	1219	CLA	C1C-NC	-2.69	1.33	1.37
14	H	1210	CLA	MG-NC	2.69	2.12	2.06
14	B	1229	CLA	MG-ND	-2.69	2.00	2.05
14	H	1219	CLA	C1C-NC	-2.69	1.33	1.37
14	A	1115	CLA	C4B-NB	-2.69	1.34	1.37
15	A	1120	F6C	C1A-C2A	2.69	1.51	1.45
14	H	1211	CLA	C3D-C2D	2.69	1.46	1.39
21	G	6001	LMT	O3'-C3'	-2.69	1.36	1.43
14	T	1401	CLA	MG-ND	-2.69	2.00	2.05
14	A	1118	CLA	MG-NC	2.69	2.12	2.06
13	a	1011	CL0	CMA-C3A	-2.69	1.48	1.53
14	H	1236	CLA	C3D-C2D	2.69	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1208	CLA	MG-NC	2.69	2.12	2.06
14	a	1103	CLA	C3D-C2D	2.69	1.46	1.39
14	B	1229	CLA	C4D-CHA	2.69	1.47	1.38
14	G	1118	CLA	C4D-CHA	2.69	1.47	1.38
14	X	1701	CLA	C3D-C2D	2.69	1.46	1.39
14	B	1233	CLA	C1B-C2B	2.69	1.49	1.43
15	G	1120	F6C	C1A-C2A	2.68	1.51	1.45
14	b	1203	CLA	C4D-CHA	2.68	1.47	1.38
14	b	1210	CLA	C4D-CHA	2.68	1.47	1.38
14	A	1118	CLA	C4D-CHA	2.68	1.47	1.38
14	x	1701	CLA	C3D-C2D	2.68	1.46	1.39
14	A	1137	CLA	C4D-CHA	2.68	1.47	1.38
14	A	1122	CLA	MG-NC	2.68	2.12	2.06
14	a	1109	CLA	C4D-CHA	2.68	1.47	1.38
15	B	1230	F6C	C1D-C2D	2.68	1.50	1.44
14	a	1133	CLA	C3D-C2D	2.68	1.46	1.39
14	a	1118	CLA	MG-NC	2.68	2.12	2.06
14	H	1238	CLA	C4D-CHA	2.68	1.47	1.38
14	a	1108	CLA	C1C-NC	-2.68	1.33	1.37
14	B	1211	CLA	C3D-C2D	2.68	1.46	1.39
14	L	1503	CLA	C4D-CHA	2.68	1.47	1.38
14	A	1110	CLA	C1C-NC	-2.68	1.33	1.37
14	k	1401	CLA	MG-ND	-2.68	2.00	2.05
14	b	1220	CLA	MG-NC	2.68	2.12	2.06
14	B	1210	CLA	C4D-CHA	2.68	1.47	1.38
14	H	1202	CLA	C4D-CHA	2.68	1.47	1.38
14	a	1122	CLA	MG-NC	2.68	2.12	2.06
14	G	1133	CLA	C3D-C2D	2.68	1.46	1.39
15	B	1237	F6C	MG-ND	-2.68	1.99	2.06
14	G	1126	CLA	MG-NC	2.68	2.12	2.06
14	B	1227	CLA	C1C-NC	-2.67	1.33	1.37
14	H	1208	CLA	MG-NC	2.67	2.12	2.06
14	A	1109	CLA	C4D-CHA	2.67	1.47	1.38
14	H	1205	CLA	C4D-CHA	2.67	1.47	1.38
14	B	1201	CLA	MG-NC	2.67	2.12	2.06
14	B	1203	CLA	C4D-CHA	2.67	1.47	1.38
14	b	1211	CLA	C4D-CHA	2.67	1.47	1.38
15	a	1120	F6C	C1A-C2A	2.67	1.51	1.45
14	B	1210	CLA	MG-NC	2.67	2.12	2.06
15	G	1120	F6C	C3C-C2C	2.67	1.45	1.38
14	B	1204	CLA	C3D-C2D	2.67	1.46	1.39
14	W	1701	CLA	C3D-C2D	2.67	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1136	CLA	C3D-C2D	2.67	1.46	1.39
14	b	1233	CLA	C1B-C2B	2.67	1.49	1.43
14	A	1136	CLA	MG-NC	2.67	2.12	2.06
14	G	1125	CLA	OBD-CAD	2.67	1.27	1.22
14	a	1125	CLA	C3D-C2D	2.67	1.46	1.39
14	A	1136	CLA	C3D-C2D	2.67	1.46	1.39
14	A	1125	CLA	OBD-CAD	2.67	1.27	1.22
14	G	1135	CLA	C4D-CHA	2.67	1.47	1.38
14	a	1123	CLA	C3D-C2D	2.67	1.46	1.39
14	a	1136	CLA	MG-NC	2.67	2.12	2.06
14	b	1221	CLA	MG-NC	2.67	2.12	2.06
14	B	1213	CLA	C1C-NC	-2.66	1.33	1.37
14	a	1125	CLA	OBD-CAD	2.66	1.27	1.22
14	B	1217	CLA	C3D-C2D	2.66	1.46	1.39
14	H	1204	CLA	C3D-C2D	2.66	1.46	1.39
14	b	1228	CLA	C4B-NB	-2.66	1.34	1.37
14	a	1126	CLA	MG-NC	2.66	2.12	2.06
14	K	1401	CLA	MG-ND	-2.66	2.00	2.05
14	b	1211	CLA	C3D-C2D	2.66	1.46	1.39
14	B	1221	CLA	MG-NC	2.66	2.12	2.06
14	a	1105	CLA	MG-NC	2.66	2.12	2.06
14	a	1136	CLA	C4B-NB	-2.66	1.34	1.37
14	A	1123	CLA	C3D-C2D	2.66	1.46	1.39
15	A	1120	F6C	C3C-C2C	2.66	1.45	1.38
14	H	1217	CLA	C3D-C2D	2.66	1.46	1.39
14	B	1209	CLA	MG-NC	2.66	2.12	2.06
14	H	1227	CLA	C1C-NC	-2.66	1.33	1.37
14	A	1102	CLA	C1C-NC	-2.66	1.33	1.37
14	a	1138	CLA	MG-NC	2.66	2.12	2.06
14	B	1202	CLA	C4D-CHA	2.66	1.47	1.38
14	b	1209	CLA	MG-NC	2.66	2.12	2.06
14	a	1130	CLA	C3D-C2D	2.66	1.46	1.39
13	G	1011	CL0	CMA-C3A	-2.66	1.48	1.53
14	b	1202	CLA	C4D-CHA	2.66	1.47	1.38
14	b	1209	CLA	C4B-NB	-2.66	1.34	1.37
14	G	1124	CLA	C3D-C2D	2.66	1.46	1.39
14	H	1232	CLA	C1C-NC	-2.66	1.33	1.37
14	b	1227	CLA	C1C-NC	-2.66	1.33	1.37
14	H	1221	CLA	MG-NC	2.66	2.12	2.06
14	B	1205	CLA	C4D-CHA	2.65	1.47	1.38
14	B	1211	CLA	C4D-CHA	2.65	1.47	1.38
14	G	1110	CLA	C1C-NC	-2.65	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1130	CLA	C3D-C2D	2.65	1.46	1.39
14	G	1138	CLA	MG-NC	2.65	2.12	2.06
14	A	1130	CLA	C3D-C2D	2.65	1.46	1.39
15	H	1230	F6C	C1D-C2D	2.65	1.49	1.44
14	G	1102	CLA	C1C-NC	-2.65	1.33	1.37
14	k	1401	CLA	C1B-NB	-2.65	1.34	1.37
14	H	1211	CLA	C4D-CHA	2.65	1.47	1.38
14	b	1217	CLA	C3D-C2D	2.65	1.46	1.39
13	A	1011	CL0	CMA-C3A	-2.65	1.48	1.53
14	G	1136	CLA	C3D-C2D	2.65	1.46	1.39
15	a	1120	F6C	C3C-C2C	2.65	1.45	1.38
14	A	1133	CLA	C3D-C2D	2.65	1.46	1.39
14	A	1135	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1135	CLA	C4D-CHA	2.65	1.47	1.38
14	B	1209	CLA	C4B-NB	-2.65	1.34	1.37
14	b	1204	CLA	C3D-C2D	2.65	1.46	1.39
14	A	1126	CLA	MG-NC	2.65	2.12	2.06
14	l	1503	CLA	C4D-CHA	2.65	1.47	1.38
14	G	1123	CLA	C3D-C2D	2.65	1.46	1.39
14	A	1124	CLA	C3D-C2D	2.65	1.46	1.39
14	b	1205	CLA	C4D-CHA	2.64	1.47	1.38
14	a	1118	CLA	C1B-C2B	2.64	1.49	1.43
14	A	1118	CLA	C1B-C2B	2.64	1.49	1.43
14	H	1222	CLA	C4D-CHA	2.64	1.47	1.38
14	L	1502	CLA	C4D-CHA	2.64	1.47	1.38
14	a	1102	CLA	C1C-NC	-2.64	1.33	1.37
14	A	1125	CLA	C3D-C2D	2.64	1.46	1.39
14	B	1218	CLA	C1C-NC	-2.64	1.33	1.37
14	U	1502	CLA	C4D-CHA	2.64	1.47	1.38
14	U	1503	CLA	C4D-CHA	2.64	1.47	1.38
14	B	1202	CLA	C3D-C2D	2.64	1.46	1.39
14	B	1222	CLA	C4D-CHA	2.64	1.47	1.38
14	B	1234	CLA	MG-NC	2.64	2.12	2.06
14	b	1211	CLA	MG-NC	2.64	2.12	2.06
14	B	1239	CLA	C3D-C2D	2.64	1.46	1.39
14	b	1202	CLA	C3D-C2D	2.64	1.46	1.39
14	H	1209	CLA	MG-NC	2.64	2.12	2.06
14	A	1138	CLA	MG-NC	2.64	2.12	2.06
14	a	1111	CLA	C3D-C2D	2.64	1.46	1.39
14	G	1118	CLA	C1B-C2B	2.64	1.49	1.43
14	G	1137	CLA	C3D-C2D	2.64	1.46	1.39
14	G	1111	CLA	C3D-C2D	2.64	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1228	CLA	MG-NC	2.63	2.12	2.06
14	A	1111	CLA	C3D-C2D	2.63	1.46	1.39
14	H	1023	CLA	C4C-C3C	2.63	1.49	1.45
14	b	1222	CLA	C4D-CHA	2.63	1.47	1.38
14	B	1231	CLA	C3D-C2D	2.63	1.46	1.39
14	H	1228	CLA	MG-NC	2.63	2.12	2.06
14	a	1137	CLA	C3D-C2D	2.63	1.46	1.39
14	b	1218	CLA	C1C-NC	-2.63	1.33	1.37
14	H	1211	CLA	MG-NC	2.63	2.12	2.06
14	H	1202	CLA	C3D-C2D	2.63	1.46	1.39
14	A	1136	CLA	C4B-NB	-2.63	1.34	1.37
14	a	1124	CLA	C3D-C2D	2.63	1.46	1.39
14	b	1223	CLA	C3D-C2D	2.63	1.46	1.39
14	B	1023	CLA	C4C-C3C	2.63	1.49	1.45
14	A	1135	CLA	C3D-C2D	2.63	1.46	1.39
14	H	1231	CLA	C3D-C2D	2.62	1.46	1.39
14	B	1211	CLA	MG-NC	2.62	2.12	2.06
14	b	1228	CLA	MG-NC	2.62	2.12	2.06
14	A	1012	CLA	MG-NC	2.62	2.12	2.06
15	a	1121	F6C	C1A-C2A	2.62	1.51	1.45
14	G	1125	CLA	C3D-C2D	2.62	1.46	1.39
14	a	1135	CLA	C3D-C2D	2.62	1.46	1.39
14	A	1101	CLA	C4B-NB	-2.62	1.34	1.37
14	A	1110	CLA	C3D-C2D	2.62	1.46	1.39
14	b	1207	CLA	MG-NC	2.62	2.12	2.06
14	G	1135	CLA	C3D-C2D	2.62	1.46	1.39
14	B	1224	CLA	C4D-CHA	2.62	1.47	1.38
14	a	1116	CLA	C4B-NB	-2.62	1.34	1.37
14	b	1239	CLA	C3D-C2D	2.62	1.46	1.39
14	H	1224	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1234	CLA	MG-NC	2.62	2.12	2.06
14	b	1224	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1231	CLA	C3D-C2D	2.62	1.46	1.39
14	B	1232	CLA	C1C-NC	-2.61	1.33	1.37
14	x	1701	CLA	C1B-C2B	2.61	1.49	1.43
14	A	1130	CLA	MG-NC	2.61	2.12	2.06
14	A	1103	CLA	C1B-C2B	2.61	1.49	1.43
14	B	1207	CLA	MG-NC	2.61	2.12	2.06
14	b	1232	CLA	C1C-NC	-2.61	1.33	1.37
14	a	1109	CLA	C1B-C2B	2.61	1.49	1.43
14	A	1116	CLA	C4B-NB	-2.61	1.34	1.37
14	W	1701	CLA	C1B-C2B	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1023	CLA	C4C-C3C	2.61	1.49	1.45
14	a	1012	CLA	MG-NC	2.61	2.12	2.06
14	a	1103	CLA	C1B-C2B	2.61	1.49	1.43
14	H	1239	CLA	C3D-C2D	2.61	1.46	1.39
14	B	1021	CLA	C3D-C2D	2.61	1.46	1.39
14	l	1502	CLA	C4D-CHA	2.61	1.47	1.38
14	a	1110	CLA	C3D-C2D	2.61	1.46	1.39
14	H	1223	CLA	C3D-C2D	2.61	1.46	1.39
14	B	1232	CLA	C4B-NB	-2.61	1.34	1.37
14	X	1701	CLA	C1B-C2B	2.61	1.49	1.43
14	A	1109	CLA	C1B-C2B	2.61	1.49	1.43
14	A	1137	CLA	C3D-C2D	2.60	1.46	1.39
14	a	1119	CLA	MG-NC	2.60	2.12	2.06
14	H	1021	CLA	C3D-C2D	2.60	1.46	1.39
14	B	1218	CLA	C4B-NB	-2.60	1.34	1.37
14	T	1401	CLA	C1B-NB	-2.60	1.34	1.37
15	B	1237	F6C	C3B-C2B	2.60	1.45	1.39
14	b	1021	CLA	C3D-C2D	2.60	1.46	1.39
14	G	1130	CLA	MG-NC	2.60	2.12	2.06
14	a	1127	CLA	C3D-C2D	2.60	1.46	1.39
14	H	1218	CLA	C4B-NB	-2.60	1.34	1.37
15	b	1237	F6C	C3B-C2B	2.60	1.45	1.39
14	H	1232	CLA	C4B-NB	-2.60	1.34	1.37
14	W	1701	CLA	C4B-NB	-2.60	1.34	1.37
14	G	1103	CLA	C1B-C2B	2.60	1.49	1.43
15	A	1121	F6C	C1A-C2A	2.60	1.51	1.45
14	H	1217	CLA	C4B-NB	-2.60	1.34	1.37
14	G	1116	CLA	C4B-NB	-2.60	1.34	1.37
14	B	1223	CLA	C3D-C2D	2.59	1.46	1.39
14	G	1110	CLA	C3D-C2D	2.59	1.46	1.39
14	b	1218	CLA	C4B-NB	-2.59	1.34	1.37
14	a	1101	CLA	C4B-NB	-2.59	1.34	1.37
14	H	1023	CLA	C4D-CHA	2.59	1.47	1.38
14	A	1107	CLA	C3D-C2D	2.59	1.46	1.39
14	H	1207	CLA	MG-NC	2.59	2.12	2.06
15	G	1121	F6C	C3C-C2C	2.59	1.45	1.38
14	b	1023	CLA	C4D-CHA	2.59	1.47	1.38
14	H	1209	CLA	C4B-NB	-2.59	1.34	1.37
14	A	1109	CLA	MG-NC	2.59	2.12	2.06
14	a	1107	CLA	C3D-C2D	2.58	1.46	1.39
15	A	1120	F6C	CMB-C2B	2.58	1.51	1.45
14	A	1110	CLA	C4B-NB	-2.58	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1237	F6C	C3B-C2B	2.58	1.45	1.39
15	b	1237	F6C	C3B-C4B	2.58	1.49	1.44
14	G	1129	CLA	C4D-CHA	2.58	1.47	1.38
14	G	1127	CLA	C3D-C2D	2.58	1.46	1.39
14	A	1119	CLA	MG-NC	2.58	2.12	2.06
14	B	1235	CLA	MG-NC	2.58	2.12	2.06
14	G	1107	CLA	C3D-C2D	2.58	1.46	1.39
14	a	1129	CLA	C4D-CHA	2.58	1.47	1.38
14	H	1234	CLA	MG-NC	2.58	2.12	2.06
14	a	1110	CLA	C4B-NB	-2.58	1.34	1.37
14	x	1701	CLA	C4B-NB	-2.58	1.34	1.37
14	G	1116	CLA	C3D-C2D	2.58	1.46	1.39
14	B	1217	CLA	C4B-NB	-2.58	1.34	1.37
15	A	1121	F6C	C4C-NC	-2.58	1.34	1.37
14	G	1012	CLA	MG-NC	2.58	2.12	2.06
14	A	1129	CLA	C4D-CHA	2.57	1.47	1.38
14	A	1127	CLA	C3D-C2D	2.57	1.46	1.39
14	K	1401	CLA	C1B-NB	-2.57	1.34	1.37
14	H	1235	CLA	MG-NC	2.57	2.12	2.06
14	G	1109	CLA	C1B-C2B	2.57	1.49	1.43
14	b	1217	CLA	C4B-NB	-2.57	1.34	1.37
14	a	1112	CLA	C1B-C2B	2.57	1.49	1.43
14	a	1130	CLA	MG-NC	2.57	2.12	2.06
14	B	1023	CLA	C4D-CHA	2.57	1.47	1.38
14	a	1113	CLA	MG-NC	2.57	2.12	2.06
14	A	1116	CLA	C3D-C2D	2.57	1.46	1.39
14	a	1116	CLA	C3D-C2D	2.57	1.46	1.39
14	X	1701	CLA	C4B-NB	-2.57	1.34	1.37
15	A	1121	F6C	C3C-C2C	2.57	1.45	1.38
21	A	6002	LMT	O3B-C3B	-2.57	1.36	1.43
15	G	1121	F6C	C4C-NC	-2.56	1.34	1.37
15	G	1121	F6C	C1A-C2A	2.56	1.50	1.45
14	G	1110	CLA	C4B-NB	-2.56	1.34	1.37
14	b	1206	CLA	MG-NC	2.56	2.12	2.06
14	b	1235	CLA	MG-NC	2.56	2.12	2.06
15	H	1237	F6C	C3B-C4B	2.56	1.49	1.44
14	a	1131	CLA	MG-NC	2.56	2.12	2.06
14	b	1215	CLA	MG-NC	2.56	2.12	2.06
14	A	1113	CLA	MG-NC	2.56	2.12	2.06
14	k	1401	CLA	C1C-NC	-2.56	1.33	1.37
14	H	1021	CLA	C4D-CHA	2.56	1.47	1.38
14	b	1021	CLA	C4D-CHA	2.56	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	C4B-NB	-2.56	1.34	1.37
14	b	1232	CLA	C4B-NB	-2.56	1.34	1.37
14	L	1502	CLA	MG-NC	2.56	2.12	2.06
14	G	1136	CLA	C4B-NB	-2.56	1.34	1.37
15	G	1120	F6C	CMB-C2B	2.55	1.51	1.45
14	H	1234	CLA	C4D-CHA	2.55	1.47	1.38
14	A	1116	CLA	C1C-NC	-2.55	1.33	1.37
14	b	1234	CLA	C4D-CHA	2.55	1.47	1.38
14	A	1128	CLA	MG-NC	2.55	2.12	2.06
15	a	1121	F6C	C3C-C2C	2.55	1.45	1.38
15	a	1120	F6C	CMB-C2B	2.55	1.51	1.45
14	T	1401	CLA	C1C-NC	-2.55	1.33	1.37
14	B	1215	CLA	MG-NC	2.55	2.12	2.06
14	a	1128	CLA	MG-NC	2.55	2.12	2.06
21	G	6002	LMT	O3B-C3B	-2.55	1.36	1.43
14	B	1229	CLA	MG-NC	2.55	2.12	2.06
21	a	6002	LMT	O3B-C3B	-2.55	1.36	1.43
14	G	1119	CLA	MG-NC	2.55	2.12	2.06
14	H	1226	CLA	MG-NC	2.55	2.12	2.06
14	A	1104	CLA	C3D-C2D	2.55	1.45	1.39
14	a	1104	CLA	C3D-C2D	2.55	1.45	1.39
14	G	1101	CLA	C4B-NB	-2.54	1.34	1.37
15	a	1121	F6C	C4C-NC	-2.54	1.34	1.37
14	B	1234	CLA	C4D-CHA	2.54	1.47	1.38
14	B	1206	CLA	MG-NC	2.54	2.12	2.06
14	b	1202	CLA	C4B-NB	-2.54	1.34	1.37
14	G	1124	CLA	MG-NC	2.54	2.12	2.06
14	a	1124	CLA	MG-NC	2.54	2.12	2.06
14	G	1116	CLA	C1C-NC	-2.54	1.33	1.37
14	A	1112	CLA	C1B-C2B	2.54	1.49	1.43
14	b	1203	CLA	OBD-CAD	2.54	1.26	1.22
14	B	1204	CLA	C4D-CHA	2.54	1.47	1.38
14	G	1104	CLA	C3D-C2D	2.54	1.45	1.39
14	G	1112	CLA	C1B-C2B	2.54	1.49	1.43
14	b	1229	CLA	MG-NC	2.54	2.12	2.06
14	H	1021	CLA	C1B-C2B	2.53	1.49	1.43
14	G	1109	CLA	MG-NC	2.53	2.12	2.06
14	A	1131	CLA	MG-NC	2.53	2.12	2.06
14	G	1133	CLA	C4B-NB	-2.53	1.34	1.37
14	H	1204	CLA	C4D-CHA	2.53	1.47	1.38
14	B	1233	CLA	C1C-NC	-2.53	1.33	1.37
14	H	1203	CLA	OBD-CAD	2.53	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1128	CLA	MG-NC	2.53	2.12	2.06
14	B	1236	CLA	C4D-CHA	2.53	1.47	1.38
14	B	1021	CLA	C4D-CHA	2.53	1.47	1.38
14	b	1226	CLA	MG-NC	2.53	2.12	2.06
14	B	1226	CLA	MG-NC	2.52	2.12	2.06
14	l	1502	CLA	MG-NC	2.52	2.12	2.06
14	H	1229	CLA	MG-NC	2.52	2.12	2.06
14	H	1206	CLA	MG-NC	2.52	2.12	2.06
14	H	1215	CLA	MG-NC	2.52	2.12	2.06
14	U	1502	CLA	MG-NC	2.52	2.12	2.06
14	b	1204	CLA	C4D-CHA	2.52	1.47	1.38
14	G	1113	CLA	MG-NC	2.52	2.12	2.06
14	a	1116	CLA	C1C-NC	-2.52	1.33	1.37
14	A	1124	CLA	MG-NC	2.52	2.12	2.06
14	H	1236	CLA	C4D-CHA	2.52	1.47	1.38
15	A	1121	F6C	C4B-NB	-2.52	1.33	1.37
14	B	1021	CLA	C1B-C2B	2.52	1.49	1.43
14	b	1233	CLA	C1C-NC	-2.52	1.33	1.37
14	b	1236	CLA	C4D-CHA	2.52	1.47	1.38
14	a	1137	CLA	C1B-C2B	2.52	1.49	1.43
14	B	1203	CLA	OBD-CAD	2.52	1.26	1.22
14	a	1109	CLA	MG-NC	2.51	2.12	2.06
15	G	1121	F6C	C4B-NB	-2.51	1.33	1.37
14	A	1133	CLA	C4B-NB	-2.51	1.34	1.37
14	H	1216	CLA	MG-NC	2.51	2.12	2.06
14	B	1216	CLA	MG-NC	2.51	2.12	2.06
14	H	1233	CLA	C1C-NC	-2.51	1.33	1.37
14	B	1236	CLA	MG-NC	2.51	2.12	2.06
15	B	1237	F6C	C3B-C4B	2.51	1.49	1.44
14	K	1401	CLA	C1C-NC	-2.51	1.33	1.37
14	b	1219	CLA	C1B-C2B	2.51	1.49	1.43
14	A	1115	CLA	C1B-C2B	2.51	1.49	1.43
14	H	1219	CLA	C1B-C2B	2.51	1.49	1.43
14	A	1107	CLA	C1B-C2B	2.50	1.49	1.43
14	b	1021	CLA	C1B-C2B	2.50	1.49	1.43
14	A	1101	CLA	C1B-C2B	2.50	1.49	1.43
15	a	1121	F6C	C4B-NB	-2.50	1.34	1.37
14	A	1123	CLA	C1B-C2B	2.50	1.49	1.43
14	B	1202	CLA	C4B-NB	-2.50	1.34	1.37
14	G	1013	CLA	C4D-CHA	2.50	1.47	1.38
14	G	1115	CLA	C1B-C2B	2.50	1.49	1.43
14	G	1131	CLA	MG-NC	2.50	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	1503	CLA	C1B-C2B	2.50	1.49	1.43
14	G	1107	CLA	C1B-C2B	2.49	1.49	1.43
14	a	1110	CLA	C1B-C2B	2.49	1.49	1.43
14	a	1115	CLA	C1B-C2B	2.49	1.49	1.43
14	b	1216	CLA	MG-NC	2.49	2.12	2.06
14	H	1202	CLA	C4B-NB	-2.49	1.34	1.37
14	B	1202	CLA	MG-NC	2.49	2.12	2.06
14	a	1013	CLA	C4D-CHA	2.49	1.46	1.38
15	H	1237	F6C	C1A-C2A	2.48	1.50	1.45
14	G	1137	CLA	C1B-C2B	2.48	1.49	1.43
14	a	1107	CLA	C1B-C2B	2.48	1.49	1.43
14	G	1117	CLA	MG-NC	2.48	2.12	2.06
14	b	1202	CLA	MG-NC	2.48	2.12	2.06
14	B	1225	CLA	C3D-C2D	2.48	1.45	1.39
14	L	1503	CLA	MG-NC	2.48	2.12	2.06
14	B	1204	CLA	MG-NC	2.48	2.12	2.06
14	b	1236	CLA	MG-NC	2.48	2.12	2.06
14	A	1137	CLA	C1B-C2B	2.48	1.48	1.43
21	a	6002	LMT	O2B-C2B	-2.48	1.36	1.43
21	G	6002	LMT	O2B-C2B	-2.48	1.36	1.43
15	H	1230	F6C	C1D-ND	-2.47	1.34	1.37
14	a	1108	CLA	C4B-NB	-2.47	1.34	1.37
14	A	1013	CLA	C4D-CHA	2.47	1.46	1.38
14	H	1202	CLA	MG-NC	2.47	2.12	2.06
14	l	1503	CLA	MG-NC	2.47	2.12	2.06
14	a	1123	CLA	C1B-C2B	2.47	1.48	1.43
14	H	1212	CLA	C1B-C2B	2.47	1.48	1.43
14	U	1503	CLA	MG-NC	2.47	2.12	2.06
15	H	1230	F6C	C4A-C3A	2.46	1.50	1.45
14	A	1110	CLA	C1B-C2B	2.46	1.48	1.43
14	H	1225	CLA	C3D-C2D	2.46	1.45	1.39
14	H	1236	CLA	MG-NC	2.46	2.12	2.06
14	b	1225	CLA	C3D-C2D	2.46	1.45	1.39
14	B	1212	CLA	C1B-C2B	2.46	1.48	1.43
14	a	1101	CLA	C1B-C2B	2.46	1.48	1.43
14	G	1140	CLA	C3B-C4B	2.46	1.49	1.42
14	a	1133	CLA	C4B-NB	-2.46	1.34	1.37
14	b	1238	CLA	C3D-C2D	2.46	1.45	1.39
14	b	1213	CLA	C1B-C2B	2.46	1.48	1.43
14	G	1110	CLA	C1B-C2B	2.46	1.48	1.43
21	A	6002	LMT	O2B-C2B	-2.46	1.36	1.43
14	a	1140	CLA	C3B-C4B	2.46	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1140	CLA	C3B-C4B	2.46	1.49	1.42
14	H	1238	CLA	C3D-C2D	2.46	1.45	1.39
14	H	1203	CLA	C1B-C2B	2.45	1.48	1.43
14	G	1108	CLA	C4B-NB	-2.45	1.34	1.37
14	G	1123	CLA	C1B-C2B	2.45	1.48	1.43
14	b	1023	CLA	C1B-C2B	2.45	1.48	1.43
18	H	4005	BCR	C30-C25	-2.45	1.50	1.53
14	b	1204	CLA	MG-NC	2.45	2.12	2.06
14	G	1101	CLA	C1B-C2B	2.45	1.48	1.43
14	H	1204	CLA	MG-NC	2.45	2.12	2.06
14	B	1023	CLA	C1B-C2B	2.45	1.48	1.43
14	A	1117	CLA	MG-NC	2.45	2.12	2.06
14	B	1203	CLA	C1B-C2B	2.45	1.48	1.43
14	B	1213	CLA	C1B-C2B	2.45	1.48	1.43
14	B	1219	CLA	C1B-C2B	2.45	1.48	1.43
14	B	1238	CLA	C3D-C2D	2.45	1.45	1.39
14	a	1117	CLA	MG-NC	2.45	2.12	2.06
15	b	1237	F6C	C1A-C2A	2.45	1.50	1.45
15	B	1237	F6C	CHB-C4A	-2.44	1.33	1.38
14	L	1503	CLA	C1B-C2B	2.44	1.48	1.43
15	B	1230	F6C	C1D-ND	-2.44	1.34	1.37
15	B	1237	F6C	C1A-C2A	2.44	1.50	1.45
14	U	1503	CLA	C1B-C2B	2.44	1.48	1.43
14	b	1203	CLA	C1B-C2B	2.44	1.48	1.43
14	G	1013	CLA	CHB-C1B	2.44	1.44	1.39
14	a	1133	CLA	C1B-C2B	2.43	1.48	1.43
14	b	1212	CLA	C1B-C2B	2.43	1.48	1.43
15	b	1230	F6C	C4A-C3A	2.43	1.50	1.45
14	A	1013	CLA	CHB-C1B	2.43	1.44	1.39
14	K	1401	CLA	C4B-NB	-2.43	1.34	1.37
14	B	1239	CLA	C1B-C2B	2.43	1.48	1.43
14	b	1236	CLA	C3B-C4B	2.43	1.49	1.42
15	b	1237	F6C	CHB-C4A	-2.43	1.33	1.38
14	G	1133	CLA	C1B-C2B	2.43	1.48	1.43
21	a	6002	LMT	O2'-C2'	-2.43	1.36	1.43
15	B	1230	F6C	C4A-C3A	2.42	1.50	1.45
14	G	1113	CLA	C1B-C2B	2.42	1.48	1.43
14	a	1129	CLA	C3D-C2D	2.42	1.45	1.39
14	B	1207	CLA	C1B-C2B	2.42	1.48	1.43
14	H	1023	CLA	C1B-C2B	2.42	1.48	1.43
14	B	1234	CLA	C3D-C2D	2.42	1.45	1.39
14	A	1129	CLA	C3D-C2D	2.42	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1230	F6C	C4C-NC	-2.42	1.34	1.37
14	G	1104	CLA	C1B-C2B	2.42	1.48	1.43
14	H	1213	CLA	C1B-C2B	2.42	1.48	1.43
14	G	1135	CLA	C1B-C2B	2.42	1.48	1.43
14	G	1129	CLA	C3D-C2D	2.42	1.45	1.39
14	A	1113	CLA	C1B-C2B	2.42	1.48	1.43
13	A	1011	CL0	C4A-C3A	-2.41	1.46	1.51
14	A	1104	CLA	C1B-C2B	2.41	1.48	1.43
21	A	6002	LMT	O2'-C2'	-2.41	1.37	1.43
14	b	1207	CLA	C1B-C2B	2.41	1.48	1.43
14	H	1236	CLA	C3B-C4B	2.41	1.49	1.42
14	a	1113	CLA	C1B-C2B	2.41	1.48	1.43
14	H	1207	CLA	C1B-C2B	2.41	1.48	1.43
13	a	1011	CL0	CBD-CGD	-2.41	1.49	1.52
15	A	1121	F6C	CHB-C4A	-2.40	1.33	1.38
14	G	1013	CLA	C3B-C4B	2.40	1.49	1.42
14	B	1236	CLA	C3B-C4B	2.40	1.49	1.42
14	a	1135	CLA	C1B-C2B	2.40	1.48	1.43
14	A	1103	CLA	MG-NC	2.40	2.12	2.06
14	A	1105	CLA	C1B-C2B	2.40	1.48	1.43
18	B	4005	BCR	C30-C25	-2.40	1.50	1.53
14	b	1239	CLA	C1B-C2B	2.40	1.48	1.43
15	H	1237	F6C	CHB-C4A	-2.40	1.33	1.38
14	H	1203	CLA	C3D-C2D	2.40	1.45	1.39
14	a	1103	CLA	MG-NC	2.40	2.12	2.06
14	a	1108	CLA	C1B-C2B	2.40	1.48	1.43
13	G	1011	CL0	CBD-CGD	-2.40	1.49	1.52
14	A	1133	CLA	C1B-C2B	2.40	1.48	1.43
14	a	1104	CLA	C1B-C2B	2.40	1.48	1.43
20	I	5006	LMG	C37-C36	-2.40	1.33	1.50
20	i	5006	LMG	C37-C36	-2.39	1.33	1.50
14	a	1013	CLA	CHB-C1B	2.39	1.44	1.39
18	b	4005	BCR	C30-C25	-2.39	1.50	1.53
15	a	1120	F6C	C4B-NB	-2.39	1.34	1.37
14	b	1209	CLA	C1B-C2B	2.39	1.48	1.43
14	k	1401	CLA	C4B-NB	-2.39	1.34	1.37
14	T	1401	CLA	C4B-NB	-2.39	1.34	1.37
14	H	1239	CLA	C1B-C2B	2.39	1.48	1.43
15	a	1121	F6C	CHB-C4A	-2.39	1.33	1.38
20	R	5006	LMG	C37-C36	-2.38	1.33	1.50
14	a	1105	CLA	C1B-C2B	2.38	1.48	1.43
14	B	1203	CLA	C3D-C2D	2.38	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1135	CLA	C1B-C2B	2.38	1.48	1.43
14	a	1013	CLA	C3B-C4B	2.38	1.49	1.42
13	a	1011	CL0	C4A-C3A	-2.38	1.46	1.51
15	A	1120	F6C	CHB-C4A	-2.38	1.33	1.38
15	a	1120	F6C	CHB-C4A	-2.38	1.33	1.38
14	G	1108	CLA	C1B-C2B	2.38	1.48	1.43
14	H	1210	CLA	C4C-C3C	2.38	1.49	1.45
14	b	1234	CLA	C3D-C2D	2.38	1.45	1.39
21	G	6002	LMT	O2'-C2'	-2.38	1.37	1.43
14	G	1103	CLA	MG-NC	2.38	2.11	2.06
13	A	1011	CL0	CBD-CGD	-2.38	1.49	1.52
14	G	1125	CLA	C1B-C2B	2.37	1.48	1.43
21	a	6001	LMT	O2B-C2B	-2.37	1.37	1.43
15	G	1120	F6C	CHB-C4A	-2.37	1.33	1.38
14	H	1234	CLA	C3D-C2D	2.37	1.45	1.39
14	A	1013	CLA	C3B-C4B	2.37	1.49	1.42
15	G	1120	F6C	C4B-NB	-2.37	1.34	1.37
14	B	1223	CLA	C1B-C2B	2.37	1.48	1.43
18	a	4007	BCR	C1-C6	-2.37	1.50	1.53
14	T	1401	CLA	C1D-C2D	2.37	1.50	1.45
14	B	1209	CLA	C1B-C2B	2.37	1.48	1.43
14	b	1203	CLA	C3D-C2D	2.37	1.45	1.39
14	b	1220	CLA	C1B-C2B	2.37	1.48	1.43
14	a	1117	CLA	MG-ND	-2.36	2.01	2.05
14	K	1401	CLA	C1D-C2D	2.36	1.50	1.45
14	B	1208	CLA	C1B-C2B	2.36	1.48	1.43
15	b	1230	F6C	C4B-NB	-2.36	1.34	1.37
13	G	1011	CL0	C4A-C3A	-2.36	1.46	1.51
14	A	1108	CLA	C1B-C2B	2.36	1.48	1.43
14	A	1122	CLA	C1B-C2B	2.36	1.48	1.43
18	A	4007	BCR	C1-C6	-2.36	1.50	1.53
14	A	1125	CLA	C1B-C2B	2.36	1.48	1.43
14	H	1211	CLA	C1B-C2B	2.36	1.48	1.43
14	H	1021	CLA	MG-NC	2.35	2.11	2.06
15	G	1121	F6C	CHB-C4A	-2.35	1.33	1.38
15	A	1120	F6C	C4B-NB	-2.35	1.34	1.37
15	b	1230	F6C	C1D-ND	-2.35	1.34	1.37
14	a	1122	CLA	C1B-C2B	2.35	1.48	1.43
15	B	1237	F6C	C3C-C2C	2.35	1.45	1.38
14	G	1122	CLA	C1B-C2B	2.35	1.48	1.43
21	A	6001	LMT	O2B-C2B	-2.35	1.37	1.43
14	H	1203	CLA	MG-NC	2.35	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1105	CLA	C1B-C2B	2.35	1.48	1.43
14	B	1021	CLA	MG-NC	2.35	2.11	2.06
14	B	1221	CLA	C1B-C2B	2.35	1.48	1.43
21	G	6002	LMT	O4'-C4B	-2.35	1.37	1.43
14	b	1223	CLA	C1B-C2B	2.35	1.48	1.43
14	H	1205	CLA	MG-NC	2.35	2.11	2.06
14	b	1208	CLA	C1B-C2B	2.35	1.48	1.43
14	G	1111	CLA	C1B-C2B	2.35	1.48	1.43
21	a	6002	LMT	O4'-C4B	-2.34	1.37	1.43
14	B	1211	CLA	C1B-C2B	2.34	1.48	1.43
14	a	1111	CLA	C1B-C2B	2.34	1.48	1.43
14	H	1209	CLA	C1B-C2B	2.34	1.48	1.43
14	B	1210	CLA	C4C-C3C	2.34	1.49	1.45
14	L	1501	CLA	C1B-C2B	2.34	1.48	1.43
14	H	1220	CLA	C1B-C2B	2.34	1.48	1.43
14	b	1203	CLA	MG-NC	2.34	2.11	2.06
14	H	1221	CLA	C1B-C2B	2.34	1.48	1.43
14	b	1205	CLA	MG-NC	2.34	2.11	2.06
14	G	1139	CLA	C3B-C4B	2.34	1.49	1.42
14	B	1220	CLA	C1B-C2B	2.34	1.48	1.43
15	G	1121	F6C	C1D-C2D	2.34	1.49	1.44
14	A	1117	CLA	MG-ND	-2.34	2.01	2.05
14	B	1205	CLA	MG-NC	2.34	2.11	2.06
14	b	1211	CLA	C1B-C2B	2.33	1.48	1.43
14	G	1139	CLA	C4B-NB	-2.33	1.34	1.37
15	A	1121	F6C	C1D-C2D	2.33	1.49	1.44
14	U	1501	CLA	C1B-C2B	2.33	1.48	1.43
14	H	1223	CLA	C1B-C2B	2.33	1.48	1.43
15	B	1230	F6C	C4B-NB	-2.33	1.34	1.37
14	k	1401	CLA	C1D-C2D	2.33	1.49	1.45
14	B	1203	CLA	MG-NC	2.33	2.11	2.06
14	G	1117	CLA	MG-ND	-2.33	2.01	2.05
14	H	1232	CLA	C1B-C2B	2.32	1.48	1.43
14	l	1501	CLA	C1B-C2B	2.32	1.48	1.43
14	H	1228	CLA	C4C-C3C	2.32	1.49	1.45
15	b	1230	F6C	C4C-NC	-2.32	1.34	1.37
14	a	1125	CLA	C1B-C2B	2.32	1.48	1.43
21	G	6001	LMT	O2B-C2B	-2.32	1.37	1.43
18	G	4007	BCR	C1-C6	-2.31	1.50	1.53
15	H	1237	F6C	C3C-C2C	2.31	1.44	1.38
14	H	1208	CLA	C1B-C2B	2.31	1.48	1.43
14	b	1021	CLA	MG-NC	2.31	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1111	CLA	C1B-C2B	2.31	1.48	1.43
14	b	1210	CLA	C4C-C3C	2.31	1.49	1.45
14	a	1104	CLA	MG-NC	2.31	2.11	2.06
14	a	1139	CLA	C3B-C4B	2.31	1.49	1.42
14	A	1104	CLA	MG-NC	2.31	2.11	2.06
14	G	1104	CLA	MG-NC	2.31	2.11	2.06
18	R	4018	BCR	C1-C6	-2.30	1.50	1.53
14	b	1222	CLA	C1B-C2B	2.30	1.48	1.43
14	A	1139	CLA	C3B-C4B	2.30	1.49	1.42
18	I	4018	BCR	C1-C6	-2.30	1.50	1.53
14	H	1229	CLA	C1B-C2B	2.30	1.48	1.43
21	A	6002	LMT	O4'-C4B	-2.30	1.37	1.43
18	i	4018	BCR	C1-C6	-2.30	1.50	1.53
14	B	1232	CLA	C1B-C2B	2.30	1.48	1.43
14	G	1140	CLA	C4B-NB	-2.30	1.34	1.37
15	B	1230	F6C	C4C-NC	-2.30	1.34	1.37
14	b	1221	CLA	C1B-C2B	2.29	1.48	1.43
15	b	1237	F6C	C3C-C2C	2.29	1.44	1.38
14	a	1116	CLA	C1B-C2B	2.28	1.48	1.43
14	B	1236	CLA	C4B-NB	-2.28	1.34	1.37
15	a	1121	F6C	C1D-C2D	2.28	1.49	1.44
18	I	4020	BCR	C1-C6	-2.28	1.50	1.53
14	H	1236	CLA	C4B-NB	-2.28	1.34	1.37
14	H	1208	CLA	C3B-C4B	2.28	1.49	1.42
14	b	1236	CLA	C4B-NB	-2.28	1.34	1.37
14	b	1229	CLA	C1B-C2B	2.28	1.48	1.43
14	b	1201	CLA	C1B-C2B	2.27	1.48	1.43
14	H	1216	CLA	C1B-C2B	2.27	1.48	1.43
14	B	1228	CLA	C4C-C3C	2.27	1.48	1.45
14	b	1232	CLA	C1B-C2B	2.27	1.48	1.43
15	B	1230	F6C	CMB-C2B	2.27	1.50	1.45
14	B	1228	CLA	C1B-C2B	2.27	1.48	1.43
14	a	1114	CLA	C1D-C2D	2.27	1.49	1.45
14	B	1201	CLA	C1B-C2B	2.27	1.48	1.43
14	H	1204	CLA	C1B-C2B	2.27	1.48	1.43
14	b	1233	CLA	C4B-NB	-2.27	1.34	1.37
14	b	1228	CLA	C4C-C3C	2.27	1.48	1.45
14	H	1228	CLA	C1B-C2B	2.27	1.48	1.43
14	b	1204	CLA	C1B-C2B	2.26	1.48	1.43
14	B	1229	CLA	C1B-C2B	2.26	1.48	1.43
14	G	1116	CLA	C1B-C2B	2.26	1.48	1.43
21	A	6001	LMT	O3B-C3B	-2.26	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1204	CLA	C1B-C2B	2.26	1.48	1.43
14	B	1222	CLA	C1B-C2B	2.26	1.48	1.43
14	a	1130	CLA	OBD-CAD	2.26	1.26	1.22
14	A	1116	CLA	C1B-C2B	2.26	1.48	1.43
14	A	1114	CLA	C1D-C2D	2.26	1.49	1.45
14	a	1139	CLA	C4B-NB	-2.25	1.34	1.37
15	b	1230	F6C	CMB-C2B	2.25	1.50	1.45
14	B	1233	CLA	C4B-NB	-2.25	1.34	1.37
14	B	1208	CLA	C3B-C4B	2.25	1.49	1.42
14	H	1222	CLA	C1B-C2B	2.25	1.48	1.43
15	H	1230	F6C	MG-ND	-2.25	2.00	2.06
14	A	1139	CLA	C4B-NB	-2.25	1.34	1.37
14	B	1216	CLA	C1B-C2B	2.25	1.48	1.43
14	H	1021	CLA	C3A-C2A	-2.25	1.48	1.54
21	G	6001	LMT	O3B-C3B	-2.25	1.37	1.43
21	a	6001	LMT	O3B-C3B	-2.25	1.37	1.43
14	H	1201	CLA	C1B-C2B	2.25	1.48	1.43
14	a	1140	CLA	C4B-NB	-2.25	1.34	1.37
14	b	1208	CLA	C3B-C4B	2.24	1.49	1.42
14	A	1140	CLA	C4B-NB	-2.24	1.34	1.37
14	B	1227	CLA	C1B-C2B	2.24	1.48	1.43
14	a	1125	CLA	MG-NC	2.24	2.11	2.06
15	b	1230	F6C	MG-ND	-2.24	2.00	2.06
14	B	1021	CLA	C3A-C2A	-2.24	1.48	1.54
14	G	1114	CLA	C4C-C3C	2.24	1.48	1.45
14	b	1228	CLA	C1B-C2B	2.23	1.48	1.43
14	B	1023	CLA	MG-NC	2.23	2.11	2.06
14	b	1216	CLA	C1B-C2B	2.23	1.48	1.43
14	H	1023	CLA	MG-NC	2.23	2.11	2.06
14	H	1208	CLA	C4B-NB	-2.23	1.34	1.37
15	H	1230	F6C	CMB-C2B	2.23	1.50	1.45
14	A	1125	CLA	MG-NC	2.23	2.11	2.06
14	G	1013	CLA	CHB-C4A	-2.23	1.32	1.37
14	a	1127	CLA	C1B-C2B	2.23	1.48	1.43
14	A	1114	CLA	C4C-C3C	2.23	1.48	1.45
14	b	1023	CLA	MG-NC	2.23	2.11	2.06
14	A	1138	CLA	C1B-C2B	2.22	1.48	1.43
18	R	4020	BCR	C1-C6	-2.22	1.50	1.53
14	a	1135	CLA	C4C-C3C	2.22	1.48	1.45
14	G	1125	CLA	MG-NC	2.22	2.11	2.06
14	G	1130	CLA	OBD-CAD	2.22	1.26	1.22
14	H	1233	CLA	C4B-NB	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1114	CLA	C1D-C2D	2.22	1.49	1.45
14	B	1239	CLA	C4C-C3C	2.22	1.48	1.45
14	T	1401	CLA	C4C-C3C	2.22	1.48	1.45
21	a	6001	LMT	O1'-C1'	-2.21	1.36	1.40
14	A	1135	CLA	C4C-C3C	2.21	1.48	1.45
14	A	1013	CLA	CHB-C4A	-2.21	1.32	1.37
14	b	1234	CLA	C1B-C2B	2.21	1.48	1.43
14	H	1239	CLA	C4C-C3C	2.21	1.48	1.45
15	H	1230	F6C	C4B-NB	-2.21	1.34	1.37
14	b	1021	CLA	C3A-C2A	-2.21	1.48	1.54
14	B	1210	CLA	C1B-C2B	2.21	1.48	1.43
14	G	1138	CLA	C1B-C2B	2.21	1.48	1.43
14	H	1226	CLA	CHB-C4A	-2.21	1.32	1.37
14	G	1133	CLA	C1A-CHA	2.21	1.52	1.43
14	H	1234	CLA	C1B-C2B	2.21	1.48	1.43
14	G	1127	CLA	C1B-C2B	2.21	1.48	1.43
15	B	1230	F6C	C1A-C2A	2.21	1.50	1.45
14	A	1133	CLA	C1A-CHA	2.20	1.52	1.43
14	b	1233	CLA	C1D-C2D	2.20	1.49	1.45
14	a	1114	CLA	C4C-C3C	2.20	1.48	1.45
14	a	1133	CLA	C1A-CHA	2.20	1.52	1.43
14	H	1210	CLA	C1B-C2B	2.20	1.48	1.43
14	k	1401	CLA	C4C-C3C	2.20	1.48	1.45
14	B	1208	CLA	C4B-NB	-2.20	1.35	1.37
14	K	1401	CLA	C4C-C3C	2.20	1.48	1.45
14	a	1013	CLA	CHB-C4A	-2.20	1.32	1.37
14	a	1138	CLA	C1B-C2B	2.19	1.48	1.43
14	B	1201	CLA	C1A-CHA	2.19	1.52	1.43
14	A	1127	CLA	C1B-C2B	2.19	1.48	1.43
14	B	1234	CLA	C1B-C2B	2.19	1.48	1.43
14	G	1126	CLA	C1B-C2B	2.19	1.48	1.43
14	H	1227	CLA	C1B-C2B	2.19	1.48	1.43
15	B	1230	F6C	MG-ND	-2.19	2.01	2.06
14	b	1210	CLA	C1B-C2B	2.19	1.48	1.43
18	i	4020	BCR	C1-C6	-2.19	1.51	1.53
14	A	1130	CLA	OBD-CAD	2.18	1.26	1.22
21	A	6001	LMT	O1'-C1'	-2.18	1.36	1.40
14	A	1013	CLA	MG-NC	2.18	2.11	2.06
21	G	6001	LMT	O1'-C1'	-2.18	1.36	1.40
14	H	1233	CLA	C1D-C2D	2.18	1.49	1.45
14	H	1201	CLA	C1A-CHA	2.18	1.52	1.43
14	b	1227	CLA	C1B-C2B	2.18	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1201	CLA	C1A-CHA	2.18	1.52	1.43
14	b	1226	CLA	CHB-C4A	-2.18	1.32	1.37
14	G	1135	CLA	C4C-C3C	2.17	1.48	1.45
14	A	1136	CLA	C1A-CHA	2.17	1.52	1.43
15	b	1230	F6C	C2B-C1B	2.17	1.49	1.44
15	A	1121	F6C	C4D-CHA	2.17	1.48	1.42
14	b	1208	CLA	C4B-NB	-2.17	1.35	1.37
14	b	1216	CLA	C1D-C2D	2.17	1.49	1.45
18	G	4011	BCR	C1-C6	-2.17	1.51	1.53
14	a	1132	CLA	C1B-C2B	2.17	1.48	1.43
14	a	1136	CLA	C1A-CHA	2.17	1.52	1.43
14	a	1013	CLA	MG-NC	2.16	2.11	2.06
14	B	1236	CLA	C1B-C2B	2.16	1.48	1.43
14	H	1231	CLA	C3B-C4B	2.16	1.49	1.42
14	B	1231	CLA	C3B-C4B	2.16	1.49	1.42
14	B	1226	CLA	CHB-C4A	-2.16	1.32	1.37
14	H	1236	CLA	C1B-C2B	2.16	1.48	1.43
14	b	1223	CLA	C1A-CHA	2.16	1.52	1.43
14	A	1139	CLA	C1B-C2B	2.16	1.48	1.43
14	G	1132	CLA	C1B-C2B	2.16	1.48	1.43
14	B	1223	CLA	C1A-CHA	2.16	1.52	1.43
14	b	1213	CLA	C1D-C2D	2.16	1.49	1.45
14	b	1239	CLA	C4C-C3C	2.16	1.48	1.45
14	H	1223	CLA	C1A-CHA	2.16	1.52	1.43
14	b	1208	CLA	C1D-C2D	2.16	1.49	1.45
14	A	1126	CLA	C1B-C2B	2.16	1.48	1.43
14	a	1126	CLA	C1B-C2B	2.15	1.48	1.43
14	B	1213	CLA	C1D-C2D	2.15	1.49	1.45
14	G	1136	CLA	C1A-CHA	2.15	1.52	1.43
14	B	1233	CLA	C1D-C2D	2.15	1.49	1.45
14	a	1139	CLA	C1B-C2B	2.15	1.48	1.43
15	b	1230	F6C	C1A-C2A	2.15	1.50	1.45
14	B	1216	CLA	C1D-C2D	2.15	1.49	1.45
14	U	1502	CLA	C1B-C2B	2.15	1.48	1.43
14	G	1139	CLA	C1B-C2B	2.15	1.48	1.43
14	A	1115	CLA	C1D-C2D	2.15	1.49	1.45
15	H	1230	F6C	C1A-C2A	2.14	1.50	1.45
14	G	1013	CLA	MG-NC	2.14	2.11	2.06
15	H	1230	F6C	C2B-C1B	2.14	1.49	1.44
14	A	1108	CLA	C1D-C2D	2.14	1.49	1.45
14	H	1208	CLA	C1D-C2D	2.14	1.49	1.45
14	L	1501	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1131	CLA	C1A-CHA	2.13	1.51	1.43
14	H	1232	CLA	C1A-CHA	2.13	1.51	1.43
14	H	1229	CLA	C1D-C2D	2.13	1.49	1.45
14	G	1112	CLA	C1A-CHA	2.13	1.51	1.43
14	A	1132	CLA	C1B-C2B	2.13	1.48	1.43
14	B	1219	CLA	C1A-CHA	2.13	1.51	1.43
14	B	1208	CLA	C1D-C2D	2.13	1.49	1.45
14	b	1231	CLA	C3B-C4B	2.13	1.48	1.42
14	G	1131	CLA	C1A-CHA	2.13	1.51	1.43
14	B	1209	CLA	C1D-C2D	2.13	1.49	1.45
14	b	1232	CLA	C1A-CHA	2.13	1.51	1.43
14	H	1219	CLA	C1A-CHA	2.13	1.51	1.43
14	b	1236	CLA	C1B-C2B	2.12	1.48	1.43
14	B	1216	CLA	C4C-C3C	2.12	1.48	1.45
14	a	1117	CLA	C1D-C2D	2.12	1.49	1.45
14	G	1108	CLA	C1D-C2D	2.12	1.49	1.45
15	a	1121	F6C	C4D-CHA	2.12	1.48	1.42
14	G	1140	CLA	C1B-C2B	2.12	1.48	1.43
14	H	1216	CLA	C4C-C3C	2.12	1.48	1.45
14	B	1232	CLA	C1A-CHA	2.12	1.51	1.43
14	a	1131	CLA	C1A-CHA	2.12	1.51	1.43
14	k	1401	CLA	C1A-CHA	2.12	1.51	1.43
14	B	1229	CLA	C1D-C2D	2.12	1.49	1.45
15	G	1121	F6C	C4D-CHA	2.12	1.48	1.42
14	K	1401	CLA	C1A-CHA	2.12	1.51	1.43
14	l	1501	CLA	C1A-CHA	2.12	1.51	1.43
18	A	4008	BCR	C30-C25	-2.12	1.51	1.53
14	a	1112	CLA	C1A-CHA	2.12	1.51	1.43
14	b	1229	CLA	C1D-C2D	2.12	1.49	1.45
14	B	1233	CLA	C4C-C3C	2.12	1.48	1.45
14	b	1216	CLA	C4C-C3C	2.12	1.48	1.45
18	B	4004	BCR	C30-C25	-2.12	1.51	1.53
14	b	1219	CLA	C1A-CHA	2.12	1.51	1.43
14	U	1501	CLA	C1A-CHA	2.12	1.51	1.43
15	G	1121	F6C	CMB-C2B	2.12	1.50	1.45
15	a	1121	F6C	CMB-C2B	2.11	1.50	1.45
18	G	4008	BCR	C30-C25	-2.11	1.51	1.53
15	B	1230	F6C	C2B-C1B	2.11	1.49	1.44
14	A	1112	CLA	C1A-CHA	2.11	1.51	1.43
14	L	1502	CLA	C1B-C2B	2.11	1.48	1.43
14	H	1216	CLA	C1D-C2D	2.11	1.49	1.45
14	l	1502	CLA	C1B-C2B	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1115	CLA	C1D-C2D	2.11	1.49	1.45
14	A	1102	CLA	C1B-C2B	2.11	1.48	1.43
14	A	1117	CLA	C1A-CHA	2.11	1.51	1.43
14	H	1209	CLA	C1D-C2D	2.11	1.49	1.45
14	a	1108	CLA	C1D-C2D	2.11	1.49	1.45
14	a	1111	CLA	C4C-C3C	2.10	1.48	1.45
14	b	1205	CLA	C1A-CHA	2.10	1.51	1.43
14	b	1023	CLA	C1A-CHA	2.10	1.51	1.43
14	H	1213	CLA	C1D-C2D	2.10	1.49	1.45
14	H	1205	CLA	C1A-CHA	2.10	1.51	1.43
14	G	1122	CLA	C1A-CHA	2.10	1.51	1.43
14	T	1401	CLA	C1A-CHA	2.10	1.51	1.43
15	A	1121	F6C	CMB-C2B	2.10	1.50	1.45
14	H	1023	CLA	C1A-CHA	2.10	1.51	1.43
14	A	1108	CLA	C3B-C4B	2.10	1.48	1.42
14	b	1209	CLA	C1D-C2D	2.10	1.49	1.45
18	H	4004	BCR	C30-C25	-2.09	1.51	1.53
14	B	1205	CLA	C1A-CHA	2.09	1.51	1.43
14	A	1122	CLA	C1A-CHA	2.09	1.51	1.43
14	a	1109	CLA	C1D-C2D	2.09	1.49	1.45
14	G	1117	CLA	C1A-CHA	2.09	1.51	1.43
14	a	1117	CLA	C1A-CHA	2.09	1.51	1.43
14	B	1226	CLA	CMB-C2B	-2.09	1.46	1.50
14	B	1023	CLA	C1A-CHA	2.09	1.51	1.43
18	A	4011	BCR	C1-C6	-2.09	1.51	1.53
14	H	1207	CLA	C3B-C4B	2.09	1.48	1.42
14	a	1122	CLA	C1A-CHA	2.08	1.51	1.43
18	a	4011	BCR	C1-C6	-2.08	1.51	1.53
14	b	1226	CLA	CMB-C2B	-2.08	1.46	1.50
15	A	1120	F6C	C4D-CHA	2.08	1.48	1.42
14	a	1140	CLA	C1B-C2B	2.08	1.48	1.43
15	a	1120	F6C	C4D-CHA	2.08	1.48	1.42
14	A	1117	CLA	C1D-C2D	2.08	1.49	1.45
14	b	1214	CLA	C4C-C3C	2.08	1.48	1.45
14	a	1102	CLA	C1B-C2B	2.08	1.48	1.43
14	a	1115	CLA	C1D-C2D	2.08	1.49	1.45
14	B	1207	CLA	C3B-C4B	2.07	1.48	1.42
14	G	1109	CLA	C1D-C2D	2.07	1.49	1.45
14	b	1212	CLA	C1A-CHA	2.07	1.51	1.43
14	H	1206	CLA	C3A-C2A	-2.07	1.48	1.54
14	A	1140	CLA	C1B-C2B	2.07	1.48	1.43
14	b	1202	CLA	C1B-C2B	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1202	CLA	C1B-C2B	2.07	1.48	1.43
18	a	4008	BCR	C30-C25	-2.07	1.51	1.53
14	G	1108	CLA	C3B-C4B	2.07	1.48	1.42
14	a	1108	CLA	C3B-C4B	2.07	1.48	1.42
14	b	1207	CLA	C3B-C4B	2.07	1.48	1.42
14	a	1112	CLA	C4C-C3C	2.07	1.48	1.45
15	G	1120	F6C	C4D-CHA	2.07	1.47	1.42
14	b	1228	CLA	C1D-C2D	2.07	1.49	1.45
14	B	1212	CLA	C1A-CHA	2.07	1.51	1.43
14	G	1112	CLA	C4C-C3C	2.07	1.48	1.45
14	G	1012	CLA	O2D-CED	-2.06	1.40	1.45
15	H	1230	F6C	C1C-C2C	2.06	1.48	1.43
14	A	1124	CLA	C3B-C4B	2.06	1.48	1.42
21	A	6001	LMT	O4'-C4B	-2.06	1.37	1.43
14	A	1110	CLA	C1A-CHA	2.06	1.51	1.43
14	A	1106	CLA	C1A-CHA	2.06	1.51	1.43
14	G	1114	CLA	C1A-CHA	2.06	1.51	1.43
14	B	1206	CLA	C3A-C2A	-2.06	1.48	1.54
14	G	1106	CLA	C1A-CHA	2.06	1.51	1.43
21	a	6001	LMT	O4'-C4B	-2.06	1.37	1.43
14	H	1233	CLA	C4C-C3C	2.06	1.48	1.45
14	H	1225	CLA	C1A-CHA	2.06	1.51	1.43
15	H	1237	F6C	C4D-CHA	2.06	1.47	1.42
14	G	1117	CLA	C1D-C2D	2.06	1.49	1.45
14	G	1124	CLA	C3B-C4B	2.06	1.48	1.42
14	H	1212	CLA	C1A-CHA	2.06	1.51	1.43
14	G	1110	CLA	C1A-CHA	2.05	1.51	1.43
15	b	1230	F6C	C1C-C2C	2.05	1.47	1.43
14	G	1013	CLA	C3A-C4A	-2.05	1.45	1.51
15	B	1237	F6C	C4D-CHA	2.05	1.47	1.42
14	G	1111	CLA	C4C-C3C	2.05	1.48	1.45
14	a	1114	CLA	C1A-CHA	2.05	1.51	1.43
14	H	1226	CLA	CMB-C2B	-2.05	1.46	1.50
15	b	1237	F6C	C4D-CHA	2.05	1.47	1.42
14	a	1012	CLA	O2D-CED	-2.05	1.40	1.45
14	B	1225	CLA	C1A-CHA	2.05	1.51	1.43
14	B	1214	CLA	C4C-C3C	2.05	1.48	1.45
14	G	1111	CLA	C1A-CHA	2.05	1.51	1.43
14	b	1206	CLA	C3A-C2A	-2.05	1.48	1.54
14	A	1114	CLA	C1A-CHA	2.05	1.51	1.43
14	A	1013	CLA	C3A-C4A	-2.05	1.45	1.51
14	A	1012	CLA	O2D-CED	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1110	CLA	C1A-CHA	2.05	1.51	1.43
14	a	1105	CLA	C1D-C2D	2.05	1.49	1.45
14	a	1013	CLA	C3A-C4A	-2.05	1.45	1.51
14	B	1228	CLA	C1D-C2D	2.05	1.49	1.45
14	H	1217	CLA	C1A-CHA	2.05	1.51	1.43
14	a	1124	CLA	C3B-C4B	2.05	1.48	1.42
18	b	4004	BCR	C30-C25	-2.05	1.51	1.53
14	A	1109	CLA	C1A-CHA	2.05	1.51	1.43
14	H	1224	CLA	C1B-C2B	2.05	1.47	1.43
14	A	1105	CLA	C1D-C2D	2.04	1.49	1.45
21	G	6001	LMT	O4'-C4B	-2.04	1.37	1.43
14	a	1112	CLA	C1D-C2D	2.04	1.49	1.45
15	B	1230	F6C	C1C-C2C	2.04	1.47	1.43
14	A	1111	CLA	C1A-CHA	2.04	1.51	1.43
14	a	1111	CLA	C1A-CHA	2.04	1.51	1.43
14	a	1109	CLA	C1A-CHA	2.04	1.51	1.43
14	b	1233	CLA	C4C-C3C	2.04	1.48	1.45
14	b	1225	CLA	C1A-CHA	2.04	1.51	1.43
14	B	1217	CLA	C1A-CHA	2.04	1.51	1.43
14	A	1111	CLA	C4C-C3C	2.04	1.48	1.45
14	b	1217	CLA	C1A-CHA	2.04	1.51	1.43
14	B	1022	CLA	C1B-C2B	2.04	1.47	1.43
14	G	1102	CLA	C1B-C2B	2.04	1.47	1.43
14	a	1106	CLA	C1A-CHA	2.04	1.51	1.43
14	A	1105	CLA	C4C-C3C	2.04	1.48	1.45
14	H	1214	CLA	C4C-C3C	2.04	1.48	1.45
14	B	1224	CLA	C1B-C2B	2.04	1.47	1.43
14	b	1209	CLA	C1A-CHA	2.04	1.51	1.43
14	A	1112	CLA	C4C-C3C	2.04	1.48	1.45
14	A	1109	CLA	C1D-C2D	2.03	1.49	1.45
14	B	1232	CLA	C1D-C2D	2.03	1.49	1.45
14	a	1131	CLA	C1B-C2B	2.03	1.47	1.43
14	A	1112	CLA	C1D-C2D	2.03	1.49	1.45
14	A	1138	CLA	C1A-CHA	2.03	1.51	1.43
14	H	1209	CLA	C1A-CHA	2.03	1.51	1.43
14	G	1109	CLA	C1A-CHA	2.03	1.51	1.43
14	B	1205	CLA	C1B-C2B	2.03	1.47	1.43
14	B	1202	CLA	C1B-C2B	2.03	1.47	1.43
14	b	1222	CLA	C3B-C4B	2.03	1.48	1.42
14	G	1112	CLA	C1D-C2D	2.03	1.49	1.45
14	H	1227	CLA	C4C-C3C	2.03	1.48	1.45
14	B	1209	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	1121	F6C	C4C-C3C	2.03	1.48	1.44
14	H	1228	CLA	C1D-C2D	2.03	1.49	1.45
14	a	1136	CLA	C3B-C4B	2.03	1.48	1.42
14	G	1105	CLA	C1D-C2D	2.02	1.49	1.45
14	b	1239	CLA	C1A-CHA	2.02	1.51	1.43
14	a	1138	CLA	C1A-CHA	2.02	1.51	1.43
14	G	1138	CLA	C1A-CHA	2.02	1.51	1.43
14	H	1239	CLA	C1A-CHA	2.02	1.51	1.43
14	G	1136	CLA	C1B-C2B	2.02	1.47	1.43
15	A	1121	F6C	C4C-C3C	2.02	1.48	1.44
14	H	1012	CLA	C1B-C2B	2.02	1.47	1.43
14	b	1232	CLA	C1D-C2D	2.02	1.49	1.45
14	b	1238	CLA	C4C-C3C	2.02	1.48	1.45
14	B	1239	CLA	C1A-CHA	2.02	1.51	1.43
14	b	1232	CLA	C4C-C3C	2.01	1.48	1.45
14	a	1136	CLA	C1B-C2B	2.01	1.47	1.43
14	G	1127	CLA	C1A-CHA	2.01	1.51	1.43
14	H	1205	CLA	C1B-C2B	2.01	1.47	1.43
14	A	1114	CLA	C1B-C2B	2.01	1.47	1.43
14	G	1131	CLA	C1B-C2B	2.01	1.47	1.43
14	a	1119	CLA	C3B-C4B	2.01	1.48	1.42
15	G	1120	F6C	C1D-C2D	2.01	1.48	1.44
14	A	1131	CLA	C1B-C2B	2.01	1.47	1.43
14	a	1138	CLA	C1D-C2D	2.01	1.49	1.45
15	a	1121	F6C	C4C-C3C	2.01	1.48	1.44
14	G	1138	CLA	C1D-C2D	2.01	1.49	1.45
15	b	1237	F6C	C4B-NB	-2.01	1.34	1.37
14	b	1022	CLA	C1B-C2B	2.01	1.47	1.43
14	G	1117	CLA	CHB-C4A	-2.01	1.32	1.37
14	a	1128	CLA	CHB-C4A	-2.00	1.32	1.37
14	B	1214	CLA	C1B-C2B	2.00	1.47	1.43
14	A	1136	CLA	C3B-C4B	2.00	1.48	1.42
14	B	1232	CLA	C4C-C3C	2.00	1.48	1.45
14	G	1124	CLA	C1A-CHA	2.00	1.51	1.43
14	A	1127	CLA	C1A-CHA	2.00	1.51	1.43
14	A	1102	CLA	C1A-CHA	2.00	1.51	1.43
14	G	1128	CLA	CHB-C4A	-2.00	1.32	1.37

All (8672) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4010	BCR	C16-C17-C18	25.54	163.10	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4010	BCR	C16-C17-C18	25.53	163.08	127.28
18	b	4010	BCR	C16-C17-C18	25.51	163.05	127.28
18	B	4017	BCR	C20-C21-C22	23.94	160.85	127.28
18	b	4017	BCR	C20-C21-C22	23.91	160.81	127.28
18	H	4017	BCR	C20-C21-C22	23.90	160.80	127.28
18	R	4018	BCR	C16-C17-C18	23.77	160.62	127.28
18	I	4018	BCR	C16-C17-C18	23.77	160.61	127.28
18	i	4018	BCR	C16-C17-C18	23.76	160.59	127.28
18	H	4016	BCR	C16-C17-C18	23.38	160.07	127.28
18	b	4016	BCR	C16-C17-C18	23.37	160.05	127.28
18	B	4016	BCR	C16-C17-C18	23.36	160.04	127.28
18	A	4007	BCR	C20-C21-C22	23.32	159.98	127.28
18	a	4007	BCR	C20-C21-C22	23.31	159.97	127.28
18	G	4007	BCR	C20-C21-C22	23.29	159.94	127.28
18	H	4016	BCR	C20-C21-C22	22.68	159.08	127.28
18	B	4016	BCR	C20-C21-C22	22.67	159.08	127.28
18	b	4016	BCR	C20-C21-C22	22.65	159.04	127.28
18	b	4009	BCR	C16-C17-C18	22.59	158.96	127.28
18	B	4009	BCR	C16-C17-C18	22.57	158.93	127.28
18	H	4009	BCR	C16-C17-C18	22.57	158.93	127.28
18	H	4006	BCR	C20-C21-C22	22.50	158.83	127.28
18	B	4006	BCR	C20-C21-C22	22.48	158.80	127.28
18	b	4006	BCR	C20-C21-C22	22.47	158.79	127.28
18	A	4001	BCR	C20-C21-C22	22.19	158.40	127.28
18	G	4001	BCR	C20-C21-C22	22.16	158.36	127.28
18	a	4001	BCR	C20-C21-C22	22.14	158.32	127.28
18	B	4010	BCR	C20-C21-C22	21.95	158.06	127.28
18	H	4010	BCR	C20-C21-C22	21.94	158.05	127.28
18	b	4010	BCR	C20-C21-C22	21.89	157.98	127.28
18	l	4019	BCR	C20-C21-C22	21.80	157.85	127.28
18	L	4019	BCR	C20-C21-C22	21.79	157.84	127.28
18	U	4019	BCR	C20-C21-C22	21.79	157.84	127.28
18	M	4021	BCR	C20-C21-C22	21.70	157.71	127.28
18	V	4021	BCR	C20-C21-C22	21.66	157.66	127.28
18	m	4021	BCR	C20-C21-C22	21.66	157.65	127.28
18	a	4003	BCR	C20-C21-C22	21.61	157.59	127.28
18	A	4003	BCR	C20-C21-C22	21.61	157.59	127.28
18	G	4003	BCR	C20-C21-C22	21.61	157.58	127.28
18	A	4007	BCR	C16-C17-C18	21.58	157.54	127.28
18	H	4014	BCR	C15-C16-C17	21.57	167.65	123.52
18	b	4014	BCR	C15-C16-C17	21.57	167.65	123.52
18	a	4007	BCR	C16-C17-C18	21.54	157.49	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4014	BCR	C15-C16-C17	21.52	167.56	123.52
18	G	4007	BCR	C16-C17-C18	21.50	157.43	127.28
18	G	4001	BCR	C15-C16-C17	21.45	167.41	123.52
18	A	4001	BCR	C15-C16-C17	21.42	167.36	123.52
18	B	4012	BCR	C20-C21-C22	21.40	157.29	127.28
18	a	4001	BCR	C15-C16-C17	21.40	167.31	123.52
18	H	4012	BCR	C20-C21-C22	21.37	157.24	127.28
18	b	4012	BCR	C20-C21-C22	21.35	157.22	127.28
18	B	4005	BCR	C20-C21-C22	21.33	157.19	127.28
18	H	4005	BCR	C20-C21-C22	21.31	157.16	127.28
18	b	4005	BCR	C20-C21-C22	21.27	157.11	127.28
18	H	4013	BCR	C16-C17-C18	21.23	157.06	127.28
18	b	4013	BCR	C16-C17-C18	21.22	157.03	127.28
18	B	4013	BCR	C20-C21-C22	21.21	157.02	127.28
18	B	4013	BCR	C16-C17-C18	21.19	157.00	127.28
18	b	4013	BCR	C20-C21-C22	21.16	156.96	127.28
18	H	4013	BCR	C20-C21-C22	21.16	156.96	127.28
18	G	4011	BCR	C16-C17-C18	21.14	156.93	127.28
18	H	4012	BCR	C15-C16-C17	21.12	166.72	123.52
18	a	4011	BCR	C16-C17-C18	21.11	156.88	127.28
18	B	4012	BCR	C15-C16-C17	21.09	166.67	123.52
18	A	4011	BCR	C16-C17-C18	21.08	156.84	127.28
18	b	4012	BCR	C15-C16-C17	21.06	166.61	123.52
18	B	4012	BCR	C16-C17-C18	21.01	156.75	127.28
18	H	4012	BCR	C16-C17-C18	20.99	156.72	127.28
18	b	4012	BCR	C16-C17-C18	20.97	156.69	127.28
18	a	4002	BCR	C15-C16-C17	20.94	166.37	123.52
18	A	4002	BCR	C15-C16-C17	20.94	166.37	123.52
18	G	4002	BCR	C15-C16-C17	20.93	166.35	123.52
18	G	4003	BCR	C16-C17-C18	20.93	156.64	127.28
18	a	4003	BCR	C16-C17-C18	20.90	156.58	127.28
18	B	4017	BCR	C16-C17-C18	20.88	156.56	127.28
18	H	4017	BCR	C16-C17-C18	20.87	156.55	127.28
18	R	4020	BCR	C20-C21-C22	20.87	156.55	127.28
18	I	4020	BCR	C20-C21-C22	20.86	156.54	127.28
18	i	4020	BCR	C20-C21-C22	20.85	156.52	127.28
18	b	4017	BCR	C16-C17-C18	20.85	156.52	127.28
18	b	4014	BCR	C20-C21-C22	20.85	156.52	127.28
18	A	4003	BCR	C16-C17-C18	20.84	156.50	127.28
18	B	4014	BCR	C20-C21-C22	20.80	156.45	127.28
18	H	4014	BCR	C20-C21-C22	20.79	156.43	127.28
18	L	4019	BCR	C15-C16-C17	20.67	165.82	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	U	4019	BCR	C15-C16-C17	20.67	165.82	123.52
18	l	4019	BCR	C15-C16-C17	20.67	165.81	123.52
18	M	4021	BCR	C15-C16-C17	20.66	165.78	123.52
18	m	4021	BCR	C15-C16-C17	20.65	165.77	123.52
18	b	4009	BCR	C20-C21-C22	20.63	156.22	127.28
18	H	4009	BCR	C20-C21-C22	20.63	156.21	127.28
18	V	4021	BCR	C15-C16-C17	20.61	165.70	123.52
18	B	4009	BCR	C20-C21-C22	20.61	156.18	127.28
18	l	4022	BCR	C20-C21-C22	20.60	156.17	127.28
18	L	4022	BCR	C20-C21-C22	20.57	156.13	127.28
18	G	4002	BCR	C20-C21-C22	20.56	156.12	127.28
18	U	4022	BCR	C20-C21-C22	20.56	156.12	127.28
18	A	4002	BCR	C20-C21-C22	20.55	156.10	127.28
18	a	4002	BCR	C20-C21-C22	20.53	156.07	127.28
18	b	4005	BCR	C16-C17-C18	20.50	156.02	127.28
18	b	4004	BCR	C15-C16-C17	20.49	165.45	123.52
18	B	4004	BCR	C15-C16-C17	20.49	165.44	123.52
18	H	4005	BCR	C15-C16-C17	20.47	165.40	123.52
18	H	4005	BCR	C16-C17-C18	20.47	155.98	127.28
18	H	4004	BCR	C15-C16-C17	20.46	165.39	123.52
18	B	4005	BCR	C15-C16-C17	20.45	165.36	123.52
18	b	4005	BCR	C15-C16-C17	20.45	165.36	123.52
18	B	4005	BCR	C16-C17-C18	20.44	155.95	127.28
18	b	4006	BCR	C16-C17-C18	20.38	155.86	127.28
18	B	4006	BCR	C16-C17-C18	20.34	155.81	127.28
18	H	4006	BCR	C16-C17-C18	20.34	155.80	127.28
18	a	4011	BCR	C15-C16-C17	20.30	165.06	123.52
18	G	4011	BCR	C15-C16-C17	20.29	165.03	123.52
18	A	4011	BCR	C15-C16-C17	20.26	164.98	123.52
18	L	4022	BCR	C15-C16-C17	20.20	164.86	123.52
18	U	4022	BCR	C15-C16-C17	20.20	164.85	123.52
18	l	4022	BCR	C15-C16-C17	20.19	164.84	123.52
18	G	4008	BCR	C20-C21-C22	20.17	155.57	127.28
18	A	4008	BCR	C20-C21-C22	20.16	155.55	127.28
18	a	4008	BCR	C20-C21-C22	20.13	155.51	127.28
18	R	4020	BCR	C16-C17-C18	20.13	155.50	127.28
18	I	4020	BCR	C16-C17-C18	20.10	155.47	127.28
18	i	4020	BCR	C16-C17-C18	20.09	155.46	127.28
18	G	4008	BCR	C15-C16-C17	19.99	164.42	123.52
18	A	4008	BCR	C15-C16-C17	19.98	164.40	123.52
18	a	4008	BCR	C15-C16-C17	19.97	164.38	123.52
18	H	4014	BCR	C16-C17-C18	19.89	155.17	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b	4014	BCR	C16-C17-C18	19.88	155.15	127.28
18	I	4020	BCR	C15-C16-C17	19.86	164.16	123.52
18	R	4020	BCR	C15-C16-C17	19.85	164.14	123.52
18	B	4014	BCR	C16-C17-C18	19.84	155.11	127.28
18	i	4020	BCR	C15-C16-C17	19.83	164.09	123.52
18	b	4006	BCR	C15-C16-C17	19.73	163.88	123.52
18	H	4006	BCR	C15-C16-C17	19.71	163.84	123.52
18	B	4006	BCR	C15-C16-C17	19.69	163.81	123.52
18	B	4017	BCR	C15-C16-C17	19.61	163.64	123.52
18	H	4009	BCR	C15-C16-C17	19.59	163.61	123.52
18	b	4009	BCR	C15-C16-C17	19.59	163.60	123.52
18	H	4017	BCR	C15-C16-C17	19.58	163.59	123.52
18	l	4022	BCR	C16-C17-C18	19.58	154.74	127.28
18	B	4009	BCR	C15-C16-C17	19.58	163.58	123.52
18	H	4004	BCR	C20-C21-C22	19.57	154.72	127.28
18	L	4022	BCR	C16-C17-C18	19.57	154.72	127.28
18	b	4017	BCR	C15-C16-C17	19.56	163.55	123.52
18	U	4022	BCR	C16-C17-C18	19.56	154.71	127.28
18	b	4004	BCR	C20-C21-C22	19.55	154.70	127.28
18	B	4004	BCR	C20-C21-C22	19.53	154.67	127.28
18	i	4018	BCR	C20-C21-C22	19.49	154.61	127.28
18	I	4018	BCR	C20-C21-C22	19.46	154.56	127.28
18	R	4018	BCR	C20-C21-C22	19.45	154.55	127.28
18	R	4018	BCR	C10-C11-C12	19.44	179.53	123.20
18	i	4018	BCR	C10-C11-C12	19.43	179.49	123.20
18	I	4018	BCR	C10-C11-C12	19.41	179.43	123.20
18	G	4008	BCR	C16-C17-C18	19.34	154.40	127.28
18	A	4008	BCR	C16-C17-C18	19.33	154.38	127.28
18	m	4021	BCR	C10-C11-C12	19.31	179.14	123.20
18	H	4004	BCR	C16-C17-C18	19.31	154.35	127.28
18	M	4021	BCR	C10-C11-C12	19.30	179.13	123.20
18	a	4008	BCR	C16-C17-C18	19.30	154.35	127.28
18	B	4004	BCR	C16-C17-C18	19.30	154.34	127.28
18	G	4003	BCR	C15-C16-C17	19.30	163.00	123.52
18	b	4004	BCR	C16-C17-C18	19.30	154.34	127.28
18	V	4021	BCR	C10-C11-C12	19.29	179.09	123.20
18	a	4003	BCR	C15-C16-C17	19.28	162.97	123.52
18	l	4019	BCR	C16-C17-C18	19.25	154.28	127.28
18	A	4011	BCR	C20-C21-C22	19.24	154.26	127.28
18	G	4011	BCR	C20-C21-C22	19.24	154.26	127.28
18	H	4006	BCR	C10-C11-C12	19.23	178.91	123.20
18	a	4011	BCR	C20-C21-C22	19.23	154.24	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4003	BCR	C15-C16-C17	19.22	162.85	123.52
18	L	4019	BCR	C16-C17-C18	19.22	154.23	127.28
18	b	4006	BCR	C10-C11-C12	19.22	178.88	123.20
18	U	4019	BCR	C16-C17-C18	19.19	154.19	127.28
18	B	4006	BCR	C10-C11-C12	19.19	178.79	123.20
18	A	4007	BCR	C15-C16-C17	19.06	162.51	123.52
18	a	4007	BCR	C15-C16-C17	19.03	162.45	123.52
18	G	4007	BCR	C15-C16-C17	19.01	162.42	123.52
18	I	4018	BCR	C15-C16-C17	18.98	162.36	123.52
18	R	4018	BCR	C15-C16-C17	18.96	162.31	123.52
18	i	4018	BCR	C15-C16-C17	18.96	162.31	123.52
18	B	4017	BCR	C10-C11-C12	18.90	177.97	123.20
18	b	4017	BCR	C10-C11-C12	18.88	177.90	123.20
18	H	4017	BCR	C10-C11-C12	18.88	177.90	123.20
18	H	4004	BCR	C10-C11-C12	18.84	177.78	123.20
18	A	4003	BCR	C10-C11-C12	18.83	177.76	123.20
18	G	4003	BCR	C10-C11-C12	18.83	177.75	123.20
18	B	4004	BCR	C10-C11-C12	18.81	177.71	123.20
18	a	4003	BCR	C10-C11-C12	18.81	177.69	123.20
18	b	4004	BCR	C10-C11-C12	18.81	177.69	123.20
18	l	4022	BCR	C10-C11-C12	18.61	177.12	123.20
18	L	4022	BCR	C10-C11-C12	18.61	177.12	123.20
18	b	4013	BCR	C10-C11-C12	18.59	177.07	123.20
18	U	4022	BCR	C10-C11-C12	18.59	177.07	123.20
18	H	4013	BCR	C10-C11-C12	18.59	177.05	123.20
18	b	4016	BCR	C10-C11-C12	18.58	177.03	123.20
18	B	4016	BCR	C10-C11-C12	18.57	177.00	123.20
18	B	4013	BCR	C10-C11-C12	18.56	176.99	123.20
18	H	4016	BCR	C10-C11-C12	18.56	176.98	123.20
18	B	4009	BCR	C10-C11-C12	18.51	176.82	123.20
18	H	4013	BCR	C15-C16-C17	18.50	161.38	123.52
18	b	4009	BCR	C10-C11-C12	18.50	176.81	123.20
18	b	4013	BCR	C15-C16-C17	18.49	161.36	123.52
18	B	4013	BCR	C15-C16-C17	18.49	161.36	123.52
18	H	4009	BCR	C10-C11-C12	18.49	176.78	123.20
18	A	4008	BCR	C10-C11-C12	18.47	176.73	123.20
18	G	4008	BCR	C10-C11-C12	18.46	176.70	123.20
18	G	4007	BCR	C10-C11-C12	18.46	176.69	123.20
18	a	4007	BCR	C10-C11-C12	18.45	176.67	123.20
18	a	4008	BCR	C10-C11-C12	18.45	176.65	123.20
18	A	4007	BCR	C10-C11-C12	18.44	176.64	123.20
18	a	4001	BCR	C10-C11-C12	18.44	176.62	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	4001	BCR	C10-C11-C12	18.43	176.60	123.20
18	A	4001	BCR	C10-C11-C12	18.42	176.56	123.20
18	H	4012	BCR	C10-C11-C12	18.41	176.53	123.20
18	b	4012	BCR	C10-C11-C12	18.40	176.52	123.20
18	L	4019	BCR	C10-C11-C12	18.40	176.52	123.20
18	B	4012	BCR	C10-C11-C12	18.39	176.50	123.20
18	A	4002	BCR	C16-C17-C18	18.39	153.07	127.28
18	a	4002	BCR	C16-C17-C18	18.39	153.07	127.28
18	l	4019	BCR	C10-C11-C12	18.36	176.41	123.20
18	U	4019	BCR	C10-C11-C12	18.36	176.40	123.20
18	G	4002	BCR	C16-C17-C18	18.36	153.03	127.28
18	H	4014	BCR	C10-C11-C12	18.26	176.12	123.20
18	b	4014	BCR	C10-C11-C12	18.24	176.05	123.20
18	B	4014	BCR	C10-C11-C12	18.24	176.05	123.20
18	b	4010	BCR	C10-C11-C12	18.20	175.93	123.20
18	B	4010	BCR	C10-C11-C12	18.19	175.90	123.20
18	H	4010	BCR	C10-C11-C12	18.17	175.86	123.20
18	M	4021	BCR	C16-C17-C18	18.15	152.73	127.28
18	m	4021	BCR	C16-C17-C18	18.12	152.69	127.28
18	V	4021	BCR	C16-C17-C18	18.06	152.61	127.28
18	I	4020	BCR	C10-C11-C12	17.97	175.28	123.20
18	R	4020	BCR	C10-C11-C12	17.96	175.25	123.20
18	i	4020	BCR	C10-C11-C12	17.96	175.23	123.20
18	b	4005	BCR	C10-C11-C12	17.84	174.90	123.20
18	B	4005	BCR	C10-C11-C12	17.84	174.88	123.20
18	H	4005	BCR	C10-C11-C12	17.81	174.82	123.20
18	B	4016	BCR	C15-C16-C17	17.76	159.86	123.52
18	H	4016	BCR	C15-C16-C17	17.75	159.85	123.52
18	b	4016	BCR	C15-C16-C17	17.75	159.83	123.52
18	G	4001	BCR	C16-C17-C18	17.48	151.79	127.28
18	A	4001	BCR	C16-C17-C18	17.45	151.76	127.28
18	a	4001	BCR	C16-C17-C18	17.41	151.69	127.28
18	G	4011	BCR	C10-C11-C12	17.29	173.31	123.20
18	a	4011	BCR	C10-C11-C12	17.29	173.30	123.20
18	A	4011	BCR	C10-C11-C12	17.29	173.30	123.20
18	A	4002	BCR	C10-C11-C12	17.03	172.55	123.20
18	G	4002	BCR	C10-C11-C12	17.03	172.55	123.20
18	a	4002	BCR	C10-C11-C12	17.02	172.52	123.20
18	H	4010	BCR	C15-C16-C17	16.64	157.56	123.52
18	b	4010	BCR	C15-C16-C17	16.63	157.55	123.52
18	B	4010	BCR	C15-C16-C17	16.61	157.51	123.52
18	V	4021	BCR	C16-C15-C14	16.28	156.83	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	M	4021	BCR	C16-C15-C14	16.24	156.75	123.52
18	m	4021	BCR	C16-C15-C14	16.24	156.74	123.52
18	a	4011	BCR	C11-C10-C9	15.91	149.58	127.28
18	G	4011	BCR	C11-C10-C9	15.87	149.53	127.28
18	A	4011	BCR	C11-C10-C9	15.86	149.53	127.28
18	i	4018	BCR	C16-C15-C14	14.96	154.14	123.52
18	b	4005	BCR	C11-C10-C9	14.96	148.26	127.28
18	R	4018	BCR	C16-C15-C14	14.95	154.10	123.52
18	I	4018	BCR	C16-C15-C14	14.93	154.07	123.52
18	B	4005	BCR	C11-C10-C9	14.92	148.20	127.28
18	H	4005	BCR	C11-C10-C9	14.92	148.20	127.28
18	H	4004	BCR	C21-C20-C19	14.91	166.41	123.20
18	b	4004	BCR	C21-C20-C19	14.89	166.34	123.20
18	B	4004	BCR	C21-C20-C19	14.89	166.33	123.20
18	G	4011	BCR	C21-C20-C19	14.75	165.93	123.20
18	a	4011	BCR	C21-C20-C19	14.73	165.89	123.20
18	A	4011	BCR	C21-C20-C19	14.73	165.88	123.20
18	H	4013	BCR	C16-C15-C14	14.62	153.43	123.52
18	b	4013	BCR	C16-C15-C14	14.62	153.43	123.52
18	B	4013	BCR	C16-C15-C14	14.61	153.42	123.52
18	A	4008	BCR	C21-C20-C19	14.53	165.29	123.20
18	G	4008	BCR	C21-C20-C19	14.53	165.29	123.20
18	a	4008	BCR	C21-C20-C19	14.51	165.25	123.20
18	b	4014	BCR	C21-C20-C19	14.51	165.25	123.20
18	H	4014	BCR	C21-C20-C19	14.50	165.22	123.20
18	B	4014	BCR	C21-C20-C19	14.49	165.19	123.20
18	H	4012	BCR	C11-C10-C9	14.42	147.51	127.28
18	b	4012	BCR	C11-C10-C9	14.40	147.47	127.28
18	B	4012	BCR	C11-C10-C9	14.35	147.41	127.28
18	l	4022	BCR	C21-C20-C19	14.31	164.67	123.20
18	L	4022	BCR	C21-C20-C19	14.30	164.64	123.20
18	U	4022	BCR	C21-C20-C19	14.29	164.61	123.20
18	A	4002	BCR	C21-C20-C19	14.29	164.60	123.20
18	G	4002	BCR	C21-C20-C19	14.29	164.59	123.20
18	a	4002	BCR	C21-C20-C19	14.27	164.55	123.20
18	b	4016	BCR	C16-C15-C14	14.19	152.55	123.52
18	B	4016	BCR	C16-C15-C14	14.18	152.53	123.52
18	H	4016	BCR	C16-C15-C14	14.16	152.50	123.52
18	b	4013	BCR	C11-C10-C9	14.12	147.08	127.28
18	H	4010	BCR	C21-C20-C19	14.10	164.04	123.20
18	b	4010	BCR	C21-C20-C19	14.09	164.03	123.20
18	B	4010	BCR	C21-C20-C19	14.09	164.01	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4013	BCR	C11-C10-C9	14.07	147.01	127.28
18	B	4013	BCR	C11-C10-C9	14.07	147.01	127.28
18	i	4018	BCR	C11-C10-C9	13.92	146.81	127.28
18	I	4018	BCR	C11-C10-C9	13.91	146.79	127.28
18	R	4018	BCR	C11-C10-C9	13.89	146.75	127.28
18	a	4001	BCR	C21-C20-C19	13.85	163.34	123.20
18	G	4001	BCR	C21-C20-C19	13.85	163.32	123.20
18	A	4001	BCR	C21-C20-C19	13.85	163.32	123.20
18	H	4009	BCR	C21-C20-C19	13.74	163.02	123.20
18	B	4009	BCR	C21-C20-C19	13.74	163.01	123.20
18	b	4009	BCR	C21-C20-C19	13.74	163.00	123.20
18	B	4010	BCR	C16-C15-C14	13.71	151.58	123.52
18	L	4022	BCR	C11-C10-C9	13.70	146.49	127.28
18	H	4010	BCR	C16-C15-C14	13.69	151.52	123.52
18	l	4022	BCR	C11-C10-C9	13.68	146.47	127.28
18	b	4010	BCR	C16-C15-C14	13.68	151.51	123.52
18	U	4022	BCR	C11-C10-C9	13.63	146.40	127.28
18	G	4003	BCR	C16-C15-C14	13.47	151.08	123.52
18	b	4009	BCR	C16-C15-C14	13.47	151.08	123.52
18	B	4009	BCR	C16-C15-C14	13.47	151.07	123.52
18	a	4003	BCR	C16-C15-C14	13.46	151.07	123.52
18	H	4009	BCR	C16-C15-C14	13.46	151.06	123.52
18	A	4003	BCR	C16-C15-C14	13.43	150.99	123.52
18	b	4016	BCR	C21-C20-C19	13.37	161.93	123.20
18	H	4006	BCR	C16-C15-C14	13.36	150.86	123.52
18	b	4006	BCR	C16-C15-C14	13.36	150.86	123.52
18	H	4016	BCR	C21-C20-C19	13.36	161.92	123.20
18	B	4016	BCR	C21-C20-C19	13.36	161.91	123.20
18	B	4006	BCR	C16-C15-C14	13.35	150.84	123.52
18	B	4014	BCR	C11-C10-C9	13.30	145.93	127.28
18	H	4014	BCR	C11-C10-C9	13.29	145.92	127.28
18	H	4004	BCR	C11-C10-C9	13.26	145.87	127.28
18	b	4014	BCR	C11-C10-C9	13.25	145.86	127.28
18	b	4004	BCR	C11-C10-C9	13.23	145.84	127.28
18	G	4007	BCR	C11-C10-C9	13.22	145.82	127.28
18	B	4004	BCR	C11-C10-C9	13.21	145.81	127.28
18	A	4007	BCR	C16-C15-C14	13.21	150.55	123.52
18	a	4007	BCR	C11-C10-C9	13.20	145.79	127.28
18	a	4007	BCR	C16-C15-C14	13.19	150.52	123.52
13	a	1011	CL0	C1B-CHB-C4A	13.19	129.81	121.32
18	G	4007	BCR	C16-C15-C14	13.18	150.50	123.52
18	l	4019	BCR	C21-C20-C19	13.18	161.38	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4007	BCR	C11-C10-C9	13.17	145.75	127.28
18	U	4019	BCR	C21-C20-C19	13.17	161.35	123.20
13	A	1011	CL0	C1B-CHB-C4A	13.17	129.79	121.32
18	L	4019	BCR	C21-C20-C19	13.16	161.34	123.20
18	H	4006	BCR	C21-C20-C19	13.13	161.25	123.20
18	b	4006	BCR	C21-C20-C19	13.12	161.22	123.20
18	H	4017	BCR	C11-C10-C9	13.11	145.67	127.28
18	B	4006	BCR	C21-C20-C19	13.11	161.20	123.20
13	G	1011	CL0	C1B-CHB-C4A	13.11	129.75	121.32
18	H	4005	BCR	C21-C20-C19	13.09	161.13	123.20
18	B	4005	BCR	C21-C20-C19	13.09	161.12	123.20
18	B	4017	BCR	C11-C10-C9	13.09	145.63	127.28
18	b	4005	BCR	C21-C20-C19	13.07	161.08	123.20
18	V	4021	BCR	C21-C20-C19	13.07	161.07	123.20
18	m	4021	BCR	C21-C20-C19	13.07	161.07	123.20
18	M	4021	BCR	C21-C20-C19	13.07	161.06	123.20
18	b	4017	BCR	C11-C10-C9	13.06	145.59	127.28
18	H	4017	BCR	C21-C20-C19	13.01	160.90	123.20
18	B	4017	BCR	C21-C20-C19	12.99	160.84	123.20
18	L	4019	BCR	C11-C10-C9	12.99	145.49	127.28
18	B	4012	BCR	C21-C20-C19	12.98	160.80	123.20
18	b	4017	BCR	C21-C20-C19	12.98	160.80	123.20
18	b	4012	BCR	C21-C20-C19	12.97	160.77	123.20
18	l	4019	BCR	C11-C10-C9	12.97	145.46	127.28
18	a	4001	BCR	C11-C10-C9	12.96	145.45	127.28
18	H	4012	BCR	C21-C20-C19	12.94	160.70	123.20
18	A	4001	BCR	C11-C10-C9	12.93	145.42	127.28
18	G	4001	BCR	C11-C10-C9	12.93	145.41	127.28
18	U	4019	BCR	C11-C10-C9	12.93	145.41	127.28
18	H	4017	BCR	C16-C15-C14	12.92	149.95	123.52
18	H	4013	BCR	C21-C20-C19	12.89	160.56	123.20
18	B	4017	BCR	C16-C15-C14	12.89	149.89	123.52
18	B	4013	BCR	C21-C20-C19	12.88	160.51	123.20
18	b	4013	BCR	C21-C20-C19	12.88	160.51	123.20
18	b	4017	BCR	C16-C15-C14	12.86	149.84	123.52
18	A	4008	BCR	C16-C15-C14	12.85	149.81	123.52
18	G	4008	BCR	C16-C15-C14	12.83	149.78	123.52
18	a	4008	BCR	C16-C15-C14	12.82	149.75	123.52
18	A	4007	BCR	C21-C20-C19	12.82	160.35	123.20
18	G	4007	BCR	C21-C20-C19	12.81	160.33	123.20
18	a	4007	BCR	C21-C20-C19	12.81	160.31	123.20
18	A	4003	BCR	C11-C10-C9	12.78	145.20	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4003	BCR	C11-C10-C9	12.77	145.18	127.28
18	G	4003	BCR	C11-C10-C9	12.76	145.17	127.28
18	b	4004	BCR	C16-C15-C14	12.74	149.58	123.52
18	I	4020	BCR	C11-C12-C13	12.73	161.28	126.36
18	i	4020	BCR	C11-C12-C13	12.73	161.28	126.36
18	B	4004	BCR	C16-C15-C14	12.73	149.57	123.52
18	H	4004	BCR	C16-C15-C14	12.73	149.57	123.52
18	R	4020	BCR	C11-C12-C13	12.73	161.27	126.36
15	a	1121	F6C	CAA-C2A-C3A	-12.69	104.10	127.87
15	G	1121	F6C	CAA-C2A-C3A	-12.68	104.12	127.87
15	A	1121	F6C	CAA-C2A-C3A	-12.67	104.13	127.87
18	I	4018	BCR	C21-C20-C19	12.48	159.36	123.20
18	i	4018	BCR	C21-C20-C19	12.47	159.34	123.20
18	R	4018	BCR	C21-C20-C19	12.46	159.31	123.20
18	B	4005	BCR	C16-C15-C14	12.36	148.81	123.52
18	H	4005	BCR	C16-C15-C14	12.35	148.79	123.52
18	b	4005	BCR	C16-C15-C14	12.35	148.78	123.52
18	U	4019	BCR	C16-C15-C14	12.29	148.68	123.52
18	L	4019	BCR	C16-C15-C14	12.29	148.67	123.52
18	a	4003	BCR	C21-C20-C19	12.28	158.79	123.20
18	l	4019	BCR	C16-C15-C14	12.28	148.65	123.52
18	A	4003	BCR	C21-C20-C19	12.28	158.79	123.20
18	b	4009	BCR	C11-C10-C9	12.28	144.50	127.28
18	G	4003	BCR	C21-C20-C19	12.28	158.78	123.20
18	B	4009	BCR	C11-C10-C9	12.28	144.50	127.28
18	H	4009	BCR	C11-C10-C9	12.21	144.40	127.28
18	G	4002	BCR	C16-C15-C14	12.07	148.21	123.52
18	A	4002	BCR	C16-C15-C14	12.06	148.19	123.52
18	a	4002	BCR	C16-C15-C14	12.06	148.19	123.52
18	U	4022	BCR	C16-C15-C14	11.91	147.88	123.52
18	L	4022	BCR	C16-C15-C14	11.90	147.87	123.52
18	l	4022	BCR	C16-C15-C14	11.89	147.85	123.52
15	a	1120	F6C	CAA-C2A-C3A	-11.88	105.62	127.87
15	G	1120	F6C	CAA-C2A-C3A	-11.87	105.63	127.87
15	A	1120	F6C	CAA-C2A-C3A	-11.86	105.65	127.87
18	a	4011	BCR	C16-C15-C14	11.70	147.46	123.52
18	G	4011	BCR	C16-C15-C14	11.68	147.42	123.52
18	A	4011	BCR	C16-C15-C14	11.68	147.42	123.52
18	B	4005	BCR	C11-C12-C13	11.65	158.32	126.36
18	b	4005	BCR	C11-C12-C13	11.65	158.31	126.36
18	A	4008	BCR	C11-C10-C9	11.65	143.62	127.28
18	H	4005	BCR	C11-C12-C13	11.62	158.24	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4006	BCR	C11-C10-C9	11.61	143.56	127.28
18	G	4008	BCR	C11-C10-C9	11.61	143.56	127.28
18	H	4012	BCR	C16-C15-C14	11.60	147.25	123.52
18	b	4006	BCR	C11-C10-C9	11.60	143.54	127.28
18	R	4020	BCR	C21-C20-C19	11.59	156.78	123.20
18	i	4020	BCR	C21-C20-C19	11.59	156.78	123.20
18	a	4008	BCR	C11-C10-C9	11.58	143.52	127.28
18	I	4020	BCR	C21-C20-C19	11.57	156.72	123.20
18	B	4012	BCR	C16-C15-C14	11.57	147.19	123.52
15	b	1237	F6C	CAA-C2A-C3A	-11.55	106.24	127.87
18	B	4006	BCR	C11-C10-C9	11.54	143.47	127.28
18	b	4012	BCR	C16-C15-C14	11.54	147.14	123.52
18	i	4020	BCR	C16-C15-C14	11.54	147.14	123.52
18	R	4020	BCR	C16-C15-C14	11.54	147.13	123.52
18	I	4020	BCR	C16-C15-C14	11.53	147.11	123.52
15	B	1237	F6C	CAA-C2A-C3A	-11.53	106.28	127.87
15	H	1237	F6C	CAA-C2A-C3A	-11.50	106.33	127.87
18	G	4001	BCR	C16-C15-C14	11.46	146.96	123.52
18	A	4001	BCR	C16-C15-C14	11.44	146.92	123.52
18	a	4001	BCR	C16-C15-C14	11.43	146.91	123.52
15	G	1120	F6C	C3B-C2B-C1B	-11.43	100.56	106.46
18	L	4019	BCR	C11-C12-C13	11.40	157.62	126.36
18	G	4001	BCR	C11-C12-C13	11.39	157.59	126.36
18	a	4001	BCR	C11-C12-C13	11.37	157.54	126.36
18	l	4019	BCR	C11-C12-C13	11.37	157.53	126.36
15	a	1120	F6C	C3B-C2B-C1B	-11.36	100.60	106.46
18	A	4001	BCR	C11-C12-C13	11.36	157.50	126.36
18	U	4019	BCR	C11-C12-C13	11.35	157.49	126.36
15	A	1120	F6C	C3B-C2B-C1B	-11.32	100.62	106.46
18	G	4008	BCR	C11-C12-C13	11.30	157.35	126.36
18	A	4008	BCR	C11-C12-C13	11.29	157.33	126.36
18	a	4008	BCR	C11-C12-C13	11.28	157.30	126.36
18	G	4011	BCR	C11-C12-C13	11.18	157.03	126.36
18	A	4011	BCR	C11-C12-C13	11.18	157.01	126.36
18	a	4011	BCR	C11-C12-C13	11.18	157.01	126.36
18	A	4007	BCR	C11-C12-C13	11.09	156.78	126.36
18	a	4007	BCR	C11-C12-C13	11.09	156.77	126.36
18	G	4007	BCR	C11-C12-C13	11.08	156.75	126.36
18	b	4014	BCR	C16-C15-C14	11.07	146.17	123.52
18	H	4014	BCR	C16-C15-C14	11.06	146.14	123.52
18	B	4014	BCR	C16-C15-C14	11.03	146.08	123.52
18	b	4016	BCR	C11-C10-C9	10.96	142.65	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	l	4022	BCR	C11-C12-C13	10.96	156.41	126.36
18	L	4022	BCR	C11-C12-C13	10.95	156.38	126.36
18	H	4016	BCR	C11-C10-C9	10.94	142.62	127.28
18	U	4022	BCR	C11-C12-C13	10.94	156.35	126.36
18	B	4016	BCR	C11-C10-C9	10.94	142.62	127.28
18	b	4012	BCR	C11-C12-C13	10.90	156.25	126.36
18	H	4012	BCR	C11-C12-C13	10.89	156.23	126.36
18	B	4012	BCR	C11-C12-C13	10.89	156.21	126.36
18	H	4004	BCR	C11-C12-C13	10.87	156.18	126.36
18	b	4004	BCR	C11-C12-C13	10.86	156.15	126.36
18	B	4004	BCR	C11-C12-C13	10.86	156.14	126.36
18	b	4010	BCR	C11-C10-C9	10.85	142.49	127.28
18	M	4021	BCR	C11-C12-C13	10.84	156.08	126.36
18	B	4010	BCR	C11-C10-C9	10.83	142.47	127.28
18	V	4021	BCR	C11-C12-C13	10.83	156.06	126.36
18	H	4006	BCR	C11-C12-C13	10.83	156.05	126.36
18	m	4021	BCR	C11-C12-C13	10.83	156.05	126.36
18	M	4021	BCR	C11-C10-C9	10.82	142.45	127.28
18	m	4021	BCR	C11-C10-C9	10.82	142.45	127.28
18	b	4006	BCR	C11-C12-C13	10.81	156.01	126.36
18	B	4006	BCR	C11-C12-C13	10.80	155.99	126.36
18	V	4021	BCR	C11-C10-C9	10.80	142.43	127.28
18	H	4010	BCR	C11-C10-C9	10.79	142.41	127.28
15	A	1121	F6C	C3B-C2B-C1B	-10.67	100.95	106.46
15	G	1121	F6C	C3B-C2B-C1B	-10.67	100.95	106.46
15	a	1121	F6C	C3B-C2B-C1B	-10.65	100.97	106.46
18	H	4010	BCR	C11-C12-C13	10.41	154.91	126.36
18	b	4010	BCR	C11-C12-C13	10.40	154.87	126.36
18	B	4010	BCR	C11-C12-C13	10.40	154.87	126.36
18	B	4014	BCR	C11-C12-C13	10.35	154.75	126.36
18	b	4014	BCR	C11-C12-C13	10.35	154.73	126.36
18	H	4014	BCR	C11-C12-C13	10.34	154.72	126.36
18	A	4002	BCR	C11-C12-C13	10.30	154.59	126.36
18	G	4002	BCR	C11-C12-C13	10.29	154.57	126.36
18	a	4002	BCR	C11-C12-C13	10.28	154.55	126.36
18	R	4020	BCR	C11-C10-C9	10.07	141.40	127.28
18	A	4003	BCR	C11-C12-C13	10.06	153.94	126.36
18	a	4003	BCR	C11-C12-C13	10.05	153.92	126.36
18	G	4003	BCR	C11-C12-C13	10.05	153.92	126.36
18	I	4020	BCR	C11-C10-C9	10.05	141.37	127.28
18	b	4013	BCR	C11-C12-C13	10.05	153.91	126.36
18	H	4013	BCR	C11-C12-C13	10.04	153.88	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4013	BCR	C11-C12-C13	10.04	153.88	126.36
18	i	4020	BCR	C11-C10-C9	10.02	141.33	127.28
15	B	1230	F6C	C3B-C2B-C1B	-10.02	101.29	106.46
15	H	1230	F6C	C3B-C2B-C1B	-9.97	101.31	106.46
18	B	4017	BCR	C11-C12-C13	9.92	153.56	126.36
18	H	4017	BCR	C11-C12-C13	9.91	153.52	126.36
18	b	4017	BCR	C11-C12-C13	9.89	153.47	126.36
15	b	1230	F6C	C3B-C2B-C1B	-9.81	101.40	106.46
13	a	1011	CL0	O2D-CGD-CBD	9.77	121.68	110.95
13	A	1011	CL0	O2D-CGD-CBD	9.75	121.66	110.95
18	b	4009	BCR	C11-C12-C13	9.75	153.09	126.36
18	H	4009	BCR	C11-C12-C13	9.74	153.07	126.36
13	G	1011	CL0	O2D-CGD-CBD	9.73	121.64	110.95
18	B	4009	BCR	C11-C12-C13	9.73	153.03	126.36
18	R	4018	BCR	C11-C12-C13	9.62	152.74	126.36
18	i	4018	BCR	C11-C12-C13	9.61	152.72	126.36
18	I	4018	BCR	C11-C12-C13	9.60	152.68	126.36
18	b	4016	BCR	C11-C12-C13	9.18	151.54	126.36
18	B	4016	BCR	C11-C12-C13	9.18	151.53	126.36
18	H	4016	BCR	C11-C12-C13	9.17	151.50	126.36
14	H	1238	CLA	CAA-C2A-C3A	-9.06	88.52	113.00
14	b	1238	CLA	CAA-C2A-C3A	-9.06	88.52	113.00
14	B	1238	CLA	CAA-C2A-C3A	-9.06	88.52	113.00
15	b	1230	F6C	C1D-ND-C4D	-9.03	102.56	106.68
15	b	1230	F6C	CAA-C2A-C3A	-9.00	111.01	127.87
15	B	1230	F6C	C1D-ND-C4D	-8.96	102.59	106.68
15	H	1230	F6C	C1D-ND-C4D	-8.86	102.64	106.68
15	B	1230	F6C	CAA-C2A-C3A	-8.86	111.28	127.87
15	B	1230	F6C	CMD-C2D-C1D	8.80	138.79	125.03
14	H	1203	CLA	CMD-C2D-C1D	8.77	140.17	124.73
14	B	1203	CLA	CMD-C2D-C1D	8.76	140.15	124.73
15	b	1230	F6C	CMD-C2D-C1D	8.75	138.70	125.03
14	b	1203	CLA	CMD-C2D-C1D	8.73	140.10	124.73
15	H	1230	F6C	CMD-C2D-C1D	8.73	138.67	125.03
18	L	4019	BCR	C24-C23-C22	-8.72	113.34	126.23
18	U	4019	BCR	C24-C23-C22	-8.71	113.35	126.23
18	l	4019	BCR	C24-C23-C22	-8.70	113.36	126.23
18	H	4012	BCR	C20-C19-C18	8.59	149.91	126.36
18	b	4012	BCR	C20-C19-C18	8.58	149.90	126.36
18	B	4012	BCR	C20-C19-C18	8.57	149.87	126.36
18	G	4007	BCR	C20-C19-C18	8.57	149.86	126.36
18	A	4007	BCR	C20-C19-C18	8.57	149.85	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4006	BCR	C20-C19-C18	8.56	149.83	126.36
18	H	4006	BCR	C20-C19-C18	8.56	149.82	126.36
18	b	4006	BCR	C20-C19-C18	8.55	149.81	126.36
18	a	4007	BCR	C20-C19-C18	8.54	149.78	126.36
18	H	4013	BCR	C20-C19-C18	8.49	149.65	126.36
18	b	4013	BCR	C20-C19-C18	8.49	149.64	126.36
18	B	4013	BCR	C20-C19-C18	8.48	149.61	126.36
18	i	4018	BCR	C20-C19-C18	8.46	149.56	126.36
18	I	4018	BCR	C20-C19-C18	8.46	149.56	126.36
18	R	4018	BCR	C20-C19-C18	8.45	149.52	126.36
15	H	1230	F6C	CAA-C2A-C3A	-8.44	112.06	127.87
14	G	1116	CLA	CMD-C2D-C1D	8.39	139.50	124.73
14	a	1116	CLA	CMD-C2D-C1D	8.37	139.47	124.73
14	A	1116	CLA	CMD-C2D-C1D	8.36	139.46	124.73
14	A	1135	CLA	CMD-C2D-C1D	8.36	139.44	124.73
14	a	1133	CLA	CMD-C2D-C1D	8.35	139.44	124.73
14	B	1023	CLA	C4A-NA-C1A	8.35	110.49	106.68
14	H	1023	CLA	C4A-NA-C1A	8.35	110.49	106.68
14	G	1133	CLA	CMD-C2D-C1D	8.34	139.41	124.73
14	G	1135	CLA	CMD-C2D-C1D	8.33	139.41	124.73
14	b	1023	CLA	C4A-NA-C1A	8.33	110.48	106.68
14	a	1135	CLA	CMD-C2D-C1D	8.33	139.39	124.73
14	b	1239	CLA	CMD-C2D-C1D	8.33	139.39	124.73
14	B	1239	CLA	CMD-C2D-C1D	8.32	139.38	124.73
14	G	1124	CLA	CMD-C2D-C1D	8.32	139.38	124.73
14	A	1133	CLA	CMD-C2D-C1D	8.31	139.37	124.73
15	a	1121	F6C	CMD-C2D-C1D	8.31	138.02	125.03
14	H	1239	CLA	CMD-C2D-C1D	8.31	139.36	124.73
14	A	1124	CLA	CMD-C2D-C1D	8.30	139.35	124.73
14	a	1104	CLA	CMD-C2D-C1D	8.30	139.35	124.73
14	A	1104	CLA	CMD-C2D-C1D	8.29	139.34	124.73
15	A	1121	F6C	CMD-C2D-C1D	8.29	137.99	125.03
14	A	1109	CLA	CMD-C2D-C1D	8.29	139.32	124.73
14	H	1231	CLA	CMD-C2D-C1D	8.28	139.32	124.73
14	a	1124	CLA	CMD-C2D-C1D	8.28	139.32	124.73
14	b	1231	CLA	CMD-C2D-C1D	8.28	139.32	124.73
14	G	1104	CLA	CMD-C2D-C1D	8.28	139.31	124.73
15	G	1121	F6C	CMD-C2D-C1D	8.27	137.96	125.03
14	B	1231	CLA	CMD-C2D-C1D	8.27	139.30	124.73
14	G	1137	CLA	CMD-C2D-C1D	8.26	139.28	124.73
14	G	1109	CLA	CMD-C2D-C1D	8.26	139.28	124.73
14	a	1109	CLA	CMD-C2D-C1D	8.26	139.28	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1137	CLA	CMD-C2D-C1D	8.26	139.27	124.73
14	a	1137	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	B	1234	CLA	CMD-C2D-C1D	8.24	139.24	124.73
15	G	1120	F6C	C1D-ND-C4D	-8.23	102.93	106.68
14	k	1401	CLA	CMD-C2D-C1D	8.23	139.21	124.73
14	H	1234	CLA	CMD-C2D-C1D	8.22	139.21	124.73
14	T	1401	CLA	CMD-C2D-C1D	8.22	139.21	124.73
14	b	1234	CLA	CMD-C2D-C1D	8.20	139.18	124.73
14	A	1105	CLA	CMD-C2D-C1D	8.20	139.17	124.73
14	a	1105	CLA	CMD-C2D-C1D	8.20	139.16	124.73
14	K	1401	CLA	CMD-C2D-C1D	8.20	139.16	124.73
14	a	1113	CLA	CMD-C2D-C1D	8.20	139.16	124.73
14	a	1110	CLA	CMD-C2D-C1D	8.19	139.16	124.73
14	G	1113	CLA	CMD-C2D-C1D	8.19	139.16	124.73
14	b	1229	CLA	CMD-C2D-C1D	8.19	139.15	124.73
14	a	1111	CLA	CMD-C2D-C1D	8.18	139.13	124.73
14	A	1110	CLA	CMD-C2D-C1D	8.18	139.13	124.73
14	B	1229	CLA	CMD-C2D-C1D	8.18	139.13	124.73
15	a	1120	F6C	C1D-ND-C4D	-8.18	102.95	106.68
14	A	1111	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	G	1130	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	G	1110	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	H	1229	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	A	1113	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	G	1111	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	G	1105	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	a	1130	CLA	CMD-C2D-C1D	8.16	139.10	124.73
14	A	1130	CLA	CMD-C2D-C1D	8.16	139.10	124.73
14	H	1233	CLA	CMD-C2D-C1D	8.15	139.08	124.73
15	A	1120	F6C	C1D-ND-C4D	-8.15	102.96	106.68
14	A	1108	CLA	CMD-C2D-C1D	8.13	139.05	124.73
14	H	1213	CLA	CMD-C2D-C1D	8.13	139.05	124.73
14	b	1233	CLA	CMD-C2D-C1D	8.12	139.03	124.73
15	b	1237	F6C	C1D-ND-C4D	-8.12	102.97	106.68
14	A	1138	CLA	CMD-C2D-C1D	8.12	139.03	124.73
14	B	1213	CLA	CMD-C2D-C1D	8.12	139.03	124.73
14	b	1213	CLA	CMD-C2D-C1D	8.12	139.02	124.73
15	H	1237	F6C	C1D-ND-C4D	-8.11	102.98	106.68
14	a	1138	CLA	CMD-C2D-C1D	8.11	139.01	124.73
14	G	1138	CLA	CMD-C2D-C1D	8.11	139.00	124.73
14	H	1232	CLA	CMD-C2D-C1D	8.10	138.99	124.73
14	B	1233	CLA	CMD-C2D-C1D	8.10	138.98	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1232	CLA	CMD-C2D-C1D	8.09	138.97	124.73
15	B	1237	F6C	C1D-ND-C4D	-8.08	102.99	106.68
14	G	1108	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	b	1232	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	a	1108	CLA	CMD-C2D-C1D	8.08	138.95	124.73
14	G	1114	CLA	CMD-C2D-C1D	8.07	138.94	124.73
14	A	1103	CLA	CMD-C2D-C1D	8.05	138.91	124.73
14	a	1114	CLA	CMD-C2D-C1D	8.05	138.90	124.73
14	G	1103	CLA	CMD-C2D-C1D	8.04	138.89	124.73
14	G	1112	CLA	CMD-C2D-C1D	8.04	138.89	124.73
14	A	1114	CLA	CMD-C2D-C1D	8.04	138.89	124.73
14	A	1112	CLA	CMD-C2D-C1D	8.02	138.86	124.73
14	a	1112	CLA	CMD-C2D-C1D	8.02	138.85	124.73
14	H	1208	CLA	CMD-C2D-C1D	8.01	138.84	124.73
15	B	1237	F6C	C3B-C2B-C1B	-8.01	102.33	106.46
14	B	1023	CLA	CAC-C3C-C4C	8.01	135.21	124.79
14	a	1103	CLA	CMD-C2D-C1D	8.01	138.83	124.73
18	H	4005	BCR	C20-C19-C18	8.01	148.31	126.36
18	b	4005	BCR	C20-C19-C18	8.00	148.30	126.36
14	a	1115	CLA	CMD-C2D-C1D	8.00	138.81	124.73
14	b	1023	CLA	CAC-C3C-C4C	7.99	135.19	124.79
18	B	4005	BCR	C20-C19-C18	7.99	148.27	126.36
14	B	1208	CLA	CMD-C2D-C1D	7.99	138.80	124.73
14	b	1208	CLA	CMD-C2D-C1D	7.99	138.79	124.73
14	b	1210	CLA	CMD-C2D-C1D	7.98	138.78	124.73
14	H	1210	CLA	CMD-C2D-C1D	7.98	138.78	124.73
14	B	1210	CLA	CMD-C2D-C1D	7.97	138.77	124.73
14	G	1115	CLA	CMD-C2D-C1D	7.97	138.77	124.73
14	A	1115	CLA	CMD-C2D-C1D	7.97	138.76	124.73
14	H	1023	CLA	CAC-C3C-C4C	7.97	135.16	124.79
14	b	1228	CLA	CMD-C2D-C1D	7.96	138.74	124.73
14	H	1228	CLA	CMD-C2D-C1D	7.95	138.73	124.73
14	B	1228	CLA	CMD-C2D-C1D	7.92	138.68	124.73
14	B	1202	CLA	CMD-C2D-C1D	7.92	138.68	124.73
15	H	1237	F6C	C3B-C2B-C1B	-7.92	102.38	106.46
18	b	4017	BCR	C20-C19-C18	7.92	148.07	126.36
18	B	4017	BCR	C20-C19-C18	7.92	148.07	126.36
14	A	1136	CLA	CMD-C2D-C1D	7.92	138.67	124.73
18	H	4017	BCR	C20-C19-C18	7.91	148.04	126.36
14	H	1201	CLA	CMD-C2D-C1D	7.90	138.64	124.73
14	b	1202	CLA	CMD-C2D-C1D	7.90	138.64	124.73
14	G	1136	CLA	CMD-C2D-C1D	7.90	138.63	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1136	CLA	CMD-C2D-C1D	7.89	138.61	124.73
14	b	1201	CLA	CMD-C2D-C1D	7.88	138.61	124.73
14	B	1201	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	H	1202	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	B	1216	CLA	CMD-C2D-C1D	7.86	138.57	124.73
14	U	1503	CLA	CMD-C2D-C1D	7.86	138.57	124.73
15	b	1237	F6C	C3B-C2B-C1B	-7.86	102.41	106.46
14	L	1503	CLA	CMD-C2D-C1D	7.85	138.55	124.73
14	B	1211	CLA	CMD-C2D-C1D	7.85	138.54	124.73
14	b	1216	CLA	CMD-C2D-C1D	7.84	138.54	124.73
14	H	1216	CLA	CMD-C2D-C1D	7.84	138.54	124.73
18	a	4003	BCR	C20-C19-C18	7.84	147.86	126.36
15	b	1237	F6C	CMD-C2D-C1D	7.84	137.28	125.03
15	B	1237	F6C	CMD-C2D-C1D	7.84	137.28	125.03
18	G	4003	BCR	C20-C19-C18	7.84	147.85	126.36
14	b	1209	CLA	CMD-C2D-C1D	7.83	138.52	124.73
14	l	1503	CLA	CMD-C2D-C1D	7.83	138.52	124.73
14	H	1214	CLA	CMD-C2D-C1D	7.83	138.52	124.73
14	B	1214	CLA	CMD-C2D-C1D	7.83	138.52	124.73
14	b	1214	CLA	CMD-C2D-C1D	7.82	138.49	124.73
14	B	1209	CLA	CMD-C2D-C1D	7.82	138.49	124.73
14	H	1209	CLA	CMD-C2D-C1D	7.81	138.49	124.73
18	A	4003	BCR	C20-C19-C18	7.81	147.78	126.36
14	G	1117	CLA	CMD-C2D-C1D	7.81	138.48	124.73
14	b	1211	CLA	CMD-C2D-C1D	7.80	138.47	124.73
14	H	1211	CLA	CMD-C2D-C1D	7.80	138.47	124.73
14	B	1217	CLA	CMD-C2D-C1D	7.80	138.47	124.73
14	A	1012	CLA	CMD-C2D-C1D	7.80	138.47	124.73
15	H	1237	F6C	CMD-C2D-C1D	7.80	137.22	125.03
14	b	1217	CLA	CMD-C2D-C1D	7.79	138.45	124.73
14	H	1217	CLA	CMD-C2D-C1D	7.79	138.45	124.73
14	G	1012	CLA	CMD-C2D-C1D	7.79	138.45	124.73
14	A	1117	CLA	CMD-C2D-C1D	7.78	138.43	124.73
14	a	1012	CLA	CMD-C2D-C1D	7.77	138.41	124.73
18	l	4019	BCR	C20-C19-C18	7.77	147.66	126.36
14	a	1117	CLA	CMD-C2D-C1D	7.76	138.40	124.73
18	U	4019	BCR	C20-C19-C18	7.76	147.63	126.36
18	L	4019	BCR	C20-C19-C18	7.75	147.62	126.36
14	X	1701	CLA	CMD-C2D-C1D	7.74	138.36	124.73
14	x	1701	CLA	CMD-C2D-C1D	7.74	138.35	124.73
14	G	1122	CLA	CMD-C2D-C1D	7.74	138.35	124.73
14	G	1118	CLA	CMD-C2D-C1D	7.73	138.35	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1215	CLA	CMD-C2D-C1D	7.73	138.34	124.73
14	W	1701	CLA	CMD-C2D-C1D	7.73	138.33	124.73
14	a	1122	CLA	CMD-C2D-C1D	7.73	138.33	124.73
14	a	1132	CLA	CMD-C2D-C1D	7.72	138.33	124.73
14	B	1215	CLA	CMD-C2D-C1D	7.72	138.33	124.73
14	A	1123	CLA	CMD-C2D-C1D	7.72	138.32	124.73
14	A	1118	CLA	CMD-C2D-C1D	7.71	138.31	124.73
14	G	1123	CLA	CMD-C2D-C1D	7.71	138.31	124.73
14	a	1118	CLA	CMD-C2D-C1D	7.71	138.30	124.73
14	b	1215	CLA	CMD-C2D-C1D	7.70	138.30	124.73
14	G	1131	CLA	CMD-C2D-C1D	7.70	138.29	124.73
14	A	1106	CLA	CMD-C2D-C1D	7.70	138.29	124.73
14	A	1131	CLA	CMD-C2D-C1D	7.70	138.28	124.73
14	A	1132	CLA	CMD-C2D-C1D	7.70	138.28	124.73
14	A	1122	CLA	CMD-C2D-C1D	7.70	138.28	124.73
14	a	1106	CLA	CMD-C2D-C1D	7.70	138.28	124.73
14	a	1102	CLA	CMD-C2D-C1D	7.69	138.27	124.73
14	a	1131	CLA	CMD-C2D-C1D	7.69	138.26	124.73
14	G	1132	CLA	CMD-C2D-C1D	7.69	138.26	124.73
14	a	1123	CLA	CMD-C2D-C1D	7.69	138.26	124.73
14	G	1106	CLA	CMD-C2D-C1D	7.68	138.26	124.73
14	H	1218	CLA	CMD-C2D-C1D	7.68	138.26	124.73
14	b	1218	CLA	CMD-C2D-C1D	7.68	138.25	124.73
14	B	1218	CLA	CMD-C2D-C1D	7.67	138.24	124.73
14	b	1222	CLA	CMD-C2D-C1D	7.67	138.23	124.73
14	B	1222	CLA	CMD-C2D-C1D	7.67	138.23	124.73
14	A	1101	CLA	CMD-C2D-C1D	7.66	138.22	124.73
14	G	1101	CLA	CMD-C2D-C1D	7.66	138.22	124.73
14	A	1102	CLA	CMD-C2D-C1D	7.66	138.21	124.73
14	G	1102	CLA	CMD-C2D-C1D	7.66	138.21	124.73
14	a	1125	CLA	CMD-C2D-C1D	7.65	138.20	124.73
14	A	1125	CLA	CMD-C2D-C1D	7.64	138.19	124.73
14	a	1101	CLA	CMD-C2D-C1D	7.64	138.18	124.73
14	G	1125	CLA	CMD-C2D-C1D	7.64	138.18	124.73
14	H	1222	CLA	CMD-C2D-C1D	7.62	138.15	124.73
14	a	1126	CLA	CMD-C2D-C1D	7.60	138.10	124.73
14	A	1126	CLA	CMD-C2D-C1D	7.59	138.09	124.73
14	G	1137	CLA	O2D-CGD-CBD	7.58	124.48	111.23
14	a	1137	CLA	O2D-CGD-CBD	7.56	124.45	111.23
14	G	1126	CLA	CMD-C2D-C1D	7.55	138.02	124.73
14	A	1137	CLA	O2D-CGD-CBD	7.54	124.42	111.23
14	l	1502	CLA	CMD-C2D-C1D	7.53	137.99	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1129	CLA	CMD-C2D-C1D	7.53	137.99	124.73
14	B	1238	CLA	CMD-C2D-C1D	7.53	137.99	124.73
14	U	1502	CLA	CMD-C2D-C1D	7.53	137.98	124.73
14	G	1129	CLA	CMD-C2D-C1D	7.52	137.98	124.73
14	L	1502	CLA	CMD-C2D-C1D	7.52	137.97	124.73
14	b	1238	CLA	CMD-C2D-C1D	7.52	137.96	124.73
14	B	1235	CLA	CMD-C2D-C1D	7.51	137.96	124.73
14	A	1129	CLA	CMD-C2D-C1D	7.51	137.96	124.73
14	H	1235	CLA	CMD-C2D-C1D	7.50	137.94	124.73
14	b	1235	CLA	CMD-C2D-C1D	7.50	137.93	124.73
14	H	1238	CLA	CMD-C2D-C1D	7.50	137.93	124.73
14	B	1236	CLA	CMD-C2D-C1D	7.49	137.92	124.73
14	b	1236	CLA	CMD-C2D-C1D	7.48	137.91	124.73
14	A	1119	CLA	CMD-C2D-C1D	7.47	137.88	124.73
14	H	1236	CLA	CMD-C2D-C1D	7.47	137.88	124.73
14	a	1132	CLA	O2D-CGD-CBD	7.46	124.27	111.23
18	b	4016	BCR	C20-C19-C18	7.45	146.80	126.36
14	A	1110	CLA	O2D-CGD-CBD	7.45	124.25	111.23
14	A	1107	CLA	CMD-C2D-C1D	7.45	137.84	124.73
18	H	4016	BCR	C20-C19-C18	7.44	146.78	126.36
14	B	1227	CLA	CMD-C2D-C1D	7.44	137.83	124.73
14	a	1119	CLA	CMD-C2D-C1D	7.44	137.83	124.73
14	G	1107	CLA	CMD-C2D-C1D	7.44	137.83	124.73
18	B	4016	BCR	C20-C19-C18	7.44	146.76	126.36
14	H	1227	CLA	CMD-C2D-C1D	7.44	137.83	124.73
14	a	1107	CLA	CMD-C2D-C1D	7.44	137.82	124.73
14	G	1119	CLA	CMD-C2D-C1D	7.43	137.81	124.73
14	G	1132	CLA	O2D-CGD-CBD	7.43	124.22	111.23
14	A	1132	CLA	O2D-CGD-CBD	7.43	124.22	111.23
14	G	1110	CLA	O2D-CGD-CBD	7.43	124.21	111.23
14	a	1110	CLA	O2D-CGD-CBD	7.42	124.21	111.23
14	b	1239	CLA	C2C-C1C-NC	7.42	117.78	109.98
14	b	1227	CLA	CMD-C2D-C1D	7.42	137.80	124.73
15	a	1120	F6C	CMD-C2D-C1D	7.41	136.61	125.03
14	H	1239	CLA	C2C-C1C-NC	7.40	117.75	109.98
14	G	1139	CLA	CMD-C2D-C1D	7.40	137.75	124.73
14	a	1139	CLA	CMD-C2D-C1D	7.39	137.75	124.73
14	B	1239	CLA	C2C-C1C-NC	7.39	117.75	109.98
14	A	1139	CLA	CMD-C2D-C1D	7.39	137.74	124.73
15	G	1120	F6C	CMD-C2D-C1D	7.39	136.58	125.03
15	A	1120	F6C	CMD-C2D-C1D	7.38	136.56	125.03
18	M	4021	BCR	C20-C19-C18	7.34	146.48	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	V	4021	BCR	C20-C19-C18	7.32	146.44	126.36
18	m	4021	BCR	C20-C19-C18	7.32	146.43	126.36
14	H	1204	CLA	CMD-C2D-C1D	7.28	137.56	124.73
14	b	1207	CLA	CMD-C2D-C1D	7.27	137.53	124.73
14	B	1204	CLA	CMD-C2D-C1D	7.27	137.53	124.73
14	b	1201	CLA	C4A-NA-C1A	7.27	110.00	106.68
14	b	1212	CLA	O2D-CGD-CBD	7.25	123.91	111.23
14	H	1207	CLA	CMD-C2D-C1D	7.25	137.50	124.73
14	B	1207	CLA	CMD-C2D-C1D	7.25	137.50	124.73
14	b	1204	CLA	CMD-C2D-C1D	7.25	137.50	124.73
14	H	1223	CLA	CMD-C2D-C1D	7.24	137.48	124.73
14	B	1223	CLA	CMD-C2D-C1D	7.24	137.47	124.73
14	H	1212	CLA	O2D-CGD-CBD	7.22	123.86	111.23
14	H	1201	CLA	C4A-NA-C1A	7.22	109.97	106.68
14	B	1212	CLA	O2D-CGD-CBD	7.22	123.85	111.23
14	A	1129	CLA	O2D-CGD-CBD	7.21	123.84	111.23
14	b	1223	CLA	CMD-C2D-C1D	7.21	137.43	124.73
14	G	1129	CLA	O2D-CGD-CBD	7.21	123.83	111.23
14	b	1220	CLA	CMD-C2D-C1D	7.20	137.41	124.73
14	a	1129	CLA	O2D-CGD-CBD	7.20	123.82	111.23
14	H	1220	CLA	CMD-C2D-C1D	7.20	137.41	124.73
14	B	1220	CLA	CMD-C2D-C1D	7.18	137.38	124.73
14	B	1201	CLA	C4A-NA-C1A	7.18	109.95	106.68
14	b	1021	CLA	C4A-NA-C1A	7.13	109.93	106.68
14	A	1140	CLA	CMD-C2D-C1D	7.10	137.24	124.73
14	G	1140	CLA	CMD-C2D-C1D	7.10	137.24	124.73
14	H	1021	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	a	1140	CLA	CMD-C2D-C1D	7.09	137.21	124.73
13	a	1011	CL0	CBC-CAC-C3C	-7.07	102.75	112.87
13	G	1011	CL0	CBC-CAC-C3C	-7.06	102.77	112.87
14	B	1219	CLA	CMD-C2D-C1D	7.05	137.14	124.73
13	A	1011	CL0	CBC-CAC-C3C	-7.04	102.79	112.87
14	H	1219	CLA	CMD-C2D-C1D	7.04	137.12	124.73
14	B	1221	CLA	CMD-C2D-C1D	7.03	137.11	124.73
14	H	1205	CLA	C4A-NA-C1A	7.03	109.89	106.68
14	B	1224	CLA	CMD-C2D-C1D	7.03	137.11	124.73
14	A	1106	CLA	O2D-CGD-CBD	7.03	123.52	111.23
14	G	1106	CLA	O2D-CGD-CBD	7.03	123.51	111.23
14	b	1219	CLA	CMD-C2D-C1D	7.02	137.09	124.73
14	b	1221	CLA	CMD-C2D-C1D	7.02	137.09	124.73
14	b	1224	CLA	CMD-C2D-C1D	7.02	137.09	124.73
14	a	1106	CLA	O2D-CGD-CBD	7.02	123.49	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1021	CLA	C4A-NA-C1A	7.01	109.88	106.68
14	H	1224	CLA	CMD-C2D-C1D	7.01	137.07	124.73
14	H	1221	CLA	CMD-C2D-C1D	7.00	137.06	124.73
18	B	4009	BCR	C20-C19-C18	6.99	145.54	126.36
14	B	1205	CLA	C4A-NA-C1A	6.98	109.86	106.68
18	b	4009	BCR	C20-C19-C18	6.98	145.50	126.36
18	H	4009	BCR	C20-C19-C18	6.97	145.47	126.36
14	b	1205	CLA	C4A-NA-C1A	6.96	109.86	106.68
14	b	1226	CLA	CMD-C2D-C1D	6.90	136.88	124.73
14	B	1212	CLA	CMD-C2D-C1D	6.89	136.85	124.73
14	B	1226	CLA	CMD-C2D-C1D	6.89	136.85	124.73
14	H	1226	CLA	CMD-C2D-C1D	6.88	136.84	124.73
14	a	1013	CLA	C2D-C1D-ND	6.87	116.93	110.13
14	H	1205	CLA	O2D-CGD-CBD	6.87	123.24	111.23
14	b	1212	CLA	CMD-C2D-C1D	6.86	136.82	124.73
14	A	1013	CLA	C2D-C1D-ND	6.85	116.91	110.13
14	H	1212	CLA	CMD-C2D-C1D	6.85	136.79	124.73
14	a	1125	CLA	O2D-CGD-CBD	6.83	123.18	111.23
14	B	1205	CLA	O2D-CGD-CBD	6.83	123.17	111.23
14	b	1205	CLA	O2D-CGD-CBD	6.83	123.17	111.23
14	A	1125	CLA	O2D-CGD-CBD	6.82	123.15	111.23
14	a	1127	CLA	CMD-C2D-C1D	6.82	136.73	124.73
14	G	1013	CLA	C2D-C1D-ND	6.81	116.87	110.13
14	b	1207	CLA	C2C-C1C-NC	6.81	117.14	109.98
14	G	1127	CLA	CMD-C2D-C1D	6.81	136.72	124.73
14	L	1501	CLA	CMD-C2D-C1D	6.80	136.70	124.73
14	H	1207	CLA	C2C-C1C-NC	6.80	117.12	109.98
14	G	1125	CLA	O2D-CGD-CBD	6.80	123.11	111.23
14	A	1127	CLA	CMD-C2D-C1D	6.79	136.69	124.73
14	U	1501	CLA	CMD-C2D-C1D	6.78	136.67	124.73
14	B	1207	CLA	C2C-C1C-NC	6.78	117.10	109.98
14	H	1012	CLA	O2D-CGD-CBD	6.77	123.07	111.23
14	l	1501	CLA	CMD-C2D-C1D	6.77	136.65	124.73
14	b	1022	CLA	O2D-CGD-CBD	6.77	123.06	111.23
14	B	1023	CLA	C2D-C1D-ND	6.75	116.80	110.13
18	L	4022	BCR	C7-C8-C9	-6.74	116.26	126.23
18	G	4001	BCR	C7-C8-C9	-6.73	116.28	126.23
18	U	4022	BCR	C7-C8-C9	-6.72	116.29	126.23
18	a	4001	BCR	C7-C8-C9	-6.72	116.30	126.23
18	B	4004	BCR	C24-C23-C22	-6.72	116.30	126.23
18	l	4022	BCR	C7-C8-C9	-6.70	116.32	126.23
14	B	1022	CLA	O2D-CGD-CBD	6.70	122.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1138	CLA	O2D-CGD-CBD	6.70	122.95	111.23
15	b	1230	F6C	CAA-C2A-C1A	-6.69	109.31	128.01
14	A	1138	CLA	O2D-CGD-CBD	6.69	122.93	111.23
14	a	1138	CLA	O2D-CGD-CBD	6.69	122.93	111.23
18	b	4004	BCR	C24-C23-C22	-6.69	116.34	126.23
18	A	4001	BCR	C7-C8-C9	-6.69	116.34	126.23
14	b	1023	CLA	C2D-C1D-ND	6.68	116.74	110.13
18	H	4004	BCR	C24-C23-C22	-6.67	116.37	126.23
14	U	1502	CLA	O2D-CGD-CBD	6.66	122.88	111.23
14	H	1023	CLA	C2D-C1D-ND	6.66	116.72	110.13
15	B	1230	F6C	CAA-C2A-C1A	-6.65	109.42	128.01
14	L	1502	CLA	O2D-CGD-CBD	6.65	122.86	111.23
15	H	1230	F6C	CAA-C2A-C1A	-6.64	109.45	128.01
14	l	1502	CLA	O2D-CGD-CBD	6.62	122.81	111.23
15	a	1121	F6C	C1D-ND-C4D	-6.62	103.66	106.68
14	b	1236	CLA	O2D-CGD-CBD	6.62	122.80	111.23
14	B	1236	CLA	O2D-CGD-CBD	6.59	122.75	111.23
14	H	1236	CLA	O2D-CGD-CBD	6.58	122.74	111.23
14	G	1133	CLA	C4A-NA-C1A	6.58	109.68	106.68
14	B	1223	CLA	O2D-CGD-CBD	6.58	122.73	111.23
14	H	1223	CLA	O2D-CGD-CBD	6.57	122.72	111.23
14	A	1128	CLA	CMD-C2D-C1D	6.56	136.28	124.73
14	A	1101	CLA	O2D-CGD-CBD	6.56	122.69	111.23
14	G	1101	CLA	O2D-CGD-CBD	6.56	122.69	111.23
14	b	1223	CLA	O2D-CGD-CBD	6.56	122.69	111.23
14	G	1128	CLA	CMD-C2D-C1D	6.55	136.27	124.73
14	H	1214	CLA	C2C-C1C-NC	6.55	116.86	109.98
14	B	1214	CLA	C2C-C1C-NC	6.54	116.86	109.98
14	a	1101	CLA	O2D-CGD-CBD	6.54	122.67	111.23
14	a	1114	CLA	C2C-C1C-NC	6.54	116.86	109.98
15	A	1121	F6C	C1D-ND-C4D	-6.54	103.69	106.68
14	b	1214	CLA	C2C-C1C-NC	6.54	116.85	109.98
14	a	1128	CLA	CMD-C2D-C1D	6.54	136.24	124.73
15	a	1120	F6C	O2D-CGD-CBD	6.54	122.66	111.23
18	A	4002	BCR	C20-C19-C18	6.54	144.29	126.36
14	B	1202	CLA	O2D-CGD-CBD	6.53	122.65	111.23
14	a	1013	CLA	C4A-NA-C1A	6.53	109.66	106.68
14	A	1114	CLA	C2C-C1C-NC	6.53	116.84	109.98
18	a	4002	BCR	C20-C19-C18	6.52	144.25	126.36
14	G	1013	CLA	C4A-NA-C1A	6.52	109.65	106.68
14	G	1114	CLA	C2C-C1C-NC	6.52	116.83	109.98
14	A	1133	CLA	C4A-NA-C1A	6.51	109.65	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	4002	BCR	C20-C19-C18	6.51	144.22	126.36
15	A	1120	F6C	O2D-CGD-CBD	6.50	122.59	111.23
14	H	1202	CLA	O2D-CGD-CBD	6.50	122.59	111.23
15	G	1120	F6C	O2D-CGD-CBD	6.49	122.58	111.23
18	b	4014	BCR	C20-C19-C18	6.49	144.16	126.36
14	b	1202	CLA	O2D-CGD-CBD	6.49	122.57	111.23
14	A	1013	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	a	1133	CLA	C4A-NA-C1A	6.48	109.64	106.68
18	H	4014	BCR	C20-C19-C18	6.48	144.13	126.36
18	B	4014	BCR	C20-C19-C18	6.46	144.07	126.36
14	A	1103	CLA	C4A-NA-C1A	6.45	109.62	106.68
15	G	1121	F6C	C1D-ND-C4D	-6.45	103.74	106.68
18	b	4010	BCR	C20-C19-C18	6.45	144.04	126.36
18	B	4010	BCR	C20-C19-C18	6.43	144.00	126.36
18	H	4010	BCR	C20-C19-C18	6.43	143.99	126.36
14	B	1215	CLA	C2C-C1C-NC	6.42	116.72	109.98
14	L	1501	CLA	O2D-CGD-CBD	6.40	122.43	111.23
14	l	1501	CLA	O2D-CGD-CBD	6.40	122.43	111.23
14	a	1103	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	G	1136	CLA	O2D-CGD-CBD	6.40	122.43	111.23
14	H	1215	CLA	C2C-C1C-NC	6.39	116.70	109.98
14	A	1136	CLA	O2D-CGD-CBD	6.39	122.41	111.23
14	U	1501	CLA	O2D-CGD-CBD	6.39	122.41	111.23
14	T	1401	CLA	C2C-C1C-NC	6.39	116.69	109.98
14	G	1103	CLA	C4A-NA-C1A	6.39	109.59	106.68
14	G	1133	CLA	C2C-C1C-NC	6.38	116.69	109.98
14	a	1137	CLA	C2C-C1C-NC	6.38	116.69	109.98
14	b	1201	CLA	O2D-CGD-CBD	6.38	122.39	111.23
14	b	1215	CLA	C2C-C1C-NC	6.38	116.68	109.98
14	a	1136	CLA	O2D-CGD-CBD	6.38	122.38	111.23
14	b	1206	CLA	CMD-C2D-C1D	6.38	135.96	124.73
14	K	1401	CLA	C2C-C1C-NC	6.38	116.68	109.98
14	B	1022	CLA	CMD-C2D-C1D	6.38	135.96	124.73
14	B	1201	CLA	O2D-CGD-CBD	6.38	122.38	111.23
14	A	1137	CLA	C2C-C1C-NC	6.37	116.67	109.98
14	k	1401	CLA	C2C-C1C-NC	6.37	116.67	109.98
14	b	1022	CLA	CMD-C2D-C1D	6.37	135.95	124.73
14	H	1206	CLA	CMD-C2D-C1D	6.37	135.94	124.73
14	H	1012	CLA	CMD-C2D-C1D	6.37	135.94	124.73
14	B	1206	CLA	CMD-C2D-C1D	6.36	135.93	124.73
14	H	1201	CLA	O2D-CGD-CBD	6.36	122.35	111.23
18	G	4002	BCR	C11-C10-C9	6.36	136.19	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4002	BCR	C11-C10-C9	6.34	136.17	127.28
14	B	1235	CLA	O2D-CGD-CBD	6.34	122.31	111.23
14	A	1133	CLA	C2C-C1C-NC	6.33	116.64	109.98
14	G	1137	CLA	C2C-C1C-NC	6.33	116.63	109.98
14	B	1215	CLA	C1C-C2C-C3C	-6.33	100.32	106.98
14	b	1235	CLA	O2D-CGD-CBD	6.33	122.30	111.23
18	G	4001	BCR	C20-C19-C18	6.33	143.72	126.36
18	a	4001	BCR	C20-C19-C18	6.33	143.71	126.36
14	a	1133	CLA	C2C-C1C-NC	6.33	116.63	109.98
18	A	4001	BCR	C20-C19-C18	6.32	143.69	126.36
14	H	1205	CLA	CMD-C2D-C1D	6.32	135.85	124.73
14	G	1118	CLA	C2C-C1C-NC	6.32	116.62	109.98
14	H	1235	CLA	O2D-CGD-CBD	6.31	122.27	111.23
14	b	1205	CLA	CMD-C2D-C1D	6.31	135.85	124.73
14	A	1118	CLA	C2C-C1C-NC	6.31	116.61	109.98
18	A	4002	BCR	C11-C10-C9	6.31	136.13	127.28
14	b	1215	CLA	C1C-C2C-C3C	-6.30	100.35	106.98
14	H	1215	CLA	C1C-C2C-C3C	-6.30	100.36	106.98
14	B	1226	CLA	C2C-C1C-NC	6.30	116.60	109.98
14	B	1205	CLA	CMD-C2D-C1D	6.29	135.81	124.73
14	G	1135	CLA	C2C-C1C-NC	6.29	116.59	109.98
14	H	1226	CLA	C2C-C1C-NC	6.29	116.59	109.98
14	b	1216	CLA	C2C-C1C-NC	6.29	116.59	109.98
14	A	1123	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	a	1125	CLA	C4A-NA-C1A	6.28	109.55	106.68
14	a	1123	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	b	1226	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	B	1225	CLA	CMD-C2D-C1D	6.28	135.78	124.73
14	A	1135	CLA	C2C-C1C-NC	6.27	116.57	109.98
14	G	1123	CLA	C2C-C1C-NC	6.27	116.56	109.98
14	H	1225	CLA	CMD-C2D-C1D	6.27	135.76	124.73
14	B	1232	CLA	C2C-C1C-NC	6.26	116.56	109.98
14	b	1225	CLA	CMD-C2D-C1D	6.26	135.76	124.73
14	G	1128	CLA	O2D-CGD-CBD	6.26	122.17	111.23
14	B	1205	CLA	O2A-CGA-O1A	-6.26	107.98	123.63
14	H	1232	CLA	C2C-C1C-NC	6.26	116.55	109.98
14	a	1128	CLA	O2D-CGD-CBD	6.26	122.17	111.23
14	a	1118	CLA	C2C-C1C-NC	6.25	116.55	109.98
14	B	1234	CLA	C2D-C1D-ND	6.25	116.31	110.13
14	b	1205	CLA	O2A-CGA-O1A	-6.25	108.00	123.63
14	H	1223	CLA	C2C-C1C-NC	6.24	116.54	109.98
14	A	1128	CLA	O2D-CGD-CBD	6.24	122.14	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1206	CLA	C2C-C1C-NC	6.23	116.53	109.98
14	H	1205	CLA	O2A-CGA-O1A	-6.23	108.04	123.63
14	b	1232	CLA	C2C-C1C-NC	6.23	116.53	109.98
14	H	1216	CLA	C2C-C1C-NC	6.23	116.52	109.98
14	b	1234	CLA	C2D-C1D-ND	6.22	116.28	110.13
14	a	1135	CLA	C2C-C1C-NC	6.22	116.51	109.98
14	B	1217	CLA	C2C-C1C-NC	6.22	116.51	109.98
14	H	1217	CLA	C2C-C1C-NC	6.22	116.51	109.98
14	A	1109	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	G	1109	CLA	C4A-NA-C1A	6.21	109.51	106.68
14	B	1206	CLA	C2C-C1C-NC	6.21	116.51	109.98
14	B	1223	CLA	C2C-C1C-NC	6.21	116.50	109.98
14	B	1216	CLA	C2C-C1C-NC	6.20	116.50	109.98
14	G	1125	CLA	C4A-NA-C1A	6.20	109.51	106.68
14	b	1206	CLA	C2C-C1C-NC	6.20	116.49	109.98
14	b	1223	CLA	C2C-C1C-NC	6.20	116.49	109.98
14	H	1234	CLA	C2D-C1D-ND	6.19	116.25	110.13
14	B	1210	CLA	O2D-CGD-CBD	6.19	122.05	111.23
18	b	4013	BCR	C24-C23-C22	-6.18	117.09	126.23
14	B	1021	CLA	CMD-C2D-C1D	6.17	135.60	124.73
14	b	1217	CLA	C2C-C1C-NC	6.17	116.47	109.98
14	H	1210	CLA	O2D-CGD-CBD	6.17	122.01	111.23
14	H	1021	CLA	CMD-C2D-C1D	6.17	135.59	124.73
18	H	4013	BCR	C24-C23-C22	-6.16	117.12	126.23
14	G	1128	CLA	C2C-C1C-NC	6.16	116.45	109.98
14	a	1109	CLA	C4A-NA-C1A	6.16	109.49	106.68
14	b	1021	CLA	CMD-C2D-C1D	6.15	135.57	124.73
14	b	1210	CLA	O2D-CGD-CBD	6.15	121.98	111.23
18	B	4013	BCR	C24-C23-C22	-6.15	117.14	126.23
18	l	4022	BCR	C20-C19-C18	6.14	143.21	126.36
14	b	1202	CLA	O2A-CGA-O1A	-6.14	108.26	123.63
14	A	1125	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	A	1128	CLA	C2C-C1C-NC	6.14	116.43	109.98
18	U	4022	BCR	C20-C19-C18	6.13	143.18	126.36
18	L	4022	BCR	C20-C19-C18	6.13	143.18	126.36
14	A	1117	CLA	C2C-C1C-NC	6.13	116.42	109.98
14	H	1213	CLA	O2D-CGD-CBD	6.12	121.94	111.23
14	B	1202	CLA	O2A-CGA-O1A	-6.12	108.31	123.63
18	G	4003	BCR	C24-C23-C22	-6.12	117.18	126.23
14	H	1202	CLA	O2A-CGA-O1A	-6.12	108.32	123.63
18	b	4005	BCR	C24-C23-C22	-6.12	117.18	126.23
14	b	1233	CLA	C2C-C1C-NC	6.11	116.40	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1128	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	b	1227	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	b	1213	CLA	O2D-CGD-CBD	6.11	121.91	111.23
14	B	1233	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	G	1117	CLA	C2C-C1C-NC	6.11	116.40	109.98
14	B	1213	CLA	O2D-CGD-CBD	6.11	121.91	111.23
14	A	1126	CLA	C3B-C2B-C1B	-6.11	99.97	107.17
18	A	4003	BCR	C24-C23-C22	-6.11	117.20	126.23
14	H	1227	CLA	C2C-C1C-NC	6.10	116.39	109.98
14	G	1126	CLA	C3B-C2B-C1B	-6.10	99.98	107.17
18	B	4005	BCR	C24-C23-C22	-6.10	117.21	126.23
14	a	1118	CLA	O2D-CGD-CBD	6.10	121.89	111.23
18	a	4003	BCR	C24-C23-C22	-6.10	117.22	126.23
14	a	1104	CLA	C4A-NA-C1A	6.10	109.46	106.68
14	G	1118	CLA	O2D-CGD-CBD	6.09	121.88	111.23
14	a	1126	CLA	C3B-C2B-C1B	-6.09	99.99	107.17
14	A	1118	CLA	C1C-C2C-C3C	-6.08	100.58	106.98
14	A	1102	CLA	O2D-CGD-CBD	6.08	121.86	111.23
14	B	1023	CLA	CMD-C2D-C1D	6.08	135.44	124.73
14	A	1104	CLA	C4A-NA-C1A	6.08	109.45	106.68
14	H	1233	CLA	C2C-C1C-NC	6.08	116.37	109.98
14	B	1227	CLA	C2C-C1C-NC	6.08	116.37	109.98
14	a	1132	CLA	C3B-C2B-C1B	-6.08	100.00	107.17
14	a	1102	CLA	O2D-CGD-CBD	6.08	121.85	111.23
14	a	1117	CLA	C2C-C1C-NC	6.07	116.36	109.98
18	H	4005	BCR	C24-C23-C22	-6.07	117.25	126.23
14	H	1239	CLA	C1C-C2C-C3C	-6.07	100.59	106.98
14	G	1102	CLA	O2D-CGD-CBD	6.07	121.84	111.23
14	A	1118	CLA	O2D-CGD-CBD	6.07	121.84	111.23
14	A	1140	CLA	O2D-CGD-CBD	6.07	121.84	111.23
14	G	1140	CLA	O2D-CGD-CBD	6.07	121.84	111.23
14	A	1107	CLA	C2C-C1C-NC	6.06	116.35	109.98
14	b	1239	CLA	C1C-C2C-C3C	-6.06	100.60	106.98
14	G	1118	CLA	C1C-C2C-C3C	-6.06	100.61	106.98
14	a	1140	CLA	O2D-CGD-CBD	6.06	121.82	111.23
14	B	1222	CLA	O2D-CGD-CBD	6.06	121.82	111.23
14	b	1023	CLA	CMD-C2D-C1D	6.05	135.38	124.73
14	a	1104	CLA	C1C-C2C-C3C	-6.05	100.62	106.98
14	a	1107	CLA	C2C-C1C-NC	6.05	116.34	109.98
14	H	1222	CLA	O2D-CGD-CBD	6.05	121.81	111.23
14	A	1131	CLA	O2D-CGD-CBD	6.05	121.81	111.23
14	a	1127	CLA	C2C-C1C-NC	6.05	116.33	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1222	CLA	O2D-CGD-CBD	6.04	121.80	111.23
14	b	1224	CLA	O2D-CGD-CBD	6.04	121.80	111.23
14	A	1106	CLA	C4A-NA-C1A	6.04	109.44	106.68
14	G	1127	CLA	C2C-C1C-NC	6.04	116.33	109.98
14	H	1023	CLA	CMD-C2D-C1D	6.04	135.37	124.73
14	G	1131	CLA	O2D-CGD-CBD	6.04	121.79	111.23
14	B	1208	CLA	C2C-C1C-NC	6.04	116.32	109.98
14	G	1107	CLA	C2C-C1C-NC	6.03	116.32	109.98
14	a	1118	CLA	C1C-C2C-C3C	-6.03	100.64	106.98
14	H	1224	CLA	O2D-CGD-CBD	6.03	121.77	111.23
14	a	1131	CLA	O2D-CGD-CBD	6.03	121.77	111.23
14	H	1208	CLA	C2C-C1C-NC	6.03	116.31	109.98
14	G	1132	CLA	C3B-C2B-C1B	-6.03	100.06	107.17
14	G	1104	CLA	C4A-NA-C1A	6.03	109.43	106.68
14	B	1239	CLA	C1C-C2C-C3C	-6.03	100.64	106.98
14	b	1203	CLA	C3D-C2D-C1D	-6.02	97.61	105.83
14	A	1133	CLA	O2D-CGD-CBD	6.02	121.76	111.23
14	B	1203	CLA	C3D-C2D-C1D	-6.02	97.61	105.83
14	H	1203	CLA	C3D-C2D-C1D	-6.02	97.61	105.83
14	B	1224	CLA	O2D-CGD-CBD	6.02	121.75	111.23
14	A	1132	CLA	C3B-C2B-C1B	-6.02	100.07	107.17
14	b	1208	CLA	C2C-C1C-NC	6.02	116.30	109.98
14	A	1104	CLA	C1C-C2C-C3C	-6.02	100.65	106.98
14	A	1127	CLA	C2C-C1C-NC	6.02	116.30	109.98
14	b	1204	CLA	C2C-C1C-NC	6.01	116.30	109.98
14	b	1201	CLA	O2A-CGA-O1A	-6.01	108.58	123.63
14	B	1201	CLA	O2A-CGA-O1A	-6.01	108.60	123.63
14	H	1201	CLA	O2A-CGA-O1A	-6.00	108.62	123.63
14	a	1133	CLA	O2D-CGD-CBD	6.00	121.71	111.23
14	a	1126	CLA	O2D-CGD-CBD	6.00	121.71	111.23
14	A	1136	CLA	C4A-NA-C1A	5.99	109.41	106.68
14	G	1133	CLA	O2D-CGD-CBD	5.99	121.71	111.23
14	G	1132	CLA	C2C-C1C-NC	5.99	116.27	109.98
14	a	1122	CLA	C4A-NA-C1A	5.98	109.41	106.68
14	H	1204	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	G	1126	CLA	O2D-CGD-CBD	5.98	121.68	111.23
14	G	1133	CLA	C1C-C2C-C3C	-5.98	100.69	106.98
14	A	1132	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	G	1104	CLA	C1C-C2C-C3C	-5.98	100.69	106.98
14	a	1132	CLA	C2C-C1C-NC	5.98	116.26	109.98
14	b	1239	CLA	C4A-NA-C1A	5.98	109.41	106.68
14	G	1106	CLA	C4A-NA-C1A	5.97	109.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1106	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	H	1218	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	A	1126	CLA	O2D-CGD-CBD	5.97	121.66	111.23
14	G	1116	CLA	C2C-C1C-NC	5.96	116.24	109.98
14	a	1136	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	G	1137	CLA	C4A-NA-C1A	5.95	109.39	106.68
14	a	1133	CLA	C1C-C2C-C3C	-5.95	100.72	106.98
14	A	1140	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	a	1012	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	B	1239	CLA	C4A-NA-C1A	5.94	109.39	106.68
14	A	1116	CLA	C2C-C1C-NC	5.94	116.22	109.98
15	G	1121	F6C	C2C-C1C-NC	5.94	116.48	110.33
14	B	1228	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	a	1116	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	B	1204	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	B	1218	CLA	C2C-C1C-NC	5.93	116.22	109.98
14	A	1137	CLA	C4A-NA-C1A	5.93	109.39	106.68
14	G	1140	CLA	C2C-C1C-NC	5.93	116.21	109.98
14	b	1202	CLA	C2C-C1C-NC	5.93	116.21	109.98
14	G	1012	CLA	C2C-C1C-NC	5.93	116.21	109.98
14	G	1013	CLA	C2B-C1B-NB	5.93	116.47	110.33
14	B	1023	CLA	C3B-C2B-C1B	-5.92	100.19	107.17
14	A	1013	CLA	C2B-C1B-NB	5.92	116.47	110.33
14	a	1103	CLA	O2D-CGD-CBD	5.92	121.58	111.23
14	a	1140	CLA	C2C-C1C-NC	5.92	116.20	109.98
15	a	1121	F6C	C2C-C1C-NC	5.92	116.47	110.33
14	A	1133	CLA	C1C-C2C-C3C	-5.92	100.75	106.98
14	G	1103	CLA	O2D-CGD-CBD	5.92	121.58	111.23
14	b	1220	CLA	C2C-C1C-NC	5.92	116.20	109.98
14	G	1136	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	L	1501	CLA	C4A-NA-C1A	5.91	109.38	106.68
14	G	1125	CLA	C3D-C2D-C1D	-5.91	97.76	105.83
14	a	1125	CLA	C3D-C2D-C1D	-5.91	97.77	105.83
14	a	1113	CLA	C2C-C1C-NC	5.91	116.19	109.98
14	b	1214	CLA	O2D-CGD-CBD	5.91	121.56	111.23
14	H	1023	CLA	C3B-C2B-C1B	-5.91	100.21	107.17
14	A	1012	CLA	C2C-C1C-NC	5.91	116.19	109.98
14	H	1239	CLA	C4A-NA-C1A	5.90	109.37	106.68
14	A	1103	CLA	O2D-CGD-CBD	5.90	121.55	111.23
14	a	1013	CLA	C2B-C1B-NB	5.90	116.45	110.33
14	G	1126	CLA	C2C-C1C-NC	5.90	116.18	109.98
14	A	1113	CLA	C3B-C2B-C1B	-5.90	100.21	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1113	CLA	C2C-C1C-NC	5.90	116.18	109.98
14	A	1111	CLA	O2D-CGD-CBD	5.90	121.54	111.23
14	a	1111	CLA	O2D-CGD-CBD	5.90	121.54	111.23
14	A	1126	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	a	1112	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	b	1228	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	G	1122	CLA	C4A-NA-C1A	5.89	109.37	106.68
14	G	1124	CLA	C3B-C2B-C1B	-5.89	100.22	107.17
14	A	1112	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	B	1217	CLA	C4A-NA-C1A	5.89	109.37	106.68
14	U	1501	CLA	C4A-NA-C1A	5.89	109.37	106.68
14	B	1220	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	H	1220	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	A	1124	CLA	C3B-C2B-C1B	-5.89	100.23	107.17
14	A	1113	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	G	1112	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	U	1503	CLA	C2C-C1C-NC	5.89	116.17	109.98
14	a	1113	CLA	C3B-C2B-C1B	-5.89	100.23	107.17
14	A	1131	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	b	1218	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	H	1219	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	H	1202	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	B	1202	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	G	1111	CLA	O2D-CGD-CBD	5.88	121.51	111.23
14	A	1122	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	B	1221	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	G	1113	CLA	C3B-C2B-C1B	-5.88	100.24	107.17
14	b	1023	CLA	C3B-C2B-C1B	-5.88	100.24	107.17
14	G	1131	CLA	C2C-C1C-NC	5.88	116.15	109.98
14	G	1118	CLA	C4A-NA-C1A	5.87	109.36	106.68
14	a	1126	CLA	C2C-C1C-NC	5.87	116.15	109.98
15	A	1121	F6C	C2C-C1C-NC	5.87	116.41	110.33
14	a	1124	CLA	C3B-C2B-C1B	-5.87	100.25	107.17
14	H	1210	CLA	C2C-C1C-NC	5.87	116.14	109.98
14	B	1210	CLA	C2C-C1C-NC	5.86	116.14	109.98
14	A	1125	CLA	C3D-C2D-C1D	-5.86	97.83	105.83
14	H	1228	CLA	C2C-C1C-NC	5.86	116.14	109.98
14	b	1210	CLA	C2C-C1C-NC	5.86	116.14	109.98
14	l	1503	CLA	C2C-C1C-NC	5.86	116.14	109.98
14	B	1204	CLA	O2D-CGD-CBD	5.86	121.48	111.23
14	b	1217	CLA	C4A-NA-C1A	5.86	109.35	106.68
14	B	1214	CLA	O2D-CGD-CBD	5.86	121.47	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1214	CLA	O2D-CGD-CBD	5.86	121.47	111.23
14	b	1204	CLA	O2D-CGD-CBD	5.86	121.47	111.23
14	A	1013	CLA	C3B-C2B-C1B	-5.85	100.27	107.17
14	B	1234	CLA	C3D-C2D-C1D	-5.85	97.84	105.83
14	H	1236	CLA	C2C-C1C-NC	5.85	116.13	109.98
14	a	1114	CLA	C1C-C2C-C3C	-5.85	100.83	106.98
14	G	1106	CLA	C2C-C1C-NC	5.85	116.12	109.98
14	B	1201	CLA	C2C-C1C-NC	5.84	116.12	109.98
18	B	4014	BCR	C24-C23-C22	-5.84	117.59	126.23
14	H	1201	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	a	1106	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	b	1234	CLA	C3D-C2D-C1D	-5.84	97.86	105.83
14	H	1204	CLA	O2D-CGD-CBD	5.84	121.44	111.23
14	a	1131	CLA	C2C-C1C-NC	5.84	116.12	109.98
15	H	1237	F6C	C1A-C2A-C3A	-5.84	100.82	106.97
14	b	1201	CLA	C2C-C1C-NC	5.84	116.11	109.98
14	a	1137	CLA	C4A-NA-C1A	5.84	109.34	106.68
14	G	1114	CLA	C1C-C2C-C3C	-5.84	100.84	106.98
14	A	1102	CLA	C2C-C1C-NC	5.84	116.11	109.98
14	A	1106	CLA	C2C-C1C-NC	5.84	116.11	109.98
14	b	1236	CLA	C2C-C1C-NC	5.84	116.11	109.98
18	A	4008	BCR	C20-C19-C18	5.83	142.36	126.36
14	b	1209	CLA	C2C-C1C-NC	5.83	116.11	109.98
18	H	4014	BCR	C24-C23-C22	-5.83	117.61	126.23
14	H	1207	CLA	C1C-C2C-C3C	-5.83	100.85	106.98
14	L	1503	CLA	C2C-C1C-NC	5.83	116.10	109.98
14	b	1219	CLA	C4A-NA-C1A	5.83	109.34	106.68
14	a	1013	CLA	C3B-C2B-C1B	-5.83	100.30	107.17
14	b	1209	CLA	O2D-CGD-CBD	5.82	121.41	111.23
14	H	1234	CLA	C3D-C2D-C1D	-5.82	97.89	105.83
18	G	4008	BCR	C20-C19-C18	5.82	142.32	126.36
14	B	1218	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	a	1126	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	B	1236	CLA	C2C-C1C-NC	5.82	116.09	109.98
14	H	1209	CLA	C2C-C1C-NC	5.82	116.09	109.98
14	G	1123	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	H	1209	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	B	1201	CLA	C3B-C2B-C1B	-5.82	100.31	107.17
14	b	1221	CLA	C4A-NA-C1A	5.82	109.33	106.68
18	H	4004	BCR	C20-C19-C18	5.82	142.31	126.36
14	A	1123	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	a	1118	CLA	C4A-NA-C1A	5.82	109.33	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1013	CLA	C3B-C2B-C1B	-5.81	100.31	107.17
14	b	1218	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	G	1102	CLA	C2C-C1C-NC	5.81	116.09	109.98
14	G	1109	CLA	C2C-C1C-NC	5.81	116.09	109.98
18	a	4008	BCR	C20-C19-C18	5.81	142.30	126.36
15	b	1237	F6C	C1A-C2A-C3A	-5.81	100.85	106.97
14	a	1123	CLA	O2D-CGD-CBD	5.81	121.39	111.23
18	b	4014	BCR	C24-C23-C22	-5.81	117.64	126.23
14	H	1201	CLA	C3B-C2B-C1B	-5.81	100.32	107.17
14	b	1201	CLA	C3B-C2B-C1B	-5.81	100.32	107.17
14	B	1219	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	B	1209	CLA	O2D-CGD-CBD	5.80	121.37	111.23
14	H	1218	CLA	O2D-CGD-CBD	5.80	121.37	111.23
14	B	1209	CLA	C2C-C1C-NC	5.80	116.08	109.98
14	G	1111	CLA	C2C-C1C-NC	5.80	116.08	109.98
14	a	1102	CLA	C2C-C1C-NC	5.80	116.08	109.98
18	B	4004	BCR	C20-C19-C18	5.80	142.26	126.36
14	A	1114	CLA	C1C-C2C-C3C	-5.80	100.88	106.98
14	H	1203	CLA	C2D-C1D-ND	5.80	115.86	110.13
15	B	1237	F6C	C1A-C2A-C3A	-5.80	100.87	106.97
18	b	4004	BCR	C20-C19-C18	5.80	142.25	126.36
14	A	1110	CLA	C2C-C1C-NC	5.79	116.07	109.98
14	A	1111	CLA	C2C-C1C-NC	5.79	116.06	109.98
14	B	1207	CLA	C1C-C2C-C3C	-5.79	100.89	106.98
14	A	1126	CLA	C4A-NA-C1A	5.79	109.32	106.68
14	a	1111	CLA	C2C-C1C-NC	5.79	116.06	109.98
14	L	1502	CLA	C2C-C1C-NC	5.78	116.06	109.98
14	U	1502	CLA	C2C-C1C-NC	5.78	116.06	109.98
14	a	1116	CLA	O2D-CGD-CBD	5.78	121.34	111.23
15	G	1120	F6C	C2D-C1D-ND	5.78	116.05	109.98
14	b	1235	CLA	C4A-NA-C1A	5.78	109.31	106.68
15	b	1230	F6C	O2D-CGD-CBD	5.78	121.33	111.23
14	G	1116	CLA	O2D-CGD-CBD	5.77	121.33	111.23
14	b	1207	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
14	A	1116	CLA	O2D-CGD-CBD	5.77	121.32	111.23
15	a	1120	F6C	C2D-C1D-ND	5.77	116.04	109.98
14	H	1217	CLA	C4A-NA-C1A	5.77	109.31	106.68
14	a	1110	CLA	C2C-C1C-NC	5.77	116.04	109.98
14	G	1110	CLA	C2C-C1C-NC	5.77	116.04	109.98
14	U	1501	CLA	C2C-C1C-NC	5.77	116.04	109.98
14	a	1109	CLA	C2C-C1C-NC	5.77	116.04	109.98
14	A	1109	CLA	C2C-C1C-NC	5.77	116.04	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1218	CLA	O2D-CGD-CBD	5.76	121.31	111.23
14	A	1131	CLA	C3B-C2B-C1B	-5.76	100.38	107.17
14	l	1501	CLA	C4A-NA-C1A	5.76	109.31	106.68
14	b	1219	CLA	C2C-C1C-NC	5.76	116.03	109.98
14	H	1221	CLA	C4A-NA-C1A	5.76	109.31	106.68
15	H	1230	F6C	O2D-CGD-CBD	5.76	121.30	111.23
14	l	1502	CLA	C2C-C1C-NC	5.76	116.03	109.98
14	H	1239	CLA	O2D-CGD-CBD	5.76	121.29	111.23
15	A	1120	F6C	C2D-C1D-ND	5.76	116.03	109.98
14	H	1235	CLA	C4A-NA-C1A	5.75	109.30	106.68
14	A	1118	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	H	1218	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	L	1501	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	b	1218	CLA	O2D-CGD-CBD	5.74	121.27	111.23
14	B	1203	CLA	C2D-C1D-ND	5.74	115.80	110.13
14	b	1203	CLA	C2D-C1D-ND	5.74	115.80	110.13
14	b	1214	CLA	C1C-C2C-C3C	-5.74	100.95	106.98
14	b	1204	CLA	C3B-C2B-C1B	-5.73	100.41	107.17
14	G	1126	CLA	C4A-NA-C1A	5.73	109.30	106.68
14	b	1239	CLA	O2D-CGD-CBD	5.73	121.25	111.23
14	a	1136	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	H	1219	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	B	1239	CLA	O2D-CGD-CBD	5.73	121.25	111.23
14	b	1219	CLA	O2D-CGD-CBD	5.73	121.25	111.23
14	a	1103	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	A	1136	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	a	1131	CLA	C3B-C2B-C1B	-5.72	100.42	107.17
14	B	1204	CLA	C3B-C2B-C1B	-5.72	100.42	107.17
14	l	1501	CLA	C2C-C1C-NC	5.72	115.99	109.98
14	B	1205	CLA	O2A-CGA-CBA	5.72	129.27	111.83
14	A	1103	CLA	C2C-C1C-NC	5.72	115.99	109.98
14	B	1214	CLA	C1C-C2C-C3C	-5.71	100.97	106.98
14	B	1023	CLA	C3D-C2D-C1D	-5.71	98.04	105.83
14	B	1219	CLA	C2C-C1C-NC	5.71	115.98	109.98
14	G	1103	CLA	C2C-C1C-NC	5.71	115.98	109.98
14	H	1205	CLA	O2A-CGA-CBA	5.71	129.24	111.83
14	b	1205	CLA	O2A-CGA-CBA	5.71	129.23	111.83
18	R	4018	BCR	C15-C14-C13	-5.70	119.28	127.28
14	H	1204	CLA	C3B-C2B-C1B	-5.70	100.45	107.17
14	B	1212	CLA	C2D-C1D-ND	5.70	115.77	110.13
18	I	4018	BCR	C15-C14-C13	-5.70	119.28	127.28
14	B	1219	CLA	O2D-CGD-CBD	5.70	121.20	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1219	CLA	O2D-CGD-CBD	5.70	121.19	111.23
14	G	1131	CLA	C3B-C2B-C1B	-5.70	100.45	107.17
14	H	1214	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
14	B	1235	CLA	C4A-NA-C1A	5.69	109.27	106.68
14	G	1108	CLA	C2C-C1C-NC	5.68	115.95	109.98
14	b	1023	CLA	C3D-C2D-C1D	-5.68	98.07	105.83
14	a	1108	CLA	C2C-C1C-NC	5.68	115.95	109.98
14	T	1401	CLA	C1C-C2C-C3C	-5.68	101.00	106.98
14	H	1226	CLA	O2D-CGD-CBD	5.68	121.16	111.23
14	H	1204	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
14	B	1226	CLA	O2D-CGD-CBD	5.68	121.15	111.23
14	b	1204	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
14	H	1219	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
14	H	1212	CLA	C2D-C1D-ND	5.67	115.74	110.13
14	b	1219	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
14	A	1138	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
14	a	1138	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
14	H	1023	CLA	C3D-C2D-C1D	-5.67	98.09	105.83
14	b	1226	CLA	O2D-CGD-CBD	5.67	121.14	111.23
14	K	1401	CLA	C1C-C2C-C3C	-5.67	101.02	106.98
18	i	4018	BCR	C15-C14-C13	-5.67	119.33	127.28
15	b	1237	F6C	O2D-CGD-CBD	5.67	121.13	111.23
14	k	1401	CLA	C1C-C2C-C3C	-5.66	101.02	106.98
14	G	1136	CLA	C2C-C1C-NC	5.66	115.93	109.98
14	B	1206	CLA	C4A-NA-C1A	5.66	109.26	106.68
14	H	1206	CLA	C4A-NA-C1A	5.66	109.26	106.68
15	B	1237	F6C	O2D-CGD-CBD	5.66	121.12	111.23
14	G	1126	CLA	O2A-CGA-O1A	-5.66	109.48	123.63
14	H	1208	CLA	C1C-C2C-C3C	-5.66	101.03	106.98
14	A	1126	CLA	O2A-CGA-O1A	-5.65	109.48	123.63
15	H	1237	F6C	O2D-CGD-CBD	5.65	121.11	111.23
14	b	1212	CLA	C2D-C1D-ND	5.65	115.72	110.13
14	A	1108	CLA	C2C-C1C-NC	5.65	115.91	109.98
14	B	1222	CLA	C3B-C2B-C1B	-5.64	100.52	107.17
14	B	1219	CLA	C3B-C2B-C1B	-5.64	100.52	107.17
15	B	1230	F6C	O2D-CGD-CBD	5.64	121.09	111.23
14	B	1225	CLA	C2C-C1C-NC	5.64	115.91	109.98
14	a	1126	CLA	O2A-CGA-O1A	-5.64	109.52	123.63
14	H	1222	CLA	C3B-C2B-C1B	-5.64	100.52	107.17
14	H	1225	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	b	1208	CLA	C1C-C2C-C3C	-5.63	101.05	106.98
14	b	1216	CLA	C3B-C2B-C1B	-5.63	100.53	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1115	CLA	C4A-NA-C1A	5.63	109.25	106.68
14	b	1211	CLA	C4A-NA-C1A	5.63	109.25	106.68
14	G	1139	CLA	C2C-C1C-NC	5.63	115.89	109.98
15	B	1237	F6C	C2C-C1C-NC	5.63	116.16	110.33
14	G	1135	CLA	C3B-C2B-C1B	-5.63	100.54	107.17
14	B	1213	CLA	C2C-C1C-NC	5.62	115.89	109.98
14	A	1103	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
14	B	1234	CLA	C1D-ND-C4D	-5.62	102.37	106.31
14	A	1139	CLA	C2C-C1C-NC	5.62	115.89	109.98
14	H	1216	CLA	C3B-C2B-C1B	-5.62	100.54	107.17
14	H	1229	CLA	C3B-C2B-C1B	-5.62	100.54	107.17
14	A	1110	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
14	A	1130	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
14	B	1211	CLA	C4A-NA-C1A	5.62	109.24	106.68
14	b	1206	CLA	C4A-NA-C1A	5.62	109.24	106.68
14	B	1224	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
14	b	1225	CLA	C2C-C1C-NC	5.62	115.88	109.98
14	b	1222	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
14	G	1138	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
14	H	1224	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
14	B	1204	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
14	B	1229	CLA	O2D-CGD-CBD	5.61	121.04	111.23
14	G	1115	CLA	C2C-C1C-NC	5.61	115.88	109.98
14	H	1213	CLA	C2C-C1C-NC	5.61	115.88	109.98
14	b	1234	CLA	C1D-ND-C4D	-5.61	102.38	106.31
14	a	1130	CLA	C3D-C2D-C1D	-5.61	98.17	105.83
14	H	1205	CLA	C2D-C1D-ND	5.61	115.68	110.13
14	b	1229	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
14	a	1112	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	A	1105	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
14	B	1216	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
14	G	1105	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
14	x	1701	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	G	1103	CLA	C3D-C2D-C1D	-5.61	98.18	105.83
14	b	1224	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
14	b	1229	CLA	O2D-CGD-CBD	5.61	121.03	111.23
14	a	1105	CLA	C3B-C2B-C1B	-5.60	100.56	107.17
14	a	1135	CLA	C3B-C2B-C1B	-5.60	100.56	107.17
14	a	1110	CLA	C3D-C2D-C1D	-5.60	98.18	105.83
14	a	1104	CLA	C2C-C1C-NC	5.60	115.87	109.98
14	B	1208	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	G	1122	CLA	C3B-C2B-C1B	-5.60	100.57	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1205	CLA	C2D-C1D-ND	5.60	115.67	110.13
14	X	1701	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	H	1217	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	b	1227	CLA	O2D-CGD-CBD	5.60	121.02	111.23
14	A	1104	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	G	1138	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	G	1130	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
14	a	1139	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	B	1220	CLA	C4A-NA-C1A	5.60	109.23	106.68
14	b	1213	CLA	C2C-C1C-NC	5.59	115.86	109.98
14	A	1135	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
14	B	1227	CLA	O2D-CGD-CBD	5.59	121.01	111.23
14	H	1220	CLA	C4A-NA-C1A	5.59	109.23	106.68
15	H	1237	F6C	C2C-C1C-NC	5.59	116.12	110.33
18	R	4020	BCR	C34-C9-C10	-5.59	113.76	122.82
14	G	1012	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
14	a	1103	CLA	C3D-C2D-C1D	-5.59	98.21	105.83
14	A	1138	CLA	C2C-C1C-NC	5.59	115.85	109.98
14	a	1138	CLA	C2C-C1C-NC	5.58	115.85	109.98
14	B	1217	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	b	1229	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	B	1229	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
14	a	1113	CLA	O2D-CGD-CBD	5.58	120.98	111.23
15	b	1237	F6C	C2C-C1C-NC	5.58	116.11	110.33
14	A	1122	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
14	A	1113	CLA	C4A-NA-C1A	5.58	109.22	106.68
14	a	1115	CLA	C4A-NA-C1A	5.58	109.22	106.68
14	a	1115	CLA	C2C-C1C-NC	5.58	115.84	109.98
14	A	1113	CLA	O2D-CGD-CBD	5.58	120.98	111.23
14	G	1112	CLA	O2D-CGD-CBD	5.58	120.98	111.23
14	a	1112	CLA	O2D-CGD-CBD	5.58	120.98	111.23
14	b	1207	CLA	O2D-CGD-CBD	5.58	120.98	111.23
14	H	1229	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
14	G	1110	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
14	B	1229	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
14	H	1227	CLA	O2D-CGD-CBD	5.57	120.97	111.23
14	W	1701	CLA	C2C-C1C-NC	5.57	115.83	109.98
14	H	1229	CLA	O2D-CGD-CBD	5.57	120.97	111.23
14	B	1235	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
14	G	1113	CLA	O2D-CGD-CBD	5.57	120.97	111.23
14	b	1207	CLA	C4A-NA-C1A	5.57	109.22	106.68
14	H	1235	CLA	C3B-C2B-C1B	-5.57	100.61	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1111	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
14	A	1012	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
14	a	1012	CLA	C3D-C2D-C1D	-5.56	98.24	105.83
14	G	1104	CLA	C2C-C1C-NC	5.56	115.83	109.98
18	i	4020	BCR	C34-C9-C10	-5.56	113.80	122.82
14	A	1136	CLA	O2A-CGA-O1A	-5.56	109.72	123.63
14	A	1106	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
14	a	1104	CLA	C2D-C1D-ND	5.56	115.63	110.13
14	B	1236	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
14	G	1104	CLA	C2D-C1D-ND	5.56	115.63	110.13
14	b	1235	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
14	a	1114	CLA	O2D-CGD-CBD	5.56	120.94	111.23
14	A	1115	CLA	C2C-C1C-NC	5.56	115.82	109.98
14	B	1205	CLA	C2D-C1D-ND	5.56	115.62	110.13
14	a	1136	CLA	O2A-CGA-O1A	-5.56	109.73	123.63
14	H	1207	CLA	O2D-CGD-CBD	5.55	120.94	111.23
14	a	1105	CLA	C2C-C1C-NC	5.55	115.82	109.98
14	a	1122	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
14	b	1217	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
18	I	4020	BCR	C34-C9-C10	-5.55	113.82	122.82
14	A	1106	CLA	C2D-C1D-ND	5.55	115.62	110.13
14	G	1106	CLA	C3B-C2B-C1B	-5.55	100.63	107.17
14	a	1122	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	H	1234	CLA	C1D-ND-C4D	-5.55	102.42	106.31
14	b	1220	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	G	1109	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	a	1111	CLA	C3D-C2D-C1D	-5.54	98.27	105.83
14	B	1207	CLA	O2D-CGD-CBD	5.54	120.92	111.23
14	G	1136	CLA	O2A-CGA-O1A	-5.54	109.76	123.63
14	a	1125	CLA	C2D-C1D-ND	5.54	115.61	110.13
14	A	1137	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	a	1106	CLA	C2D-C1D-ND	5.54	115.61	110.13
14	A	1112	CLA	O2D-CGD-CBD	5.53	120.91	111.23
14	a	1106	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
14	A	1109	CLA	C1C-C2C-C3C	-5.53	101.16	106.98
14	K	1401	CLA	C4A-NA-C1A	5.53	109.20	106.68
15	b	1230	F6C	C2C-C1C-NC	5.53	116.06	110.33
14	b	1222	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	b	1236	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
18	b	4009	BCR	C24-C23-C22	-5.52	118.07	126.23
14	H	1236	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
14	a	1112	CLA	C3B-C2B-C1B	-5.52	100.66	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1212	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	A	1111	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
15	A	1121	F6C	CAA-C2A-C1A	-5.51	112.60	128.01
14	a	1137	CLA	C1C-C2C-C3C	-5.51	101.18	106.98
14	H	1021	CLA	C2D-C1D-ND	5.51	115.58	110.13
14	B	1222	CLA	C2C-C1C-NC	5.51	115.77	109.98
15	a	1121	F6C	CAA-C2A-C1A	-5.51	112.61	128.01
14	H	1211	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	G	1112	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
14	A	1130	CLA	O2D-CGD-CBD	5.51	120.86	111.23
14	G	1106	CLA	C2D-C1D-ND	5.51	115.58	110.13
14	G	1104	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
14	A	1123	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	G	1114	CLA	O2D-CGD-CBD	5.51	120.86	111.23
14	H	1213	CLA	C3B-C2B-C1B	-5.51	100.68	107.17
14	A	1104	CLA	C2D-C1D-ND	5.51	115.58	110.13
14	b	1213	CLA	C3B-C2B-C1B	-5.51	100.68	107.17
14	a	1113	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	G	1122	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	l	1502	CLA	C2D-C1D-ND	5.50	115.57	110.13
18	m	4021	BCR	C24-C23-C22	-5.50	118.09	126.23
14	A	1114	CLA	O2D-CGD-CBD	5.50	120.85	111.23
14	a	1130	CLA	O2D-CGD-CBD	5.50	120.85	111.23
14	H	1207	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	b	1235	CLA	O2A-CGA-O1A	-5.50	109.87	123.63
14	a	1109	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
14	A	1105	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	G	1105	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	H	1235	CLA	O2A-CGA-O1A	-5.50	109.87	123.63
14	B	1021	CLA	C2D-C1D-ND	5.50	115.57	110.13
14	H	1229	CLA	C2C-C1C-NC	5.50	115.76	109.98
18	M	4021	BCR	C24-C23-C22	-5.50	118.10	126.23
14	A	1125	CLA	C2D-C1D-ND	5.50	115.57	110.13
14	G	1137	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
14	G	1125	CLA	C2D-C1D-ND	5.50	115.56	110.13
14	b	1021	CLA	C2D-C1D-ND	5.50	115.56	110.13
14	b	1208	CLA	O2D-CGD-CBD	5.50	120.84	111.23
14	G	1115	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	A	1112	CLA	C3B-C2B-C1B	-5.49	100.69	107.17
14	H	1212	CLA	C2C-C1C-NC	5.49	115.75	109.98
14	a	1130	CLA	C2C-C1C-NC	5.49	115.75	109.98
15	G	1121	F6C	CAA-C2A-C1A	-5.49	112.67	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	V	4021	BCR	C24-C23-C22	-5.49	118.11	126.23
14	L	1501	CLA	C2D-C1D-ND	5.49	115.56	110.13
14	a	1104	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
14	B	1213	CLA	C3B-C2B-C1B	-5.49	100.70	107.17
14	B	1208	CLA	O2D-CGD-CBD	5.49	120.83	111.23
18	H	4009	BCR	C24-C23-C22	-5.49	118.12	126.23
14	H	1208	CLA	O2D-CGD-CBD	5.49	120.82	111.23
14	b	1215	CLA	O2D-CGD-CBD	5.49	120.82	111.23
14	A	1131	CLA	C1C-C2C-C3C	-5.49	101.21	106.98
14	a	1113	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
14	T	1401	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	G	1130	CLA	O2D-CGD-CBD	5.48	120.82	111.23
14	A	1104	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
14	G	1111	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
14	a	1111	CLA	C3B-C2B-C1B	-5.48	100.71	107.17
15	A	1121	F6C	C1A-C2A-C3A	-5.48	101.20	106.97
14	U	1502	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
14	L	1502	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	G	1123	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
14	B	1207	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	A	1129	CLA	C2C-C1C-NC	5.48	115.73	109.98
14	b	1212	CLA	C2C-C1C-NC	5.48	115.73	109.98
14	L	1502	CLA	C2D-C1D-ND	5.48	115.55	110.13
15	G	1121	F6C	C1A-C2A-C3A	-5.48	101.20	106.97
14	b	1229	CLA	C2C-C1C-NC	5.48	115.73	109.98
14	B	1235	CLA	O2A-CGA-O1A	-5.48	109.93	123.63
14	B	1211	CLA	C2C-C1C-NC	5.48	115.73	109.98
14	U	1501	CLA	C2D-C1D-ND	5.48	115.55	110.13
14	G	1113	CLA	C4A-NA-C1A	5.47	109.18	106.68
14	L	1502	CLA	C1C-C2C-C3C	-5.47	101.22	106.98
15	H	1230	F6C	C2C-C1C-NC	5.47	116.00	110.33
14	H	1218	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
14	a	1123	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
14	H	1238	CLA	C3B-C2B-C1B	-5.47	100.72	107.17
14	A	1122	CLA	C2C-C1C-NC	5.47	115.73	109.98
14	a	1131	CLA	C4A-NA-C1A	5.47	109.17	106.68
14	G	1119	CLA	C2C-C1C-NC	5.47	115.72	109.98
14	B	1203	CLA	C1C-C2C-C3C	-5.47	101.23	106.98
14	A	1112	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	H	1222	CLA	C2C-C1C-NC	5.46	115.72	109.98
14	a	1106	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
15	a	1120	F6C	C2C-C1C-NC	5.46	115.99	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1235	CLA	C2C-C1C-NC	5.46	115.72	109.98
14	A	1111	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
14	B	1238	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
14	l	1502	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
15	a	1121	F6C	C1A-C2A-C3A	-5.46	101.22	106.97
18	B	4009	BCR	C24-C23-C22	-5.46	118.16	126.23
14	B	1235	CLA	C2C-C1C-NC	5.46	115.72	109.98
14	k	1401	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	a	1104	CLA	C3B-C2B-C1B	-5.46	100.74	107.17
14	H	1215	CLA	O2D-CGD-CBD	5.46	120.77	111.23
14	b	1238	CLA	C3B-C2B-C1B	-5.45	100.74	107.17
14	B	1215	CLA	O2D-CGD-CBD	5.45	120.76	111.23
14	B	1229	CLA	C2C-C1C-NC	5.45	115.71	109.98
14	U	1502	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
14	A	1106	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
14	H	1203	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
18	m	4021	BCR	C15-C14-C13	-5.45	119.64	127.28
14	G	1131	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
14	b	1203	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
14	A	1119	CLA	C2C-C1C-NC	5.45	115.70	109.98
14	b	1211	CLA	C2C-C1C-NC	5.44	115.70	109.98
14	H	1210	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
14	b	1231	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
15	A	1120	F6C	C2C-C1C-NC	5.44	115.97	110.33
14	B	1202	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	G	1113	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	b	1021	CLA	C2C-C1C-NC	5.44	115.70	109.98
14	H	1021	CLA	C2C-C1C-NC	5.44	115.70	109.98
14	L	1502	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	H	1232	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	G	1129	CLA	C2C-C1C-NC	5.44	115.69	109.98
14	B	1231	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
14	B	1218	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	B	1203	CLA	C2C-C1C-NC	5.44	115.69	109.98
14	A	1128	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	A	1113	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	G	1104	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
18	a	4011	BCR	C7-C8-C9	-5.44	118.19	126.23
14	G	1130	CLA	C2C-C1C-NC	5.44	115.69	109.98
14	A	1113	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
14	G	1131	CLA	C4A-NA-C1A	5.43	109.16	106.68
14	l	1502	CLA	C4A-NA-C1A	5.43	109.16	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1104	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
14	a	1119	CLA	C2C-C1C-NC	5.43	115.69	109.98
14	B	1232	CLA	C1C-C2C-C3C	-5.43	101.27	106.98
14	a	1129	CLA	C2C-C1C-NC	5.43	115.69	109.98
14	U	1502	CLA	C2D-C1D-ND	5.43	115.50	110.13
14	b	1203	CLA	C2C-C1C-NC	5.43	115.68	109.98
14	l	1501	CLA	C2D-C1D-ND	5.43	115.50	110.13
18	M	4021	BCR	C15-C14-C13	-5.43	119.67	127.28
14	A	1130	CLA	C2C-C1C-NC	5.43	115.68	109.98
18	A	4011	BCR	C7-C8-C9	-5.43	118.21	126.23
14	l	1502	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
14	B	1021	CLA	C2C-C1C-NC	5.42	115.68	109.98
14	A	1124	CLA	C2C-C1C-NC	5.42	115.68	109.98
14	a	1113	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
14	A	1136	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
14	b	1218	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
14	A	1103	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
14	b	1220	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
14	G	1112	CLA	C4A-NA-C1A	5.42	109.15	106.68
14	U	1502	CLA	C4A-NA-C1A	5.42	109.15	106.68
14	b	1232	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
14	G	1115	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
14	b	1202	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
14	H	1203	CLA	C2C-C1C-NC	5.42	115.67	109.98
14	b	1235	CLA	C2C-C1C-NC	5.42	115.67	109.98
14	A	1110	CLA	C2D-C1D-ND	5.42	115.49	110.13
14	G	1106	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
14	H	1211	CLA	C2C-C1C-NC	5.41	115.67	109.98
14	H	1207	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
14	H	1223	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	a	1110	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	a	1115	CLA	C3B-C2B-C1B	-5.41	100.79	107.17
14	H	1201	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	B	1220	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
18	V	4021	BCR	C15-C14-C13	-5.41	119.69	127.28
14	A	1130	CLA	C3B-C2B-C1B	-5.41	100.80	107.17
14	B	1201	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	a	1131	CLA	C1C-C2C-C3C	-5.41	101.29	106.98
14	a	1130	CLA	C3B-C2B-C1B	-5.41	100.80	107.17
18	G	4011	BCR	C7-C8-C9	-5.41	118.24	126.23
14	H	1231	CLA	C3B-C2B-C1B	-5.41	100.80	107.17
14	G	1113	CLA	C1C-C2C-C3C	-5.40	101.30	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1233	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	A	1131	CLA	C4A-NA-C1A	5.40	109.14	106.68
14	G	1116	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	A	1012	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
14	a	1124	CLA	C2C-C1C-NC	5.40	115.65	109.98
14	B	1022	CLA	C2D-C1D-ND	5.39	115.47	110.13
14	H	1023	CLA	O2D-CGD-CBD	5.39	120.66	111.23
14	H	1220	CLA	C3D-C2D-C1D	-5.39	98.47	105.83
14	B	1210	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
14	b	1201	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
14	G	1103	CLA	C3B-C2B-C1B	-5.39	100.82	107.17
14	G	1124	CLA	C2C-C1C-NC	5.39	115.64	109.98
14	W	1701	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	b	1022	CLA	C3B-C2B-C1B	-5.39	100.82	107.17
14	b	1223	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
14	G	1110	CLA	C2D-C1D-ND	5.39	115.46	110.13
14	a	1136	CLA	C3D-C2D-C1D	-5.39	98.48	105.83
14	B	1209	CLA	C1C-C2C-C3C	-5.39	101.32	106.98
14	G	1136	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
14	B	1022	CLA	C3B-C2B-C1B	-5.38	100.82	107.17
15	B	1230	F6C	C2C-C1C-NC	5.38	115.91	110.33
14	b	1022	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	A	1140	CLA	C4A-NA-C1A	5.38	109.14	106.68
14	G	1117	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	b	1207	CLA	C3D-C2D-C1D	-5.38	98.48	105.83
14	A	1116	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	a	1103	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
14	H	1212	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	B	1223	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	a	1116	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	A	1115	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
14	B	1021	CLA	O2D-CGD-CBD	5.38	120.63	111.23
14	B	1212	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	A	1132	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	H	1233	CLA	C1C-C2C-C3C	-5.38	101.33	106.98
14	H	1021	CLA	O2D-CGD-CBD	5.38	120.63	111.23
14	B	1233	CLA	C1C-C2C-C3C	-5.38	101.33	106.98
15	G	1120	F6C	C2C-C1C-NC	5.37	115.90	110.33
14	H	1211	CLA	C3B-C2B-C1B	-5.37	100.83	107.17
14	b	1021	CLA	O2D-CGD-CBD	5.37	120.62	111.23
14	B	1203	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	B	1207	CLA	C3D-C2D-C1D	-5.37	98.50	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1130	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
14	H	1228	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
14	H	1218	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
14	G	1125	CLA	C2C-C1C-NC	5.37	115.62	109.98
14	b	1220	CLA	C2D-C1D-ND	5.37	115.44	110.13
14	B	1023	CLA	O2D-CGD-CBD	5.37	120.61	111.23
14	H	1210	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	b	1211	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
14	b	1212	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	H	1202	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	H	1209	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	G	1117	CLA	C4A-NA-C1A	5.36	109.12	106.68
14	b	1227	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	b	1210	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
14	H	1012	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
14	H	1203	CLA	C4A-NA-C1A	5.36	109.12	106.68
14	B	1211	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
14	H	1227	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	B	1218	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
14	x	1701	CLA	C4A-NA-C1A	5.36	109.12	106.68
14	A	1102	CLA	C3B-C2B-C1B	-5.36	100.86	107.17
14	G	1132	CLA	C1C-C2C-C3C	-5.36	101.35	106.98
14	B	1220	CLA	C2D-C1D-ND	5.35	115.42	110.13
14	A	1117	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
18	H	4012	BCR	C1-C6-C5	-5.35	115.32	122.64
14	H	1012	CLA	C2D-C1D-ND	5.35	115.42	110.13
14	a	1012	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
14	B	1212	CLA	C4A-NA-C1A	5.35	109.12	106.68
14	H	1228	CLA	C4A-NA-C1A	5.35	109.12	106.68
14	b	1228	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
14	b	1223	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
14	G	1101	CLA	C2C-C1C-NC	5.35	115.60	109.98
14	a	1117	CLA	C1C-C2C-C3C	-5.35	101.36	106.98
18	B	4012	BCR	C1-C6-C5	-5.34	115.33	122.64
14	H	1236	CLA	C1D-ND-C4D	-5.34	102.56	106.31
14	b	1023	CLA	O2D-CGD-CBD	5.34	120.57	111.23
14	a	1012	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
14	B	1228	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	a	1101	CLA	C2C-C1C-NC	5.34	115.59	109.98
14	a	1102	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
14	a	1137	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
14	b	1210	CLA	C3D-C2D-C1D	-5.34	98.54	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1210	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	L	1501	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
14	b	1209	CLA	C1C-C2C-C3C	-5.34	101.36	106.98
14	A	1101	CLA	C2C-C1C-NC	5.34	115.59	109.98
14	b	1218	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	A	1108	CLA	C4A-NA-C1A	5.34	109.11	106.68
14	H	1202	CLA	C4A-NA-C1A	5.34	109.11	106.68
14	H	1212	CLA	C4A-NA-C1A	5.34	109.11	106.68
14	a	1102	CLA	C4A-NA-C1A	5.34	109.11	106.68
14	a	1133	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
14	B	1223	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
14	H	1223	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	B	1221	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
15	b	1230	F6C	C1A-C2A-C3A	-5.34	101.35	106.97
18	b	4012	BCR	C1-C6-C5	-5.33	115.35	122.64
14	A	1012	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
14	L	1501	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
14	a	1128	CLA	C4A-NA-C1A	5.33	109.11	106.68
14	H	1203	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
14	A	1102	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
15	H	1230	F6C	C1A-C2A-C3A	-5.33	101.36	106.97
14	A	1107	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
14	a	1013	CLA	C1D-ND-C4D	-5.33	102.57	106.31
14	G	1137	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
14	a	1117	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	G	1128	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	a	1131	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	b	1203	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
14	G	1102	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
14	B	1236	CLA	C2D-C1D-ND	5.32	115.39	110.13
14	a	1107	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
14	G	1133	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	H	1220	CLA	C2D-C1D-ND	5.32	115.39	110.13
14	B	1236	CLA	C1D-ND-C4D	-5.32	102.58	106.31
14	G	1012	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
14	a	1102	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
14	G	1012	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	x	1701	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	B	1227	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	a	1132	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	X	1701	CLA	C4A-NA-C1A	5.31	109.10	106.68
14	a	1115	CLA	O2D-CGD-CBD	5.31	120.52	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1137	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	U	1501	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	G	1102	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	a	1137	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	b	1221	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	B	1203	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	H	1223	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	A	1125	CLA	C2C-C1C-NC	5.31	115.56	109.98
14	a	1013	CLA	O2D-CGD-CBD	5.31	120.51	111.23
14	b	1236	CLA	C1D-ND-C4D	-5.31	102.59	106.31
14	H	1234	CLA	O2D-CGD-CBD	5.31	120.51	111.23
14	A	1137	CLA	C3B-C2B-C1B	-5.31	100.92	107.17
14	H	1218	CLA	C2D-C1D-ND	5.30	115.38	110.13
14	B	1223	CLA	C3D-C2D-C1D	-5.30	98.59	105.83
14	l	1501	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
14	A	1136	CLA	C2D-C1D-ND	5.30	115.38	110.13
14	A	1013	CLA	O2D-CGD-CBD	5.30	120.50	111.23
14	H	1221	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
14	H	1236	CLA	C2D-C1D-ND	5.30	115.37	110.13
14	H	1226	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
14	b	1223	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	G	1131	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	H	1229	CLA	CAA-C2A-C3A	-5.30	98.68	113.00
14	A	1131	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	A	1133	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	B	1229	CLA	CAA-C2A-C3A	-5.30	98.68	113.00
14	b	1229	CLA	CAA-C2A-C3A	-5.30	98.68	113.00
14	U	1501	CLA	CAA-C2A-C3A	-5.30	98.68	113.00
14	A	1013	CLA	C1D-ND-C4D	-5.30	102.60	106.31
14	X	1701	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
15	B	1230	F6C	C1A-C2A-C3A	-5.29	101.39	106.97
14	H	1221	CLA	C2C-C1C-NC	5.29	115.54	109.98
14	l	1501	CLA	CAA-C2A-C3A	-5.29	98.69	113.00
14	B	1021	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
14	A	1137	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
14	B	1224	CLA	C2D-C1D-ND	5.29	115.36	110.13
14	x	1701	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
14	G	1138	CLA	C4A-NA-C1A	5.29	109.09	106.68
14	A	1115	CLA	O2D-CGD-CBD	5.29	120.48	111.23
14	B	1234	CLA	O2D-CGD-CBD	5.29	120.48	111.23
14	b	1236	CLA	C2D-C1D-ND	5.29	115.36	110.13
14	b	1234	CLA	O2D-CGD-CBD	5.29	120.48	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1115	CLA	O2D-CGD-CBD	5.29	120.47	111.23
14	l	1501	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
14	L	1501	CLA	CAA-C2A-C3A	-5.29	98.71	113.00
14	H	1233	CLA	O2D-CGD-CBD	5.29	120.47	111.23
14	b	1218	CLA	C2D-C1D-ND	5.29	115.36	110.13
14	A	1107	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	A	1138	CLA	C4A-NA-C1A	5.28	109.09	106.68
14	b	1203	CLA	C4A-NA-C1A	5.28	109.09	106.68
14	b	1233	CLA	O2D-CGD-CBD	5.28	120.47	111.23
14	B	1218	CLA	C2D-C1D-ND	5.28	115.36	110.13
14	b	1224	CLA	C2D-C1D-ND	5.28	115.36	110.13
14	X	1701	CLA	C3B-C2B-C1B	-5.28	100.94	107.17
14	b	1218	CLA	C3B-C2B-C1B	-5.28	100.94	107.17
14	U	1501	CLA	C3B-C2B-C1B	-5.28	100.94	107.17
14	G	1107	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
14	a	1124	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
14	G	1136	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	G	1107	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
14	H	1224	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	a	1136	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	G	1013	CLA	O2D-CGD-CBD	5.28	120.46	111.23
14	b	1213	CLA	O2A-CGA-O1A	-5.28	110.43	123.63
14	B	1023	CLA	C1D-ND-C4D	-5.28	102.61	106.31
14	a	1107	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
14	B	1202	CLA	C4A-NA-C1A	5.27	109.08	106.68
14	a	1138	CLA	C4A-NA-C1A	5.27	109.08	106.68
15	A	1120	F6C	CAA-C2A-C1A	-5.27	113.28	128.01
14	B	1226	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	b	1228	CLA	C4A-NA-C1A	5.27	109.08	106.68
14	A	1126	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	U	1501	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	B	1218	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
18	I	4020	BCR	C20-C19-C18	5.27	140.81	126.36
14	H	1021	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	H	1239	CLA	O2A-CGA-O1A	-5.27	110.45	123.63
14	b	1210	CLA	CAC-C3C-C4C	5.27	131.64	124.79
14	L	1501	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	W	1701	CLA	C3B-C2B-C1B	-5.27	100.96	107.17
14	L	1503	CLA	O2D-CGD-CBD	5.26	120.43	111.23
14	A	1124	CLA	C1C-C2C-C3C	-5.26	101.44	106.98
14	b	1021	CLA	C1C-C2C-C3C	-5.26	101.44	106.98
14	a	1125	CLA	C2C-C1C-NC	5.26	115.51	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1117	CLA	C4A-NA-C1A	5.26	109.08	106.68
14	B	1233	CLA	O2D-CGD-CBD	5.26	120.43	111.23
14	a	1104	CLA	O2D-CGD-CBD	5.26	120.43	111.23
14	B	1213	CLA	O2A-CGA-O1A	-5.26	110.47	123.63
14	b	1023	CLA	C1D-ND-C4D	-5.26	102.62	106.31
18	A	4001	BCR	C28-C27-C26	-5.26	104.67	114.06
14	H	1213	CLA	O2A-CGA-O1A	-5.26	110.47	123.63
14	A	1104	CLA	O2D-CGD-CBD	5.26	120.42	111.23
14	A	1108	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
18	R	4020	BCR	C20-C19-C18	5.26	140.78	126.36
14	A	1123	CLA	C4A-NA-C1A	5.26	109.08	106.68
14	H	1218	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
14	b	1221	CLA	C2C-C1C-NC	5.26	115.50	109.98
14	b	1202	CLA	C4A-NA-C1A	5.26	109.08	106.68
14	k	1401	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
14	l	1503	CLA	O2D-CGD-CBD	5.26	120.42	111.23
14	B	1210	CLA	CAC-C3C-C4C	5.26	131.63	124.79
14	B	1212	CLA	C3B-C2B-C1B	-5.25	100.97	107.17
14	l	1501	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	B	1205	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
14	T	1401	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
18	G	4001	BCR	C28-C27-C26	-5.25	104.69	114.06
14	A	1119	CLA	C4A-NA-C1A	5.25	109.08	106.68
14	B	1239	CLA	O2A-CGA-O1A	-5.25	110.49	123.63
14	G	1013	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	G	1135	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	b	1226	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	W	1701	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
15	G	1120	F6C	CAA-C2A-C1A	-5.25	113.35	128.01
14	A	1140	CLA	C2D-C1D-ND	5.25	115.32	110.13
18	i	4020	BCR	C20-C19-C18	5.25	140.75	126.36
14	B	1228	CLA	C4A-NA-C1A	5.25	109.07	106.68
14	G	1104	CLA	O2D-CGD-CBD	5.25	120.40	111.23
14	U	1503	CLA	O2D-CGD-CBD	5.25	120.40	111.23
14	a	1126	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	H	1210	CLA	CAC-C3C-C4C	5.24	131.61	124.79
14	b	1205	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
14	H	1215	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
14	G	1013	CLA	C1D-ND-C4D	-5.24	102.63	106.31
14	A	1101	CLA	C3B-C2B-C1B	-5.24	100.99	107.17
14	H	1222	CLA	O2A-CGA-O1A	-5.24	110.52	123.63
15	a	1120	F6C	CAA-C2A-C1A	-5.24	113.37	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4001	BCR	C28-C27-C26	-5.24	104.71	114.06
14	A	1102	CLA	C4A-NA-C1A	5.24	109.07	106.68
14	G	1108	CLA	O2D-CGD-CBD	5.24	120.39	111.23
14	H	1224	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
14	b	1212	CLA	C4A-NA-C1A	5.24	109.07	106.68
14	B	1215	CLA	C3D-C2D-C1D	-5.24	98.69	105.83
14	B	1224	CLA	C3D-C2D-C1D	-5.24	98.69	105.83
14	A	1138	CLA	C1C-C2C-C3C	-5.23	101.47	106.98
14	G	1124	CLA	C1C-C2C-C3C	-5.23	101.47	106.98
14	K	1401	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	b	1208	CLA	O2A-CGA-O1A	-5.23	110.53	123.63
14	A	1115	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	a	1013	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	a	1127	CLA	C1C-C2C-C3C	-5.23	101.47	106.98
14	A	1013	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
14	B	1222	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
14	b	1231	CLA	O2D-CGD-CBD	5.23	120.38	111.23
14	H	1231	CLA	O2D-CGD-CBD	5.23	120.38	111.23
14	G	1126	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	G	1012	CLA	O2D-CGD-CBD	5.23	120.38	111.23
14	H	1208	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
14	b	1212	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
14	b	1239	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
14	G	1108	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
14	G	1138	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	b	1222	CLA	O2A-CGA-O1A	-5.23	110.55	123.63
14	G	1112	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
14	a	1012	CLA	O2D-CGD-CBD	5.23	120.37	111.23
14	H	1023	CLA	C1D-ND-C4D	-5.23	102.64	106.31
14	H	1012	CLA	C2C-C1C-NC	5.23	115.47	109.98
14	a	1140	CLA	C4A-NA-C1A	5.23	109.06	106.68
14	H	1212	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
14	B	1221	CLA	C2C-C1C-NC	5.23	115.47	109.98
14	G	1101	CLA	C3B-C2B-C1B	-5.22	101.01	107.17
14	B	1231	CLA	O2D-CGD-CBD	5.22	120.36	111.23
14	G	1102	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	G	1108	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	G	1140	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	H	1023	CLA	C2C-C1C-NC	5.22	115.47	109.98
14	B	1208	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
14	H	1226	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
14	B	1211	CLA	C1C-C2C-C3C	-5.22	101.49	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1127	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
14	a	1108	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	b	1216	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	B	1023	CLA	C2C-C1C-NC	5.22	115.46	109.98
15	G	1120	F6C	C3D-C2D-C1D	-5.22	98.28	105.83
14	A	1136	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
14	H	1216	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	b	1226	CLA	O2A-CGA-O1A	-5.21	110.58	123.63
14	A	1110	CLA	C4A-NA-C1A	5.21	109.06	106.68
14	G	1115	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	b	1224	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	A	1111	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
14	k	1401	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
14	B	1229	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
14	b	1215	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	a	1111	CLA	O2A-CGA-O1A	-5.21	110.59	123.63
14	H	1235	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	a	1138	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	A	1136	CLA	O2A-CGA-CBA	5.21	127.72	111.83
14	A	1127	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	G	1140	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	H	1219	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	b	1211	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	A	1112	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
14	G	1119	CLA	C3D-C2D-C1D	-5.21	98.73	105.83
14	b	1238	CLA	C2C-C1C-NC	5.21	115.45	109.98
14	a	1112	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	H	1229	CLA	O2A-CGA-O1A	-5.20	110.61	123.63
14	G	1103	CLA	C2D-C1D-ND	5.20	115.28	110.13
14	H	1205	CLA	C3B-C2B-C1B	-5.20	101.03	107.17
14	a	1101	CLA	C3B-C2B-C1B	-5.20	101.03	107.17
14	A	1110	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	A	1135	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	A	1119	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	A	1135	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	b	1209	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
14	b	1229	CLA	O2A-CGA-O1A	-5.20	110.62	123.63
15	A	1120	F6C	C3D-C2D-C1D	-5.20	98.30	105.83
14	b	1022	CLA	C2C-C1C-NC	5.20	115.44	109.98
14	a	1108	CLA	O2D-CGD-CBD	5.20	120.32	111.23
14	a	1109	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	B	1226	CLA	O2A-CGA-O1A	-5.20	110.62	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1109	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
18	L	4022	BCR	C24-C23-C22	-5.20	118.54	126.23
14	a	1136	CLA	O2A-CGA-CBA	5.20	127.69	111.83
14	B	1235	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	B	1222	CLA	C2D-C1D-ND	5.20	115.27	110.13
14	B	1022	CLA	C2C-C1C-NC	5.20	115.44	109.98
14	G	1136	CLA	O2A-CGA-CBA	5.20	127.68	111.83
14	G	1111	CLA	O2A-CGA-O1A	-5.20	110.63	123.63
14	a	1103	CLA	C2D-C1D-ND	5.20	115.27	110.13
14	A	1109	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	G	1109	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
18	U	4022	BCR	C24-C23-C22	-5.20	118.55	126.23
14	L	1503	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	a	1115	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
14	G	1110	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	b	1235	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	b	1202	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	B	1206	CLA	C2D-C1D-ND	5.19	115.27	110.13
14	b	1229	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	B	1209	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
14	a	1136	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	H	1202	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
18	l	4022	BCR	C24-C23-C22	-5.19	118.56	126.23
14	a	1110	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	a	1140	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	b	1023	CLA	C2C-C1C-NC	5.19	115.43	109.98
14	A	1103	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	A	1108	CLA	O2D-CGD-CBD	5.18	120.29	111.23
14	H	1211	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	a	1109	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
14	H	1206	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	b	1233	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	G	1110	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
14	G	1125	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
14	a	1110	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
14	l	1503	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	U	1503	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	B	1217	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
14	A	1012	CLA	O2D-CGD-CBD	5.18	120.29	111.23
14	A	1107	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	a	1107	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	H	1238	CLA	C2C-C1C-NC	5.18	115.42	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1401	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
14	G	1124	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	B	1202	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
14	B	1216	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	B	1219	CLA	C2D-C1D-ND	5.18	115.25	110.13
14	b	1222	CLA	C2D-C1D-ND	5.18	115.25	110.13
14	L	1503	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
14	A	1110	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
14	K	1401	CLA	C3B-C2B-C1B	-5.18	101.07	107.17
14	b	1206	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
14	G	1115	CLA	O2A-CGA-O1A	-5.18	110.68	123.63
14	a	1108	CLA	C1C-C2C-C3C	-5.18	101.54	106.98
14	G	1135	CLA	O2D-CGD-CBD	5.18	120.28	111.23
14	G	1110	CLA	C4A-NA-C1A	5.17	109.04	106.68
14	b	1219	CLA	C2D-C1D-ND	5.17	115.24	110.13
14	G	1109	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
14	H	1217	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
15	a	1120	F6C	C3D-C2D-C1D	-5.17	98.34	105.83
14	H	1233	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
15	A	1121	F6C	CMA-C3A-C4A	-5.17	115.62	124.73
14	H	1012	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
15	a	1121	F6C	CMA-C3A-C4A	-5.17	115.63	124.73
14	a	1108	CLA	C4A-NA-C1A	5.17	109.04	106.68
14	b	1217	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
14	b	1204	CLA	O2A-CGA-O1A	-5.17	110.70	123.63
14	b	1228	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
14	a	1135	CLA	O2D-CGD-CBD	5.17	120.26	111.23
14	G	1123	CLA	C4A-NA-C1A	5.17	109.04	106.68
14	a	1139	CLA	O2D-CGD-CBD	5.16	120.26	111.23
14	B	1228	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
14	A	1115	CLA	O2A-CGA-O1A	-5.16	110.71	123.63
14	H	1204	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
15	G	1121	F6C	CMA-C3A-C4A	-5.16	115.64	124.73
14	a	1119	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	H	1234	CLA	C4A-NA-C1A	5.16	109.03	106.68
14	G	1135	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	H	1206	CLA	C2D-C1D-ND	5.16	115.23	110.13
14	B	1204	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
14	H	1229	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	B	1229	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	b	1213	CLA	C4A-NA-C1A	5.16	109.03	106.68
14	B	1238	CLA	C2C-C1C-NC	5.16	115.40	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1121	F6C	O2D-CGD-CBD	5.16	120.25	111.23
14	B	1022	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	G	1136	CLA	C1C-C2C-C3C	-5.16	101.56	106.98
14	b	1022	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
15	G	1121	F6C	O2D-CGD-CBD	5.16	120.24	111.23
14	A	1125	CLA	C3B-C2B-C1B	-5.15	101.09	107.17
14	B	1206	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	a	1110	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	a	1115	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
14	H	1228	CLA	C3B-C2B-C1B	-5.15	101.09	107.17
14	A	1108	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	b	1206	CLA	C2D-C1D-ND	5.15	115.22	110.13
14	B	1213	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
14	A	1139	CLA	O2D-CGD-CBD	5.15	120.23	111.23
14	H	1209	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
14	A	1115	CLA	C1C-C2C-C3C	-5.15	101.57	106.98
14	a	1130	CLA	C1C-C2C-C3C	-5.15	101.57	106.98
14	G	1108	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	G	1128	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	H	1223	CLA	C2D-C1D-ND	5.14	115.22	110.13
14	H	1213	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	a	1125	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
14	H	1222	CLA	C2D-C1D-ND	5.14	115.22	110.13
15	B	1237	F6C	CAA-C2A-C1A	-5.14	113.64	128.01
14	a	1135	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	b	1216	CLA	C1C-C2C-C3C	-5.14	101.57	106.98
14	H	1213	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
15	a	1121	F6C	O2D-CGD-CBD	5.14	120.22	111.23
14	B	1221	CLA	O2D-CGD-CBD	5.14	120.21	111.23
14	H	1221	CLA	O2D-CGD-CBD	5.14	120.21	111.23
14	b	1224	CLA	C2C-C1C-NC	5.14	115.38	109.98
14	b	1231	CLA	C2C-C1C-NC	5.14	115.38	109.98
14	G	1139	CLA	O2D-CGD-CBD	5.14	120.21	111.23
14	A	1101	CLA	C2D-C1D-ND	5.14	115.21	110.13
14	H	1235	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
14	H	1231	CLA	C2C-C1C-NC	5.13	115.38	109.98
14	H	1219	CLA	C3D-C2D-C1D	-5.13	98.82	105.83
14	B	1235	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	a	1123	CLA	C4A-NA-C1A	5.13	109.02	106.68
14	l	1503	CLA	C4A-NA-C1A	5.13	109.02	106.68
14	a	1128	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
14	a	1124	CLA	C3D-C2D-C1D	-5.13	98.83	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1140	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	b	1234	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
15	b	1237	F6C	C2D-C1D-ND	5.13	115.37	109.98
14	B	1234	CLA	C4A-NA-C1A	5.13	109.02	106.68
14	b	1213	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	B	1206	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	G	1130	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
14	b	1202	CLA	O2A-CGA-CBA	5.13	127.47	111.83
14	b	1221	CLA	O2D-CGD-CBD	5.13	120.19	111.23
14	b	1235	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	A	1135	CLA	O2D-CGD-CBD	5.13	120.19	111.23
14	B	1202	CLA	O2A-CGA-CBA	5.13	127.47	111.83
14	A	1128	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
14	U	1503	CLA	C1C-C2C-C3C	-5.13	101.59	106.98
14	A	1124	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
15	b	1237	F6C	CAA-C2A-C1A	-5.12	113.69	128.01
14	H	1234	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
15	H	1237	F6C	CAA-C2A-C1A	-5.12	113.69	128.01
14	G	1115	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
14	a	1135	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	U	1503	CLA	C4A-NA-C1A	5.12	109.02	106.68
14	A	1130	CLA	C1C-C2C-C3C	-5.12	101.59	106.98
14	G	1140	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	l	1503	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
14	A	1101	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	a	1115	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
14	b	1213	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
14	G	1107	CLA	C4A-NA-C1A	5.12	109.01	106.68
14	a	1118	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
14	H	1202	CLA	O2A-CGA-CBA	5.12	127.43	111.83
14	B	1233	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
14	A	1127	CLA	O2D-CGD-CBD	5.11	120.17	111.23
14	B	1231	CLA	C2C-C1C-NC	5.11	115.35	109.98
14	x	1701	CLA	C2D-C1D-ND	5.11	115.19	110.13
18	A	4011	BCR	C20-C19-C18	5.11	140.38	126.36
14	A	1118	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
14	G	1125	CLA	O2A-CGA-O1A	-5.11	110.84	123.63
14	a	1140	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
18	G	4011	BCR	C20-C19-C18	5.11	140.37	126.36
14	A	1125	CLA	O2A-CGA-O1A	-5.11	110.85	123.63
14	G	1127	CLA	O2D-CGD-CBD	5.11	120.16	111.23
14	b	1206	CLA	C3D-C2D-C1D	-5.11	98.86	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1234	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
15	B	1237	F6C	C2D-C1D-ND	5.11	115.35	109.98
14	b	1219	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	a	1106	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	B	1213	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
14	X	1701	CLA	C2D-C1D-ND	5.10	115.18	110.13
14	a	1101	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	B	1224	CLA	C2C-C1C-NC	5.10	115.34	109.98
14	G	1101	CLA	C2D-C1D-ND	5.10	115.17	110.13
15	H	1237	F6C	C2D-C1D-ND	5.10	115.34	109.98
14	G	1101	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	B	1223	CLA	C4A-NA-C1A	5.10	109.00	106.68
14	a	1119	CLA	C4A-NA-C1A	5.10	109.00	106.68
14	l	1501	CLA	O2A-CGA-O1A	-5.10	110.88	123.63
14	H	1206	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	A	1127	CLA	C4A-NA-C1A	5.10	109.00	106.68
14	H	1213	CLA	C4A-NA-C1A	5.10	109.00	106.68
14	G	1107	CLA	O2D-CGD-CBD	5.10	120.14	111.23
14	B	1202	CLA	C2D-C1D-ND	5.10	115.17	110.13
14	a	1125	CLA	O2A-CGA-O1A	-5.09	110.88	123.63
14	H	1210	CLA	C2D-C1D-ND	5.09	115.17	110.13
14	B	1219	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	W	1701	CLA	C2D-C1D-ND	5.09	115.17	110.13
14	A	1105	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	B	1201	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
14	a	1101	CLA	C2D-C1D-ND	5.09	115.17	110.13
14	L	1503	CLA	C1C-C2C-C3C	-5.09	101.62	106.98
18	a	4011	BCR	C20-C19-C18	5.09	140.33	126.36
14	G	1118	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
14	a	1127	CLA	O2D-CGD-CBD	5.09	120.13	111.23
14	H	1201	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	B	1220	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
14	b	1223	CLA	C2D-C1D-ND	5.09	115.16	110.13
14	a	1122	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	a	1140	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
14	G	1104	CLA	C1D-ND-C4D	-5.09	102.74	106.31
15	A	1120	F6C	C1C-C2C-C3C	-5.09	100.99	106.82
14	b	1209	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	G	1140	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
14	H	1231	CLA	O2A-CGA-O1A	-5.09	110.91	123.63
14	G	1122	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
14	H	1202	CLA	C2D-C1D-ND	5.08	115.16	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1231	CLA	O2A-CGA-O1A	-5.08	110.91	123.63
14	B	1232	CLA	C4A-NA-C1A	5.08	109.00	106.68
14	b	1202	CLA	C2D-C1D-ND	5.08	115.16	110.13
14	B	1217	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	H	1224	CLA	C2C-C1C-NC	5.08	115.32	109.98
14	b	1219	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	U	1501	CLA	O2A-CGA-O1A	-5.08	110.92	123.63
14	a	1111	CLA	C2D-C1D-ND	5.08	115.15	110.13
14	b	1217	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	a	1105	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	G	1106	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	b	1234	CLA	C4A-NA-C1A	5.08	109.00	106.68
18	b	4004	BCR	C7-C8-C9	-5.08	118.72	126.23
14	b	1201	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	H	1219	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	H	1208	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	A	1106	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	G	1119	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	B	1209	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	B	1223	CLA	C2D-C1D-ND	5.07	115.15	110.13
14	H	1228	CLA	C2D-C1D-ND	5.07	115.15	110.13
14	L	1501	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
14	b	1231	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
18	H	4004	BCR	C7-C8-C9	-5.07	118.73	126.23
14	a	1122	CLA	C2D-C1D-ND	5.07	115.15	110.13
14	A	1104	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
14	B	1214	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	A	1107	CLA	O2D-CGD-CBD	5.07	120.09	111.23
14	A	1122	CLA	C3D-C2D-C1D	-5.07	98.92	105.83
14	H	1216	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
14	b	1220	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
14	B	1213	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	a	1104	CLA	C1D-ND-C4D	-5.06	102.76	106.31
14	H	1223	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	H	1214	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
18	B	4004	BCR	C7-C8-C9	-5.06	118.75	126.23
14	a	1013	CLA	O2A-CGA-O1A	-5.06	110.97	123.63
14	B	1208	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
15	a	1120	F6C	C1C-C2C-C3C	-5.06	101.02	106.82
14	H	1209	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
14	A	1140	CLA	C1C-C2C-C3C	-5.06	101.66	106.98
14	H	1217	CLA	C3D-C2D-C1D	-5.06	98.93	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1102	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
14	B	1238	CLA	O2A-CGA-O1A	-5.06	110.98	123.63
14	G	1111	CLA	C2D-C1D-ND	5.06	115.13	110.13
14	a	1107	CLA	O2D-CGD-CBD	5.05	120.06	111.23
14	G	1122	CLA	C2D-C1D-ND	5.05	115.13	110.13
14	b	1238	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
14	G	1013	CLA	O2A-CGA-O1A	-5.05	110.99	123.63
14	G	1104	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	b	1210	CLA	C2D-C1D-ND	5.05	115.12	110.13
14	G	1105	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	H	1238	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	a	1117	CLA	O2D-CGD-CBD	5.05	120.05	111.23
14	b	1228	CLA	C2D-C1D-ND	5.05	115.12	110.13
14	B	1216	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
14	a	1128	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	a	1104	CLA	O2A-CGA-O1A	-5.05	111.01	123.63
14	B	1219	CLA	C1C-C2C-C3C	-5.04	101.67	106.98
14	G	1139	CLA	C2D-C1D-ND	5.04	115.12	110.13
14	b	1208	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	A	1129	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
14	G	1013	CLA	O2A-C1-C2	5.04	127.51	108.11
14	G	1117	CLA	O2D-CGD-CBD	5.04	120.04	111.23
14	H	1232	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	G	1105	CLA	O2D-CGD-CBD	5.04	120.04	111.23
14	b	1225	CLA	C4A-NA-C1A	5.04	108.98	106.68
14	b	1214	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
14	G	1128	CLA	O2A-CGA-O1A	-5.04	111.03	123.63
14	B	1228	CLA	C2D-C1D-ND	5.04	115.11	110.13
14	a	1116	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	U	1502	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
14	a	1128	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	A	1013	CLA	O2A-CGA-O1A	-5.04	111.03	123.63
14	A	1128	CLA	O2A-CGA-O1A	-5.04	111.03	123.63
14	A	1111	CLA	C2D-C1D-ND	5.03	115.11	110.13
15	G	1120	F6C	C1C-C2C-C3C	-5.03	101.05	106.82
14	A	1117	CLA	O2D-CGD-CBD	5.03	120.03	111.23
14	A	1105	CLA	O2D-CGD-CBD	5.03	120.03	111.23
14	a	1123	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
14	G	1129	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	H	1220	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	H	1214	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
14	a	1013	CLA	O2A-C1-C2	5.03	127.46	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1102	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	A	1013	CLA	O2A-C1-C2	5.03	127.46	108.11
14	B	1232	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	G	1116	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	A	1123	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
14	H	1231	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	G	1102	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	A	1108	CLA	C2D-C1D-ND	5.03	115.10	110.13
14	B	1210	CLA	C2D-C1D-ND	5.02	115.10	110.13
14	G	1128	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	a	1105	CLA	O2D-CGD-CBD	5.02	120.01	111.23
14	a	1129	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	b	1232	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	b	1207	CLA	O2A-CGA-O1A	-5.02	110.42	123.33
18	H	4010	BCR	C24-C23-C22	-5.02	118.81	126.23
14	A	1128	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	a	1116	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
14	B	1222	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	b	1214	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	G	1117	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	B	1216	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
18	b	4010	BCR	C24-C23-C22	-5.01	118.82	126.23
14	b	1209	CLA	C4A-NA-C1A	5.01	108.97	106.68
14	a	1132	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	B	1231	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	G	1123	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
14	b	1216	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	A	1139	CLA	C2D-C1D-ND	5.01	115.08	110.13
14	a	1117	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
14	H	1207	CLA	O2A-CGA-O1A	-5.01	110.45	123.33
14	A	1122	CLA	C2D-C1D-ND	5.01	115.08	110.13
14	A	1116	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
14	B	1207	CLA	O2A-CGA-O1A	-5.00	110.47	123.33
14	A	1132	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	B	1201	CLA	O2A-CGA-CBA	5.00	127.08	111.83
14	H	1209	CLA	C4A-NA-C1A	5.00	108.96	106.68
14	b	1232	CLA	C4A-NA-C1A	5.00	108.96	106.68
14	B	1222	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	B	1221	CLA	C2D-C1D-ND	5.00	115.07	110.13
18	B	4010	BCR	C24-C23-C22	-5.00	118.84	126.23
14	A	1137	CLA	O2A-CGA-O1A	-5.00	110.48	123.33
14	G	1137	CLA	O2A-CGA-O1A	-5.00	110.48	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1135	CLA	O2A-CGA-O1A	-4.99	111.14	123.63
14	b	1201	CLA	O2A-CGA-CBA	4.99	127.06	111.83
14	b	1229	CLA	C2D-C1D-ND	4.99	115.07	110.13
14	A	1123	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	A	1135	CLA	O2A-CGA-O1A	-4.99	111.14	123.63
14	B	1214	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
14	G	1132	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	G	1124	CLA	C2D-C1D-ND	4.99	115.06	110.13
14	k	1401	CLA	C2D-C1D-ND	4.99	115.06	110.13
14	b	1231	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	a	1105	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
18	i	4018	BCR	C24-C23-C22	-4.99	118.86	126.23
14	a	1127	CLA	C4A-NA-C1A	4.99	108.95	106.68
14	L	1502	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
14	B	1228	CLA	O2D-CGD-CBD	4.99	119.94	111.23
14	H	1201	CLA	O2A-CGA-CBA	4.98	127.03	111.83
14	l	1502	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
14	G	1012	CLA	C2D-C1D-ND	4.98	115.06	110.13
14	b	1233	CLA	C4A-NA-C1A	4.98	108.95	106.68
14	H	1205	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	B	1205	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	a	1114	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	a	1137	CLA	O2A-CGA-O1A	-4.98	110.53	123.33
14	A	1116	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
14	H	1216	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	A	1116	CLA	O2A-CGA-O1A	-4.98	111.18	123.63
14	b	1222	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	b	1205	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	G	1135	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
14	B	1236	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
14	G	1116	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
14	H	1236	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
14	a	1139	CLA	C2D-C1D-ND	4.97	115.05	110.13
14	A	1117	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	A	1104	CLA	C1D-ND-C4D	-4.97	102.83	106.31
14	x	1701	CLA	O2D-CGD-CBD	4.97	119.91	111.23
14	a	1116	CLA	O2A-CGA-O1A	-4.97	111.21	123.63
14	L	1503	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	a	1105	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	T	1401	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	a	1115	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	G	1116	CLA	O2A-CGA-O1A	-4.96	111.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1012	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	a	1138	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	a	1123	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	1105	CLA	C2D-C1D-ND	4.96	115.03	110.13
14	W	1701	CLA	O2D-CGD-CBD	4.96	119.90	111.23
14	U	1503	CLA	C2D-C1D-ND	4.95	115.03	110.13
13	a	1011	CL0	CAA-C2A-C3A	-4.95	99.61	113.00
14	G	1139	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
14	G	1114	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
14	B	1229	CLA	C2D-C1D-ND	4.95	115.03	110.13
14	H	1229	CLA	C2D-C1D-ND	4.95	115.03	110.13
14	a	1127	CLA	O2A-CGA-O1A	-4.95	111.24	123.63
14	b	1223	CLA	C4A-NA-C1A	4.95	108.94	106.68
14	A	1105	CLA	C1C-C2C-C3C	-4.95	101.77	106.98
13	A	1011	CL0	CAA-C2A-C3A	-4.95	99.62	113.00
18	I	4018	BCR	C24-C23-C22	-4.95	118.91	126.23
14	H	1227	CLA	O2A-CGA-O1A	-4.95	110.60	123.33
14	B	1235	CLA	C2D-C1D-ND	4.95	115.02	110.13
14	l	1503	CLA	C2D-C1D-ND	4.95	115.02	110.13
14	G	1105	CLA	C1C-C2C-C3C	-4.95	101.78	106.98
14	A	1103	CLA	O2A-CGA-O1A	-4.95	111.25	123.63
14	G	1108	CLA	C2D-C1D-ND	4.95	115.02	110.13
14	H	1222	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
13	G	1011	CL0	CAA-C2A-C3A	-4.95	99.63	113.00
14	B	1216	CLA	O2D-CGD-CBD	4.95	119.88	111.23
14	A	1124	CLA	C2D-C1D-ND	4.94	115.02	110.13
14	A	1114	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	b	1221	CLA	C2D-C1D-ND	4.94	115.02	110.13
14	H	1228	CLA	O2D-CGD-CBD	4.94	119.87	111.23
15	a	1121	F6C	O2A-CGA-O1A	-4.94	110.62	123.33
14	A	1138	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
18	R	4018	BCR	C24-C23-C22	-4.94	118.93	126.23
14	H	1233	CLA	C4A-NA-C1A	4.94	108.93	106.68
14	H	1216	CLA	O2D-CGD-CBD	4.94	119.87	111.23
14	X	1701	CLA	O2D-CGD-CBD	4.94	119.87	111.23
14	a	1103	CLA	O2A-CGA-O1A	-4.94	111.27	123.63
14	H	1221	CLA	C2D-C1D-ND	4.94	115.02	110.13
14	G	1138	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	A	1118	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	G	1103	CLA	O2A-CGA-O1A	-4.94	111.28	123.63
14	G	1105	CLA	C2D-C1D-ND	4.94	115.01	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1201	CLA	C2D-C1D-ND	4.93	115.01	110.13
14	b	1235	CLA	C2D-C1D-ND	4.93	115.01	110.13
14	B	1209	CLA	C4A-NA-C1A	4.93	108.93	106.68
14	G	1127	CLA	O2A-CGA-O1A	-4.93	111.29	123.63
14	A	1109	CLA	O2D-CGD-CBD	4.93	119.85	111.23
14	b	1236	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
14	H	1231	CLA	C4A-NA-C1A	4.93	108.93	106.68
14	H	1235	CLA	C2D-C1D-ND	4.93	115.01	110.13
14	a	1012	CLA	C2D-C1D-ND	4.93	115.01	110.13
14	B	1221	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
14	H	1203	CLA	C1D-ND-C4D	-4.93	102.85	106.31
14	b	1216	CLA	O2D-CGD-CBD	4.93	119.85	111.23
14	H	1222	CLA	C4A-NA-C1A	4.93	108.93	106.68
14	H	1232	CLA	C4A-NA-C1A	4.93	108.93	106.68
14	a	1108	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	A	1109	CLA	C2D-C1D-ND	4.93	115.00	110.13
14	b	1205	CLA	O2A-C1-C2	4.93	127.07	108.11
15	A	1121	F6C	O2A-CGA-O1A	-4.93	110.66	123.33
14	b	1228	CLA	O2D-CGD-CBD	4.93	119.84	111.23
14	b	1221	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
14	a	1139	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
14	A	1135	CLA	C2D-C1D-ND	4.93	115.00	110.13
14	A	1139	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
14	B	1207	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	A	1127	CLA	O2A-CGA-O1A	-4.92	111.31	123.63
14	B	1217	CLA	O2A-CGA-O1A	-4.92	111.31	123.63
14	B	1227	CLA	O2A-CGA-O1A	-4.92	110.67	123.33
14	B	1201	CLA	C2D-C1D-ND	4.92	115.00	110.13
14	H	1217	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
14	b	1217	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
18	B	4004	BCR	C3-C4-C5	-4.92	105.28	114.06
14	H	1204	CLA	C2D-C1D-ND	4.92	114.99	110.13
14	a	1108	CLA	C2D-C1D-ND	4.92	114.99	110.13
14	G	1137	CLA	C2D-C1D-ND	4.92	114.99	110.13
14	a	1118	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
14	B	1205	CLA	O2A-C1-C2	4.92	127.03	108.11
14	a	1139	CLA	C1C-C2C-C3C	-4.91	101.81	106.98
14	a	1124	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	a	1133	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	b	1207	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	H	1225	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	G	1109	CLA	O2D-CGD-CBD	4.91	119.82	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1108	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
14	H	1207	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	K	1401	CLA	C2D-C1D-ND	4.91	114.99	110.13
14	G	1115	CLA	C2D-C1D-ND	4.91	114.99	110.13
15	a	1120	F6C	C1A-C2A-C3A	-4.91	101.80	106.97
14	A	1101	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	b	1227	CLA	O2A-CGA-O1A	-4.91	110.70	123.33
14	G	1118	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
14	b	1222	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	G	1139	CLA	C1C-C2C-C3C	-4.91	101.82	106.98
18	b	4004	BCR	C3-C4-C5	-4.91	105.30	114.06
14	b	1206	CLA	O2A-CGA-O1A	-4.91	110.71	123.33
14	H	1234	CLA	C2C-C1C-NC	4.91	115.14	109.98
14	G	1127	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
14	a	1127	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
14	G	1109	CLA	C2D-C1D-ND	4.91	114.98	110.13
14	b	1201	CLA	C2D-C1D-ND	4.91	114.98	110.13
14	b	1207	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
14	a	1118	CLA	O2A-CGA-O1A	-4.90	111.36	123.63
14	A	1102	CLA	O2A-CGA-O1A	-4.90	111.36	123.63
14	A	1133	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	A	1115	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	B	1206	CLA	O2A-CGA-O1A	-4.90	110.72	123.33
14	H	1206	CLA	O2A-CGA-O1A	-4.90	110.72	123.33
14	H	1205	CLA	O2A-C1-C2	4.90	126.97	108.11
14	A	1119	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	H	1221	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
15	A	1120	F6C	C1A-C2A-C3A	-4.90	101.81	106.97
14	A	1137	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	a	1109	CLA	C2D-C1D-ND	4.90	114.98	110.13
15	G	1121	F6C	O2A-CGA-O1A	-4.90	110.73	123.33
14	b	1239	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
15	G	1120	F6C	C1A-C2A-C3A	-4.90	101.81	106.97
18	H	4004	BCR	C3-C4-C5	-4.90	105.32	114.06
14	G	1127	CLA	C4A-NA-C1A	4.90	108.91	106.68
14	a	1137	CLA	C2D-C1D-ND	4.90	114.97	110.13
14	a	1109	CLA	O2D-CGD-CBD	4.90	119.79	111.23
14	G	1102	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
14	a	1102	CLA	O2A-CGA-O1A	-4.89	111.39	123.63
14	A	1112	CLA	C1C-C2C-C3C	-4.89	101.83	106.98
14	B	1215	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
14	b	1234	CLA	C2C-C1C-NC	4.89	115.12	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1215	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
14	H	1217	CLA	C2D-C1D-ND	4.89	114.97	110.13
14	H	1225	CLA	O2A-CGA-O1A	-4.89	111.40	123.63
14	G	1119	CLA	C2D-C1D-ND	4.89	114.97	110.13
14	A	1139	CLA	C1C-C2C-C3C	-4.89	101.84	106.98
14	H	1215	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
14	B	1021	CLA	O2A-CGA-CBA	4.89	126.74	111.83
14	a	1101	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	b	1209	CLA	C2D-C1D-ND	4.89	114.96	110.13
14	b	1217	CLA	C2D-C1D-ND	4.89	114.96	110.13
14	H	1216	CLA	O2A-CGA-O1A	-4.89	111.40	123.63
14	B	1216	CLA	O2A-CGA-O1A	-4.89	111.41	123.63
14	G	1112	CLA	C2D-C1D-ND	4.89	114.96	110.13
14	b	1225	CLA	O2A-CGA-O1A	-4.88	111.41	123.63
14	G	1135	CLA	C2D-C1D-ND	4.88	114.96	110.13
14	H	1236	CLA	O2A-CGA-O1A	-4.88	110.77	123.33
14	A	1118	CLA	O2A-CGA-O1A	-4.88	111.41	123.63
14	B	1225	CLA	C4A-NA-C1A	4.88	108.91	106.68
14	b	1021	CLA	O2A-CGA-CBA	4.88	126.72	111.83
14	B	1211	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
14	B	1204	CLA	C2D-C1D-ND	4.88	114.96	110.13
14	G	1133	CLA	C2D-C1D-ND	4.88	114.96	110.13
14	A	1139	CLA	C4A-NA-C1A	4.88	108.91	106.68
14	a	1112	CLA	C1C-C2C-C3C	-4.88	101.85	106.98
14	b	1216	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
14	A	1112	CLA	C2D-C1D-ND	4.88	114.96	110.13
14	a	1124	CLA	O2D-CGD-CBD	4.88	119.76	111.23
14	H	1021	CLA	O2A-CGA-CBA	4.88	126.72	111.83
14	b	1224	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
14	G	1132	CLA	O2A-CGA-O1A	-4.88	111.42	123.63
14	H	1207	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
14	B	1225	CLA	O2A-CGA-O1A	-4.88	111.43	123.63
14	G	1101	CLA	C4A-NA-C1A	4.88	108.90	106.68
14	A	1129	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
14	B	1236	CLA	O2A-CGA-O1A	-4.88	110.79	123.33
14	a	1129	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
14	b	1231	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	A	1108	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
14	G	1118	CLA	O2A-CGA-O1A	-4.87	111.44	123.63
14	b	1203	CLA	C1D-ND-C4D	-4.87	102.89	106.31
14	H	1212	CLA	O2A-CGA-O1A	-4.87	110.80	123.33
14	B	1239	CLA	C3D-C2D-C1D	-4.87	99.18	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1124	CLA	O2D-CGD-CBD	4.87	119.74	111.23
14	G	1129	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
14	B	1217	CLA	C2D-C1D-ND	4.87	114.94	110.13
14	H	1239	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
14	a	1119	CLA	O2D-CGD-CBD	4.87	119.74	111.23
14	b	1212	CLA	O2A-CGA-O1A	-4.87	110.82	123.33
14	G	1112	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
14	b	1231	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
14	b	1204	CLA	C2D-C1D-ND	4.87	114.94	110.13
14	H	1227	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
14	B	1207	CLA	C2D-C1D-ND	4.86	114.94	110.13
14	B	1233	CLA	C4A-NA-C1A	4.86	108.90	106.68
14	B	1212	CLA	O2A-CGA-O1A	-4.86	110.82	123.33
14	B	1227	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
14	B	1209	CLA	C2D-C1D-ND	4.86	114.94	110.13
14	H	1224	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
14	H	1211	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
14	G	1119	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
14	A	1119	CLA	O2A-CGA-O1A	-4.86	111.47	123.63
15	B	1230	F6C	O2A-CGA-O1A	-4.86	110.84	123.33
14	B	1234	CLA	C2C-C1C-NC	4.86	115.08	109.98
14	a	1119	CLA	C2D-C1D-ND	4.86	114.93	110.13
14	A	1119	CLA	O2D-CGD-CBD	4.86	119.72	111.23
14	B	1224	CLA	O2A-CGA-O1A	-4.86	111.48	123.63
14	a	1135	CLA	C2D-C1D-ND	4.85	114.93	110.13
14	A	1127	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
14	H	1209	CLA	C2D-C1D-ND	4.85	114.93	110.13
14	A	1126	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
14	A	1123	CLA	O2A-CGA-O1A	-4.85	111.49	123.63
14	A	1132	CLA	O2A-CGA-O1A	-4.85	111.49	123.63
14	G	1124	CLA	O2D-CGD-CBD	4.85	119.71	111.23
14	a	1139	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
14	b	1236	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
14	A	1125	CLA	OBD-CAD-C3D	-4.85	117.08	128.42
14	a	1123	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	B	1220	CLA	O2D-CGD-CBD	4.85	119.71	111.23
14	X	1701	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
14	W	1701	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
14	b	1211	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	H	1231	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
14	H	1220	CLA	O2D-CGD-CBD	4.84	119.70	111.23
14	G	1126	CLA	C3D-C2D-C1D	-4.84	99.22	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1132	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
14	b	1233	CLA	O2A-CGA-O1A	-4.84	110.88	123.33
14	G	1140	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
14	a	1125	CLA	OBD-CAD-C3D	-4.84	117.11	128.42
14	A	1139	CLA	O2A-CGA-O1A	-4.84	110.89	123.33
14	a	1119	CLA	O2A-CGA-O1A	-4.84	111.53	123.63
14	G	1129	CLA	C4A-NA-C1A	4.84	108.89	106.68
14	B	1222	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
14	B	1203	CLA	C1D-ND-C4D	-4.84	102.92	106.31
14	a	1127	CLA	C2D-C1D-ND	4.84	114.91	110.13
14	B	1231	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
14	a	1112	CLA	C2D-C1D-ND	4.83	114.91	110.13
14	a	1140	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
14	b	1222	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	H	1223	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
15	H	1230	F6C	O2A-CGA-O1A	-4.83	110.90	123.33
14	X	1701	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	a	1119	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
14	H	1233	CLA	O2A-CGA-O1A	-4.83	110.90	123.33
14	a	1126	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
14	G	1123	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
14	A	1103	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	G	1119	CLA	O2D-CGD-CBD	4.83	119.67	111.23
14	b	1220	CLA	O2D-CGD-CBD	4.83	119.67	111.23
14	a	1103	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	x	1701	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	G	1119	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
14	B	1223	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
14	G	1139	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	G	1125	CLA	OBD-CAD-C3D	-4.83	117.13	128.42
14	x	1701	CLA	O2A-CGA-O1A	-4.83	110.92	123.33
14	H	1220	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
14	A	1119	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
15	H	1230	F6C	C2D-C1D-ND	4.83	115.05	109.98
14	A	1140	CLA	O2A-CGA-O1A	-4.82	111.56	123.63
15	b	1230	F6C	C2D-C1D-ND	4.82	115.05	109.98
14	B	1233	CLA	O2A-CGA-O1A	-4.82	110.93	123.33
14	B	1203	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	b	1223	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	b	1203	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	H	1203	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	b	1220	CLA	C3B-C2B-C1B	-4.82	101.49	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1231	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	W	1701	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
15	B	1230	F6C	C2D-C1D-ND	4.82	115.04	109.98
14	H	1232	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
14	l	1503	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
14	G	1103	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
14	G	1105	CLA	O2A-CGA-O1A	-4.81	110.95	123.33
14	B	1220	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
14	a	1105	CLA	O2A-CGA-O1A	-4.81	110.96	123.33
14	b	1227	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
14	A	1012	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
14	H	1222	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
14	B	1226	CLA	C4A-NA-C1A	4.81	108.87	106.68
14	H	1233	CLA	C2D-C1D-ND	4.81	114.88	110.13
14	a	1012	CLA	O2A-CGA-O1A	-4.81	111.61	123.63
14	H	1021	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
14	G	1127	CLA	C2D-C1D-ND	4.80	114.88	110.13
14	B	1232	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
14	L	1503	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
14	b	1021	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
14	G	1012	CLA	O2A-CGA-O1A	-4.80	111.62	123.63
14	A	1105	CLA	O2A-CGA-O1A	-4.80	110.99	123.33
15	G	1121	F6C	C1C-C2C-C3C	-4.80	101.32	106.82
14	B	1215	CLA	O2A-CGA-CBA	4.80	126.46	111.83
14	H	1021	CLA	O2A-CGA-O1A	-4.80	111.63	123.63
14	B	1021	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
14	b	1231	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	b	1233	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	b	1214	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
14	B	1214	CLA	O2A-CGA-O1A	-4.79	111.64	123.63
14	H	1213	CLA	C2D-C1D-ND	4.79	114.87	110.13
13	a	1011	CL0	O2A-CGA-O1A	-4.79	111.65	123.63
14	b	1021	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
14	H	1214	CLA	O2A-CGA-O1A	-4.78	111.66	123.63
14	H	1021	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
14	G	1109	CLA	O2A-CGA-O1A	-4.78	111.03	123.33
14	B	1021	CLA	O2A-CGA-O1A	-4.78	111.66	123.63
14	b	1021	CLA	O2A-CGA-O1A	-4.78	111.66	123.63
14	U	1503	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
14	H	1236	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	H	1215	CLA	O2A-CGA-CBA	4.78	126.41	111.83
14	b	1232	CLA	C3B-C2B-C1B	-4.78	101.53	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1231	CLA	C2D-C1D-ND	4.78	114.86	110.13
13	A	1011	CL0	O2A-CGA-O1A	-4.78	111.67	123.63
14	G	1116	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	G	1124	CLA	C2B-C1B-NB	4.78	115.28	110.33
14	b	1229	CLA	C1D-ND-C4D	-4.77	102.96	106.31
14	A	1109	CLA	O2A-CGA-O1A	-4.77	111.05	123.33
14	B	1021	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
14	G	1114	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
14	a	1114	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
14	a	1124	CLA	C2B-C1B-NB	4.77	115.27	110.33
14	b	1220	CLA	O2A-CGA-O1A	-4.77	111.70	123.63
14	A	1107	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
14	a	1109	CLA	O2A-CGA-O1A	-4.77	111.06	123.33
14	A	1124	CLA	C2B-C1B-NB	4.77	115.27	110.33
14	A	1135	CLA	C4A-NA-C1A	4.77	108.85	106.68
14	B	1220	CLA	O2A-CGA-O1A	-4.77	111.70	123.63
14	A	1131	CLA	C2B-C1B-NB	4.77	115.27	110.33
13	G	1011	CL0	O2A-CGA-O1A	-4.77	111.71	123.63
14	A	1129	CLA	C4A-NA-C1A	4.77	108.85	106.68
14	B	1224	CLA	C4A-NA-C1A	4.77	108.85	106.68
14	H	1206	CLA	O2D-CGD-CBD	4.76	119.56	111.23
14	H	1212	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
14	G	1107	CLA	O2A-CGA-O1A	-4.76	111.08	123.33
15	b	1237	F6C	C3D-C2D-C1D	-4.76	98.93	105.83
14	b	1215	CLA	O2A-CGA-CBA	4.76	126.36	111.83
14	B	1212	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
15	a	1121	F6C	C1C-C2C-C3C	-4.76	101.36	106.82
15	b	1230	F6C	C3D-C2D-C1D	-4.76	98.94	105.83
15	H	1230	F6C	C3D-C2D-C1D	-4.76	98.94	105.83
14	B	1206	CLA	O2D-CGD-CBD	4.76	119.55	111.23
13	a	1011	CL0	O2A-CGA-CBA	4.76	126.34	111.83
14	A	1127	CLA	C2D-C1D-ND	4.76	114.83	110.13
14	H	1220	CLA	O2A-CGA-O1A	-4.76	111.73	123.63
14	H	1021	CLA	C1D-ND-C4D	-4.76	102.97	106.31
14	B	1233	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	A	1114	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
14	b	1212	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
14	H	1215	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	b	1021	CLA	C1D-ND-C4D	-4.75	102.98	106.31
15	H	1237	F6C	C3D-C2D-C1D	-4.75	98.95	105.83
15	B	1237	F6C	C3D-C2D-C1D	-4.75	98.95	105.83
14	A	1113	CLA	O2A-CGA-O1A	-4.75	111.11	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1213	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	a	1107	CLA	O2A-CGA-O1A	-4.75	111.12	123.33
15	A	1121	F6C	C1C-C2C-C3C	-4.75	101.38	106.82
14	b	1213	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	b	1206	CLA	O2D-CGD-CBD	4.75	119.53	111.23
15	B	1237	F6C	O2A-CGA-O1A	-4.74	111.76	123.63
14	B	1215	CLA	C2D-C1D-ND	4.74	114.82	110.13
15	B	1230	F6C	C3D-C2D-C1D	-4.74	98.96	105.83
14	a	1129	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	G	1112	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
14	a	1139	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	a	1112	CLA	O2A-CGA-O1A	-4.74	111.14	123.33
14	A	1112	CLA	O2A-CGA-O1A	-4.74	111.15	123.33
13	G	1011	CL0	O2A-CGA-CBA	4.74	126.27	111.83
14	A	1124	CLA	C4A-NA-C1A	4.73	108.84	106.68
14	G	1135	CLA	C4A-NA-C1A	4.73	108.84	106.68
14	a	1135	CLA	C4A-NA-C1A	4.73	108.84	106.68
14	B	1231	CLA	C2D-C1D-ND	4.73	114.81	110.13
15	b	1237	F6C	O2A-CGA-O1A	-4.73	111.79	123.63
14	B	1219	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
14	A	1108	CLA	O2A-CGA-O1A	-4.73	111.16	123.33
15	A	1120	F6C	O2A-CGA-O1A	-4.73	111.17	123.33
14	a	1113	CLA	O2A-CGA-O1A	-4.73	111.17	123.33
14	b	1219	CLA	O2A-CGA-O1A	-4.73	111.17	123.33
14	A	1122	CLA	O2A-CGA-O1A	-4.73	111.81	123.63
14	b	1215	CLA	C2D-C1D-ND	4.73	114.80	110.13
13	A	1011	CL0	O2A-CGA-CBA	4.73	126.24	111.83
14	B	1232	CLA	O2A-CGA-O1A	-4.72	111.18	123.33
15	H	1237	F6C	O2A-CGA-O1A	-4.72	111.81	123.63
14	G	1106	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	a	1122	CLA	O2A-CGA-O1A	-4.72	111.81	123.63
15	a	1120	F6C	O2A-CGA-O1A	-4.72	111.19	123.33
14	a	1106	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	G	1131	CLA	C2B-C1B-NB	4.72	115.22	110.33
14	A	1106	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	B	1228	CLA	C1C-C2C-C3C	-4.72	102.02	106.98
14	b	1225	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	H	1229	CLA	C1D-ND-C4D	-4.72	103.00	106.31
14	a	1138	CLA	O2A-CGA-O1A	-4.72	111.82	123.63
14	H	1219	CLA	O2A-CGA-O1A	-4.72	111.19	123.33
14	b	1232	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
15	G	1120	F6C	O2A-CGA-O1A	-4.72	111.20	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1202	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
14	a	1108	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
14	A	1101	CLA	C1C-C2C-C3C	-4.71	102.02	106.98
14	B	1225	CLA	C2D-C1D-ND	4.71	114.79	110.13
14	b	1205	CLA	C1D-ND-C4D	-4.71	103.00	106.31
14	B	1205	CLA	C2C-C1C-NC	4.71	114.93	109.98
14	H	1205	CLA	C1D-ND-C4D	-4.71	103.01	106.31
14	G	1131	CLA	C2D-C1D-ND	4.71	114.79	110.13
15	b	1230	F6C	O2A-CGA-O1A	-4.71	111.22	123.33
14	G	1113	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
14	b	1202	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
14	G	1138	CLA	O2A-CGA-O1A	-4.71	111.85	123.63
14	H	1023	CLA	O2A-CGA-O1A	-4.71	111.85	123.63
14	G	1127	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
14	H	1208	CLA	C2D-C1D-ND	4.71	114.78	110.13
14	a	1130	CLA	O2A-CGA-O1A	-4.70	111.86	123.63
14	B	1023	CLA	O2A-CGA-O1A	-4.70	111.86	123.63
14	G	1108	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
14	a	1131	CLA	C2B-C1B-NB	4.70	115.20	110.33
14	A	1130	CLA	O2A-CGA-O1A	-4.70	111.87	123.63
14	A	1138	CLA	O2A-CGA-O1A	-4.70	111.87	123.63
14	L	1502	CLA	O2A-CGA-O1A	-4.70	111.88	123.63
14	H	1225	CLA	C2D-C1D-ND	4.70	114.78	110.13
14	b	1023	CLA	O2A-CGA-O1A	-4.70	111.88	123.63
14	G	1139	CLA	C4A-NA-C1A	4.70	108.82	106.68
14	a	1127	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
14	G	1122	CLA	O2A-CGA-O1A	-4.70	111.88	123.63
14	H	1226	CLA	O2A-CGA-CBA	4.70	126.15	111.83
14	B	1218	CLA	O2A-CGA-O1A	-4.70	111.26	123.33
14	A	1116	CLA	C4A-NA-C1A	4.70	108.82	106.68
14	H	1226	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
14	B	1226	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
14	H	1218	CLA	O2A-CGA-O1A	-4.69	111.26	123.33
14	a	1131	CLA	C2D-C1D-ND	4.69	114.77	110.13
14	H	1232	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	B	1226	CLA	O2A-CGA-CBA	4.69	126.14	111.83
14	G	1106	CLA	C1D-ND-C4D	-4.69	103.02	106.31
14	A	1131	CLA	C2D-C1D-ND	4.69	114.77	110.13
14	A	1106	CLA	C1D-ND-C4D	-4.69	103.02	106.31
14	G	1129	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	b	1226	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
14	G	1101	CLA	C1C-C2C-C3C	-4.68	102.05	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1228	CLA	C1C-C2C-C3C	-4.68	102.05	106.98
14	B	1208	CLA	C2D-C1D-ND	4.68	114.76	110.13
14	G	1130	CLA	O2A-CGA-O1A	-4.68	111.91	123.63
14	B	1202	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
14	H	1204	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
14	a	1101	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
14	H	1217	CLA	O2D-CGD-CBD	4.68	119.42	111.23
14	b	1226	CLA	O2A-CGA-CBA	4.68	126.11	111.83
14	b	1217	CLA	O2D-CGD-CBD	4.68	119.41	111.23
14	B	1204	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
14	b	1218	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
14	B	1222	CLA	C1D-ND-C4D	-4.68	103.03	106.31
14	G	1111	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
14	H	1222	CLA	C1D-ND-C4D	-4.68	103.03	106.31
14	U	1502	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
14	l	1502	CLA	O2A-CGA-O1A	-4.68	111.93	123.63
14	A	1129	CLA	O2A-CGA-O1A	-4.68	111.30	123.33
14	L	1501	CLA	O2A-C1-C2	4.67	126.08	108.11
14	a	1111	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
14	B	1021	CLA	C1D-ND-C4D	-4.67	103.03	106.31
14	B	1217	CLA	O2D-CGD-CBD	4.67	119.39	111.23
14	a	1116	CLA	C4A-NA-C1A	4.67	108.81	106.68
15	b	1230	F6C	C1C-C2C-C3C	-4.67	101.47	106.82
14	b	1205	CLA	C2C-C1C-NC	4.67	114.89	109.98
15	A	1121	F6C	C3D-C2D-C1D	-4.67	99.07	105.83
14	A	1127	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
14	a	1106	CLA	C1D-ND-C4D	-4.66	103.04	106.31
14	G	1102	CLA	C2B-C1B-NB	4.66	115.16	110.33
14	G	1110	CLA	O2A-CGA-O1A	-4.66	111.34	123.33
14	a	1114	CLA	O2A-CGA-O1A	-4.66	111.34	123.33
14	B	1229	CLA	C1D-ND-C4D	-4.66	103.04	106.31
14	a	1129	CLA	O2A-CGA-O1A	-4.66	111.35	123.33
14	H	1228	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
14	B	1211	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
14	G	1130	CLA	C2D-C1D-ND	4.66	114.74	110.13
14	U	1501	CLA	O2A-C1-C2	4.66	126.03	108.11
14	H	1226	CLA	C4A-NA-C1A	4.66	108.80	106.68
15	a	1121	F6C	C3D-C2D-C1D	-4.66	99.09	105.83
14	H	1221	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
14	G	1114	CLA	O2A-CGA-O1A	-4.66	111.36	123.33
14	b	1228	CLA	O2A-CGA-O1A	-4.66	111.36	123.33
14	b	1233	CLA	C3B-C2B-C1B	-4.66	101.68	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	1502	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	H	1205	CLA	C2C-C1C-NC	4.65	114.87	109.98
14	A	1110	CLA	O2A-CGA-O1A	-4.65	111.36	123.33
14	B	1225	CLA	C1C-C2C-C3C	-4.65	102.09	106.98
14	B	1233	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
14	k	1401	CLA	O2A-CGA-O1A	-4.65	111.37	123.33
14	b	1022	CLA	C1C-C2C-C3C	-4.65	102.09	106.98
14	l	1502	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	a	1113	CLA	C2D-C1D-ND	4.65	114.73	110.13
14	A	1102	CLA	C2B-C1B-NB	4.65	115.15	110.33
14	A	1114	CLA	O2A-CGA-O1A	-4.65	111.38	123.33
14	l	1501	CLA	O2A-C1-C2	4.65	125.99	108.11
14	b	1222	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	T	1401	CLA	O2A-CGA-O1A	-4.65	111.38	123.33
14	H	1228	CLA	O2A-CGA-O1A	-4.65	111.38	123.33
14	a	1102	CLA	C2B-C1B-NB	4.64	115.14	110.33
14	A	1111	CLA	C1C-C2C-C3C	-4.64	102.09	106.98
14	B	1228	CLA	O2A-CGA-O1A	-4.64	111.39	123.33
14	b	1204	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
14	b	1208	CLA	C2D-C1D-ND	4.64	114.72	110.13
14	H	1224	CLA	C4A-NA-C1A	4.64	108.80	106.68
14	H	1233	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
14	a	1116	CLA	C2D-C1D-ND	4.64	114.72	110.13
14	b	1204	CLA	C1D-ND-C4D	-4.64	103.06	106.31
14	K	1401	CLA	O2A-CGA-O1A	-4.64	111.40	123.33
14	b	1224	CLA	C4A-NA-C1A	4.64	108.80	106.68
14	B	1205	CLA	C1D-ND-C4D	-4.64	103.06	106.31
14	H	1204	CLA	C1D-ND-C4D	-4.64	103.06	106.31
14	A	1131	CLA	O2A-CGA-O1A	-4.64	112.03	123.63
14	a	1110	CLA	O2A-CGA-O1A	-4.64	111.41	123.33
15	H	1230	F6C	C1C-C2C-C3C	-4.64	101.51	106.82
14	A	1130	CLA	C2D-C1D-ND	4.63	114.71	110.13
14	B	1221	CLA	O2A-CGA-O1A	-4.63	112.05	123.63
14	b	1221	CLA	O2A-CGA-O1A	-4.63	112.05	123.63
14	B	1212	CLA	C1D-ND-C4D	-4.63	103.06	106.31
15	G	1121	F6C	C3D-C2D-C1D	-4.63	99.13	105.83
14	B	1022	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
14	a	1139	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
14	A	1139	CLA	C3B-C2B-C1B	-4.63	101.72	107.17
14	b	1226	CLA	C4A-NA-C1A	4.62	108.79	106.68
14	A	1123	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	G	1133	CLA	O2A-CGA-O1A	-4.62	112.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1105	CLA	C1D-ND-C4D	-4.62	103.07	106.31
14	G	1116	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	G	1124	CLA	O2A-CGA-O1A	-4.62	112.07	123.63
14	a	1101	CLA	C1D-ND-C4D	-4.62	103.07	106.31
14	G	1131	CLA	O2A-CGA-O1A	-4.62	112.07	123.63
14	A	1124	CLA	O2A-CGA-O1A	-4.62	112.08	123.63
14	b	1225	CLA	C1C-C2C-C3C	-4.62	102.12	106.98
14	a	1102	CLA	C2D-C1D-ND	4.62	114.69	110.13
14	H	1012	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
14	B	1231	CLA	C2B-C1B-NB	4.61	115.11	110.33
14	a	1124	CLA	O2A-CGA-O1A	-4.61	112.09	123.63
14	B	1205	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
14	b	1211	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
14	a	1131	CLA	O2A-CGA-O1A	-4.61	112.10	123.63
14	G	1013	CLA	CAA-C2A-C3A	-4.61	100.55	113.00
14	A	1113	CLA	C2D-C1D-ND	4.61	114.69	110.13
14	A	1101	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	a	1133	CLA	O2A-CGA-O1A	-4.61	112.11	123.63
18	a	4002	BCR	C8-C9-C10	4.61	126.25	119.01
14	a	1124	CLA	C4A-NA-C1A	4.61	108.78	106.68
14	H	1212	CLA	C1D-ND-C4D	-4.60	103.08	106.31
14	A	1013	CLA	CAA-C2A-C3A	-4.60	100.56	113.00
14	H	1211	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
13	A	1011	CL0	CHA-C1A-C2A	-4.60	122.50	133.31
13	a	1011	CL0	CHA-C1A-C2A	-4.60	122.50	133.31
14	H	1205	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
14	G	1139	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
13	G	1011	CL0	CHA-C1A-C2A	-4.60	122.51	133.31
18	G	4002	BCR	C8-C9-C10	4.60	126.24	119.01
14	G	1101	CLA	C1D-ND-C4D	-4.59	103.09	106.31
14	B	1236	CLA	C4A-NA-C1A	4.59	108.78	106.68
15	B	1237	F6C	C1C-C2C-C3C	-4.59	101.56	106.82
14	b	1022	CLA	O2A-CGA-O1A	-4.59	112.14	123.63
14	A	1133	CLA	O2A-CGA-O1A	-4.59	112.14	123.63
14	a	1013	CLA	CAA-C2A-C3A	-4.59	100.59	113.00
14	a	1130	CLA	C2D-C1D-ND	4.59	114.67	110.13
18	G	4011	BCR	C24-C23-C22	-4.59	119.45	126.23
14	b	1205	CLA	C1C-C2C-C3C	-4.59	102.16	106.98
14	G	1113	CLA	C2D-C1D-ND	4.59	114.67	110.13
14	H	1221	CLA	C1C-C2C-C3C	-4.59	102.16	106.98
14	H	1225	CLA	C1C-C2C-C3C	-4.59	102.16	106.98
14	B	1208	CLA	C4A-NA-C1A	4.59	108.77	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1022	CLA	O2A-CGA-O1A	-4.59	112.16	123.63
14	G	1105	CLA	C1D-ND-C4D	-4.58	103.09	106.31
14	B	1225	CLA	O2D-CGD-CBD	4.58	119.24	111.23
14	b	1231	CLA	C2B-C1B-NB	4.58	115.08	110.33
14	B	1204	CLA	C1D-ND-C4D	-4.58	103.10	106.31
14	H	1012	CLA	O2A-CGA-O1A	-4.58	112.17	123.63
14	H	1221	CLA	O2A-CGA-CBA	4.58	125.80	111.83
14	U	1503	CLA	O2A-CGA-O1A	-4.58	112.18	123.63
14	A	1105	CLA	C1D-ND-C4D	-4.58	103.10	106.31
14	H	1210	CLA	C4A-NA-C1A	4.58	108.77	106.68
14	B	1221	CLA	C1C-C2C-C3C	-4.58	102.17	106.98
14	G	1123	CLA	C2D-C1D-ND	4.58	114.66	110.13
14	H	1209	CLA	O2A-CGA-O1A	-4.58	111.56	123.33
14	B	1222	CLA	O2A-CGA-CBA	4.58	125.79	111.83
14	A	1116	CLA	C2D-C1D-ND	4.58	114.65	110.13
14	A	1101	CLA	O2A-CGA-O1A	-4.57	111.57	123.33
14	B	1022	CLA	C4A-NA-C1A	4.57	108.77	106.68
18	A	4002	BCR	C8-C9-C10	4.57	126.20	119.01
14	b	1222	CLA	O2A-CGA-CBA	4.57	125.77	111.83
18	G	4002	BCR	C24-C23-C22	-4.57	119.47	126.23
14	H	1222	CLA	O2A-CGA-CBA	4.57	125.77	111.83
14	G	1102	CLA	C2D-C1D-ND	4.57	114.65	110.13
14	G	1101	CLA	O2A-CGA-O1A	-4.57	111.58	123.33
14	b	1221	CLA	C1C-C2C-C3C	-4.57	102.17	106.98
14	G	1124	CLA	C4A-NA-C1A	4.57	108.76	106.68
14	H	1238	CLA	O2D-CGD-CBD	4.57	119.21	111.23
14	b	1209	CLA	O2A-CGA-O1A	-4.57	111.59	123.33
18	a	4011	BCR	C24-C23-C22	-4.56	119.48	126.23
15	b	1237	F6C	C1C-C2C-C3C	-4.56	101.59	106.82
14	B	1221	CLA	O2A-CGA-CBA	4.56	125.75	111.83
18	A	4011	BCR	C24-C23-C22	-4.56	119.48	126.23
14	b	1221	CLA	O2A-CGA-CBA	4.56	125.75	111.83
14	l	1503	CLA	O2A-CGA-O1A	-4.56	112.22	123.63
14	A	1109	CLA	C1D-ND-C4D	-4.56	103.11	106.31
14	H	1229	CLA	C4A-NA-C1A	4.56	108.76	106.68
14	H	1225	CLA	O2D-CGD-CBD	4.56	119.20	111.23
14	b	1236	CLA	C4A-NA-C1A	4.56	108.76	106.68
14	a	1101	CLA	O2A-CGA-O1A	-4.56	111.61	123.33
14	G	1128	CLA	C2D-C1D-ND	4.56	114.64	110.13
14	B	1238	CLA	O2D-CGD-CBD	4.56	119.20	111.23
14	G	1118	CLA	C2D-C1D-ND	4.56	114.64	110.13
14	L	1503	CLA	O2A-CGA-O1A	-4.56	112.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	U	1502	CLA	C1D-ND-C4D	-4.56	103.12	106.31
14	b	1225	CLA	O2D-CGD-CBD	4.55	119.19	111.23
18	L	4019	BCR	C33-C5-C6	-4.55	119.51	124.48
14	a	1013	CLA	CMD-C2D-C1D	4.55	132.75	124.73
14	b	1212	CLA	C1D-ND-C4D	-4.55	103.12	106.31
14	G	1117	CLA	O2A-CGA-O1A	-4.55	112.24	123.63
14	a	1117	CLA	O2A-CGA-O1A	-4.55	112.24	123.63
15	H	1237	F6C	C1C-C2C-C3C	-4.55	101.60	106.82
14	A	1118	CLA	C2D-C1D-ND	4.55	114.63	110.13
15	B	1230	F6C	C1C-C2C-C3C	-4.55	101.61	106.82
14	B	1209	CLA	O2A-CGA-O1A	-4.55	111.63	123.33
14	b	1238	CLA	O2D-CGD-CBD	4.55	119.18	111.23
14	A	1013	CLA	CMD-C2D-C1D	4.55	132.74	124.73
14	G	1136	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
14	A	1117	CLA	O2A-CGA-O1A	-4.55	112.25	123.63
14	A	1102	CLA	C2D-C1D-ND	4.55	114.63	110.13
14	H	1012	CLA	C4A-NA-C1A	4.55	108.75	106.68
14	A	1136	CLA	C3B-C2B-C1B	-4.54	101.81	107.17
14	H	1231	CLA	C2B-C1B-NB	4.54	115.04	110.33
14	b	1208	CLA	C4A-NA-C1A	4.54	108.75	106.68
14	b	1218	CLA	C1D-ND-C4D	-4.54	103.13	106.31
18	a	4002	BCR	C24-C23-C22	-4.54	119.52	126.23
14	G	1013	CLA	CMD-C2D-C1D	4.54	132.72	124.73
14	a	1123	CLA	C2D-C1D-ND	4.54	114.62	110.13
18	l	4019	BCR	C33-C5-C6	-4.54	119.53	124.48
14	a	1136	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
14	B	1022	CLA	O2A-C1-C2	4.53	125.55	108.11
14	A	1128	CLA	C2D-C1D-ND	4.53	114.61	110.13
14	H	1012	CLA	O2A-C1-C2	4.53	125.54	108.11
14	b	1022	CLA	O2A-C1-C2	4.53	125.54	108.11
14	A	1139	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	H	1210	CLA	C1D-ND-C4D	-4.53	103.14	106.31
14	a	1138	CLA	C2B-C1B-NB	4.53	115.02	110.33
14	b	1232	CLA	O2D-CGD-CBD	4.52	119.14	111.23
14	H	1224	CLA	O2A-C1-C2	4.52	125.51	108.11
14	a	1118	CLA	C2D-C1D-ND	4.52	114.60	110.13
14	b	1224	CLA	O2A-C1-C2	4.52	125.51	108.11
14	B	1219	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	G	1109	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	G	1126	CLA	C2B-C1B-NB	4.52	115.01	110.33
16	H	2002	PQN	C14-C13-C15	4.51	123.06	115.23
14	H	1204	CLA	O2A-CGA-CBA	4.51	125.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1208	CLA	C4A-NA-C1A	4.51	108.74	106.68
14	b	1204	CLA	O2A-CGA-CBA	4.51	125.59	111.83
14	A	1126	CLA	C2B-C1B-NB	4.51	115.00	110.33
14	H	1218	CLA	C1D-ND-C4D	-4.51	103.15	106.31
14	B	1224	CLA	O2A-C1-C2	4.51	125.46	108.11
14	A	1138	CLA	C2B-C1B-NB	4.51	115.00	110.33
18	U	4019	BCR	C33-C5-C6	-4.51	119.56	124.48
14	L	1503	CLA	C1D-ND-C4D	-4.51	103.15	106.31
14	H	1232	CLA	O2D-CGD-CBD	4.50	119.11	111.23
14	a	1109	CLA	C1D-ND-C4D	-4.50	103.15	106.31
18	A	4002	BCR	C24-C23-C22	-4.50	119.57	126.23
16	b	2002	PQN	C14-C13-C15	4.50	123.04	115.23
14	l	1503	CLA	C1D-ND-C4D	-4.50	103.16	106.31
14	G	1139	CLA	C1D-ND-C4D	-4.50	103.16	106.31
18	G	4002	BCR	C34-C9-C10	-4.50	115.53	122.82
14	A	1128	CLA	O2A-CGA-CBA	4.50	125.55	111.83
14	b	1239	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
14	B	1232	CLA	O2D-CGD-CBD	4.50	119.09	111.23
14	B	1204	CLA	O2A-CGA-CBA	4.50	125.54	111.83
14	G	1127	CLA	O2A-C1-C2	4.49	125.40	108.11
14	H	1201	CLA	C2B-C1B-NB	4.49	114.98	110.33
14	a	1127	CLA	O2A-C1-C2	4.49	125.40	108.11
14	a	1128	CLA	O2A-CGA-CBA	4.49	125.53	111.83
14	G	1138	CLA	C2B-C1B-NB	4.49	114.98	110.33
14	A	1127	CLA	O2A-C1-C2	4.49	125.39	108.11
14	a	1126	CLA	C2B-C1B-NB	4.49	114.98	110.33
14	B	1225	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
16	B	2002	PQN	C14-C13-C15	4.49	123.02	115.23
14	A	1108	CLA	C1D-ND-C4D	-4.49	103.16	106.31
14	B	1218	CLA	C1D-ND-C4D	-4.49	103.16	106.31
14	B	1239	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
14	b	1225	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
14	b	1201	CLA	C2B-C1B-NB	4.49	114.98	110.33
14	B	1201	CLA	C2B-C1B-NB	4.48	114.98	110.33
14	B	1236	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
18	a	4002	BCR	C34-C9-C10	-4.48	115.56	122.82
14	A	1140	CLA	C1D-ND-C4D	-4.48	103.17	106.31
14	B	1210	CLA	C4A-NA-C1A	4.48	108.72	106.68
14	G	1128	CLA	O2A-CGA-CBA	4.48	125.49	111.83
14	G	1129	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
14	a	1128	CLA	C2D-C1D-ND	4.48	114.56	110.13
14	H	1227	CLA	C4A-NA-C1A	4.48	108.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1236	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
14	a	1129	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	B	1238	CLA	C2D-C1D-ND	4.47	114.55	110.13
14	a	1107	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	A	1107	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
14	G	1117	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
14	b	1022	CLA	C4A-NA-C1A	4.47	108.72	106.68
14	B	1229	CLA	O2A-CGA-CBA	4.47	125.45	111.83
14	G	1107	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
18	A	4002	BCR	C34-C9-C10	-4.46	115.58	122.82
14	l	1503	CLA	O2A-C1-C2	4.46	125.29	108.11
18	a	4011	BCR	C3-C4-C5	-4.46	106.10	114.06
14	U	1503	CLA	O2A-C1-C2	4.46	125.28	108.11
14	b	1235	CLA	C1D-ND-C4D	-4.46	103.18	106.31
18	A	4011	BCR	C3-C4-C5	-4.46	106.10	114.06
14	B	1235	CLA	C2B-C1B-NB	4.46	114.95	110.33
14	a	1132	CLA	C2D-C1D-ND	4.46	114.54	110.13
14	H	1232	CLA	C2D-C1D-ND	4.46	114.54	110.13
14	U	1503	CLA	C1D-ND-C4D	-4.46	103.19	106.31
14	H	1239	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
14	a	1132	CLA	C4A-NA-C1A	4.45	108.71	106.68
14	B	1232	CLA	C2D-C1D-ND	4.45	114.53	110.13
14	H	1239	CLA	O2A-CGA-CBA	4.45	125.41	111.83
14	b	1236	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
14	H	1235	CLA	C2B-C1B-NB	4.45	114.94	110.33
14	B	1224	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
14	a	1139	CLA	C1D-ND-C4D	-4.45	103.19	106.31
14	L	1503	CLA	O2A-C1-C2	4.45	125.24	108.11
18	G	4007	BCR	C31-C1-C6	-4.45	103.26	110.24
14	H	1225	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
14	G	1108	CLA	C1D-ND-C4D	-4.45	103.19	106.31
14	A	1140	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
14	b	1224	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
14	b	1232	CLA	C2D-C1D-ND	4.45	114.53	110.13
14	b	1210	CLA	C1D-ND-C4D	-4.45	103.19	106.31
14	b	1229	CLA	O2A-CGA-CBA	4.45	125.39	111.83
14	H	1229	CLA	O2A-CGA-CBA	4.44	125.39	111.83
14	G	1119	CLA	C1C-C2C-C3C	-4.44	102.31	106.98
14	G	1135	CLA	C1D-ND-C4D	-4.44	103.19	106.31
14	A	1119	CLA	C1C-C2C-C3C	-4.44	102.31	106.98
18	G	4011	BCR	C3-C4-C5	-4.44	106.14	114.06
14	A	1105	CLA	C4A-NA-C1A	4.44	108.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1401	CLA	C1D-ND-C4D	-4.44	103.20	106.31
14	a	1126	CLA	C2D-C1D-ND	4.44	114.52	110.13
14	H	1219	CLA	C1D-ND-C4D	-4.44	103.20	106.31
14	A	1122	CLA	C1D-ND-C4D	-4.44	103.20	106.31
14	B	1210	CLA	C1D-ND-C4D	-4.44	103.20	106.31
14	G	1124	CLA	C1D-ND-C4D	-4.44	103.20	106.31
14	A	1132	CLA	C4A-NA-C1A	4.44	108.70	106.68
14	G	1140	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
18	a	4007	BCR	C31-C1-C6	-4.44	103.29	110.24
14	B	1239	CLA	O2A-CGA-CBA	4.43	125.36	111.83
18	A	4007	BCR	C31-C1-C6	-4.43	103.29	110.24
14	A	1102	CLA	O2A-C1-C2	4.43	125.17	108.11
14	b	1239	CLA	O2A-CGA-CBA	4.43	125.35	111.83
14	H	1224	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
14	B	1211	CLA	C2D-C1D-ND	4.43	114.51	110.13
14	b	1235	CLA	O2A-CGA-CBA	4.43	125.34	111.83
14	b	1235	CLA	C2B-C1B-NB	4.43	114.92	110.33
18	i	4018	BCR	C7-C8-C9	-4.43	119.68	126.23
14	b	1219	CLA	C1D-ND-C4D	-4.43	103.20	106.31
14	H	1211	CLA	O2D-CGD-CBD	4.43	118.97	111.23
14	a	1102	CLA	O2A-C1-C2	4.43	125.15	108.11
14	G	1102	CLA	O2A-C1-C2	4.43	125.14	108.11
14	A	1132	CLA	C2D-C1D-ND	4.43	114.51	110.13
14	a	1117	CLA	C3B-C2B-C1B	-4.42	101.95	107.17
14	a	1122	CLA	C1D-ND-C4D	-4.42	103.21	106.31
20	i	5006	LMG	O7-C10-C11	4.42	121.05	111.48
14	A	1126	CLA	C2D-C1D-ND	4.42	114.50	110.13
14	a	1140	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
14	U	1501	CLA	C1D-ND-C4D	-4.42	103.21	106.31
14	k	1401	CLA	C1D-ND-C4D	-4.42	103.21	106.31
14	l	1501	CLA	C1D-ND-C4D	-4.42	103.21	106.31
14	B	1235	CLA	O2A-CGA-CBA	4.42	125.31	111.83
18	R	4018	BCR	C7-C8-C9	-4.42	119.70	126.23
14	G	1132	CLA	C2D-C1D-ND	4.42	114.50	110.13
14	B	1238	CLA	O2A-CGA-CBA	4.42	125.30	111.83
14	B	1222	CLA	C2B-C1B-NB	4.42	114.91	110.33
14	a	1119	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
14	A	1129	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
14	B	1229	CLA	C4A-NA-C1A	4.42	108.69	106.68
14	G	1132	CLA	C4A-NA-C1A	4.42	108.69	106.68
14	B	1211	CLA	O2D-CGD-CBD	4.42	118.95	111.23
14	G	1111	CLA	O2A-CGA-CBA	4.42	125.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1129	CLA	C2D-C1D-ND	4.42	114.50	110.13
14	G	1136	CLA	C1D-ND-C4D	-4.42	103.21	106.31
20	R	5006	LMG	O7-C10-C11	4.41	121.03	111.48
14	A	1124	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	a	1136	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	A	1111	CLA	O2A-CGA-CBA	4.41	125.29	111.83
14	H	1238	CLA	C2D-C1D-ND	4.41	114.49	110.13
14	H	1235	CLA	O2A-CGA-CBA	4.41	125.28	111.83
14	A	1135	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	L	1501	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	b	1211	CLA	O2D-CGD-CBD	4.41	118.93	111.23
20	G	5005	LMG	O7-C10-C11	4.41	121.01	111.48
14	a	1111	CLA	O2A-CGA-CBA	4.41	125.27	111.83
20	I	5006	LMG	O7-C10-C11	4.40	121.01	111.48
14	b	1229	CLA	C4A-NA-C1A	4.40	108.69	106.68
14	G	1117	CLA	C2D-C1D-ND	4.40	114.48	110.13
20	A	5005	LMG	O7-C10-C11	4.40	121.01	111.48
14	G	1140	CLA	C1D-ND-C4D	-4.40	103.22	106.31
14	b	1231	CLA	C1D-ND-C4D	-4.40	103.22	106.31
15	b	1237	F6C	C4A-NA-C1A	4.40	109.40	106.31
14	A	1012	CLA	O2A-CGA-CBA	4.40	125.26	111.83
14	b	1238	CLA	O2A-CGA-CBA	4.40	125.25	111.83
14	a	1140	CLA	C1D-ND-C4D	-4.40	103.22	106.31
14	H	1238	CLA	O2A-CGA-CBA	4.40	125.25	111.83
14	G	1122	CLA	C1D-ND-C4D	-4.40	103.23	106.31
14	b	1238	CLA	C2D-C1D-ND	4.40	114.48	110.13
14	H	1222	CLA	C2B-C1B-NB	4.40	114.89	110.33
14	B	1209	CLA	C1D-ND-C4D	-4.40	103.23	106.31
14	b	1208	CLA	O2A-CGA-CBA	4.40	125.24	111.83
15	B	1237	F6C	C4A-NA-C1A	4.39	109.39	106.31
14	G	1126	CLA	C2D-C1D-ND	4.39	114.47	110.13
14	a	1012	CLA	O2A-CGA-CBA	4.39	125.23	111.83
14	A	1117	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
14	b	1210	CLA	C4A-NA-C1A	4.39	108.68	106.68
18	I	4018	BCR	C7-C8-C9	-4.39	119.74	126.23
14	a	1108	CLA	C1D-ND-C4D	-4.39	103.23	106.31
14	G	1129	CLA	C2D-C1D-ND	4.39	114.47	110.13
20	a	5005	LMG	O7-C10-C11	4.39	120.97	111.48
14	b	1211	CLA	C2D-C1D-ND	4.39	114.47	110.13
14	A	1129	CLA	C2D-C1D-ND	4.39	114.47	110.13
14	a	1124	CLA	C1D-ND-C4D	-4.39	103.23	106.31
14	B	1208	CLA	O2A-CGA-CBA	4.38	125.20	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1216	CLA	C2D-C1D-ND	4.38	114.47	110.13
14	H	1211	CLA	C2D-C1D-ND	4.38	114.47	110.13
14	G	1012	CLA	O2A-CGA-CBA	4.38	125.20	111.83
14	a	1135	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	B	1239	CLA	C2D-C1D-ND	4.38	114.46	110.13
14	H	1231	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	A	1110	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	B	1235	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	b	1209	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	B	1225	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
14	b	1222	CLA	C2B-C1B-NB	4.37	114.86	110.33
14	b	1239	CLA	C2D-C1D-ND	4.37	114.45	110.13
14	H	1235	CLA	C1D-ND-C4D	-4.37	103.25	106.31
14	b	1225	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
14	A	1136	CLA	C1D-ND-C4D	-4.37	103.25	106.31
14	b	1205	CLA	C2B-C1B-NB	4.37	114.86	110.33
14	H	1239	CLA	C2D-C1D-ND	4.37	114.45	110.13
14	H	1213	CLA	C1D-ND-C4D	-4.37	103.25	106.31
14	H	1225	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
14	A	1114	CLA	C4A-NA-C1A	4.37	108.67	106.68
14	H	1208	CLA	O2A-CGA-CBA	4.36	125.14	111.83
14	B	1205	CLA	C2B-C1B-NB	4.36	114.85	110.33
14	B	1214	CLA	C4A-NA-C1A	4.36	108.67	106.68
14	W	1701	CLA	C1D-ND-C4D	-4.36	103.25	106.31
14	H	1238	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
14	B	1215	CLA	C4A-NA-C1A	4.36	108.67	106.68
14	b	1216	CLA	C2D-C1D-ND	4.36	114.44	110.13
14	H	1216	CLA	C2D-C1D-ND	4.35	114.44	110.13
14	b	1238	CLA	C1C-C2C-C3C	-4.35	102.40	106.98
14	B	1203	CLA	CAA-C2A-C3A	-4.35	101.23	113.00
14	H	1239	CLA	O2A-C1-C2	4.35	124.86	108.11
14	G	1103	CLA	CAA-C2A-C3A	-4.35	101.24	113.00
14	b	1239	CLA	O2A-C1-C2	4.35	124.85	108.11
14	B	1238	CLA	C1C-C2C-C3C	-4.35	102.41	106.98
14	H	1220	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	X	1701	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	B	1239	CLA	O2A-C1-C2	4.35	124.85	108.11
14	H	1203	CLA	O2A-CGA-CBA	4.35	125.10	111.83
14	b	1203	CLA	O2A-CGA-CBA	4.35	125.10	111.83
15	a	1121	F6C	C2D-C1D-ND	4.35	114.55	109.98
14	A	1103	CLA	CAA-C2A-C3A	-4.35	101.25	113.00
14	B	1203	CLA	O2A-CGA-CBA	4.35	125.09	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1103	CLA	CAA-C2A-C3A	-4.35	101.25	113.00
18	A	4003	BCR	C7-C8-C9	-4.35	119.80	126.23
14	K	1401	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	H	1209	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	a	1138	CLA	C2D-C1D-ND	4.34	114.42	110.13
14	A	1117	CLA	C2D-C1D-ND	4.34	114.42	110.13
14	b	1210	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
14	G	1105	CLA	C4A-NA-C1A	4.34	108.66	106.68
14	B	1220	CLA	C1D-ND-C4D	-4.34	103.27	106.31
14	b	1217	CLA	C1D-ND-C4D	-4.34	103.27	106.31
14	b	1220	CLA	C1D-ND-C4D	-4.34	103.27	106.31
14	G	1103	CLA	C1D-ND-C4D	-4.34	103.27	106.31
15	H	1237	F6C	C4A-NA-C1A	4.33	109.35	106.31
14	x	1701	CLA	C1D-ND-C4D	-4.33	103.27	106.31
14	b	1234	CLA	O2A-CGA-O1A	-4.33	112.79	123.63
14	a	1131	CLA	O2A-C1-C2	4.33	124.78	108.11
14	A	1131	CLA	O2A-C1-C2	4.33	124.77	108.11
14	G	1110	CLA	C1D-ND-C4D	-4.33	103.28	106.31
14	a	1110	CLA	C1D-ND-C4D	-4.33	103.28	106.31
15	B	1237	F6C	O2A-C1-C2	4.33	124.76	108.11
18	H	4009	BCR	C15-C14-C13	-4.33	121.21	127.28
15	b	1237	F6C	O2A-C1-C2	4.33	124.75	108.11
14	G	1131	CLA	O2A-C1-C2	4.33	124.75	108.11
14	a	1117	CLA	C2D-C1D-ND	4.32	114.41	110.13
14	a	1133	CLA	C3B-C2B-C1B	-4.32	102.07	107.17
15	H	1237	F6C	O2A-C1-C2	4.32	124.74	108.11
14	H	1023	CLA	C2B-C1B-NB	4.32	114.81	110.33
14	b	1203	CLA	CAA-C2A-C3A	-4.32	101.32	113.00
14	B	1228	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	B	1219	CLA	C2B-C1B-NB	4.32	114.81	110.33
14	a	1124	CLA	O2A-C1-C2	4.32	124.73	108.11
18	a	4008	BCR	C15-C14-C13	-4.32	121.22	127.28
14	A	1138	CLA	C2D-C1D-ND	4.32	114.40	110.13
14	b	1224	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	H	1205	CLA	C2B-C1B-NB	4.32	114.80	110.33
14	H	1203	CLA	CAA-C2A-C3A	-4.32	101.33	113.00
15	B	1237	F6C	O2A-CGA-CBA	4.32	125.00	111.83
14	B	1231	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	H	1211	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	G	1124	CLA	O2A-C1-C2	4.32	124.72	108.11
14	B	1210	CLA	C1C-C2C-C3C	-4.32	102.44	106.98
18	G	4008	BCR	C15-C14-C13	-4.31	121.23	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1213	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	H	1234	CLA	O2A-CGA-O1A	-4.31	112.84	123.63
15	b	1237	F6C	O2A-CGA-CBA	4.31	124.98	111.83
18	H	4017	BCR	C24-C23-C22	-4.31	119.86	126.23
18	b	4017	BCR	C24-C23-C22	-4.31	119.86	126.23
14	A	1124	CLA	O2A-C1-C2	4.31	124.70	108.11
15	A	1121	F6C	C2D-C1D-ND	4.31	114.51	109.98
14	H	1228	CLA	C1D-ND-C4D	-4.31	103.29	106.31
18	a	4003	BCR	C7-C8-C9	-4.31	119.86	126.23
14	a	1105	CLA	C4A-NA-C1A	4.31	108.64	106.68
14	H	1221	CLA	C1D-ND-C4D	-4.31	103.29	106.31
18	B	4013	BCR	C15-C14-C13	-4.31	121.24	127.28
18	G	4003	BCR	C7-C8-C9	-4.31	119.86	126.23
14	B	1234	CLA	O2A-CGA-O1A	-4.30	112.86	123.63
14	B	1211	CLA	C1D-ND-C4D	-4.30	103.29	106.31
14	b	1215	CLA	C4A-NA-C1A	4.30	108.64	106.68
18	B	4017	BCR	C24-C23-C22	-4.30	119.87	126.23
18	H	4006	BCR	C24-C23-C22	-4.30	119.87	126.23
18	b	4013	BCR	C15-C14-C13	-4.30	121.25	127.28
14	H	1210	CLA	C1C-C2C-C3C	-4.30	102.46	106.98
14	H	1215	CLA	C4A-NA-C1A	4.30	108.64	106.68
15	H	1237	F6C	O2A-CGA-CBA	4.30	124.94	111.83
14	G	1138	CLA	C2D-C1D-ND	4.30	114.38	110.13
18	b	4009	BCR	C15-C14-C13	-4.30	121.25	127.28
14	A	1133	CLA	C3B-C2B-C1B	-4.30	102.11	107.17
14	H	1217	CLA	C1D-ND-C4D	-4.29	103.30	106.31
18	B	4006	BCR	C24-C23-C22	-4.29	119.88	126.23
14	B	1023	CLA	C2B-C1B-NB	4.29	114.78	110.33
14	G	1125	CLA	O2A-CGA-CBA	4.29	124.92	111.83
14	H	1224	CLA	C1D-ND-C4D	-4.29	103.30	106.31
14	H	1238	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
14	a	1113	CLA	C2B-C1B-NB	4.29	114.77	110.33
18	b	4006	BCR	C24-C23-C22	-4.28	119.90	126.23
14	B	1233	CLA	C1D-ND-C4D	-4.28	103.31	106.31
14	b	1227	CLA	C4A-NA-C1A	4.28	108.63	106.68
14	a	1103	CLA	C1D-ND-C4D	-4.28	103.31	106.31
14	b	1208	CLA	C3B-C2B-C1B	-4.28	102.12	107.17
14	B	1213	CLA	O2A-CGA-CBA	4.28	124.89	111.83
18	B	4017	BCR	C3-C4-C5	-4.28	106.42	114.06
14	B	1224	CLA	C1D-ND-C4D	-4.28	103.31	106.31
14	b	1219	CLA	C2B-C1B-NB	4.28	114.76	110.33
14	G	1133	CLA	C3B-C2B-C1B	-4.28	102.13	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1129	CLA	C1D-ND-C4D	-4.28	103.31	106.31
18	H	4013	BCR	C15-C14-C13	-4.28	121.28	127.28
14	B	1208	CLA	C3B-C2B-C1B	-4.28	102.13	107.17
14	b	1238	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
14	G	1129	CLA	C1D-ND-C4D	-4.28	103.31	106.31
14	a	1115	CLA	C1D-ND-C4D	-4.28	103.31	106.31
14	a	1125	CLA	O2A-CGA-CBA	4.28	124.87	111.83
18	A	4008	BCR	C15-C14-C13	-4.28	121.28	127.28
14	b	1220	CLA	O2A-CGA-CBA	4.28	124.87	111.83
14	G	1122	CLA	C1C-C2C-C3C	-4.27	102.48	106.98
18	B	4009	BCR	C15-C14-C13	-4.27	121.28	127.28
14	B	1220	CLA	O2A-CGA-CBA	4.27	124.87	111.83
14	b	1228	CLA	C1D-ND-C4D	-4.27	103.31	106.31
14	A	1125	CLA	O2A-CGA-CBA	4.27	124.86	111.83
14	a	1122	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
14	b	1213	CLA	O2A-CGA-CBA	4.27	124.86	111.83
14	B	1238	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
14	A	1140	CLA	O2A-CGA-CBA	4.27	124.86	111.83
14	H	1213	CLA	O2A-CGA-CBA	4.27	124.86	111.83
14	H	1214	CLA	C4A-NA-C1A	4.27	108.63	106.68
14	b	1211	CLA	C1D-ND-C4D	-4.27	103.32	106.31
14	B	1217	CLA	C1D-ND-C4D	-4.27	103.32	106.31
18	H	4017	BCR	C3-C4-C5	-4.27	106.45	114.06
14	B	1023	CLA	O2A-CGA-CBA	4.27	124.84	111.83
14	a	1129	CLA	C1D-ND-C4D	-4.27	103.32	106.31
14	b	1233	CLA	C1D-ND-C4D	-4.27	103.32	106.31
14	b	1023	CLA	O2A-CGA-CBA	4.26	124.84	111.83
18	a	4011	BCR	C33-C5-C6	-4.26	119.83	124.48
14	a	1127	CLA	O2A-CGA-CBA	4.26	124.83	111.83
18	G	4011	BCR	C33-C5-C6	-4.26	119.84	124.48
14	a	1140	CLA	O2A-CGA-CBA	4.26	124.82	111.83
14	H	1023	CLA	O2A-CGA-CBA	4.26	124.82	111.83
14	A	1103	CLA	C1D-ND-C4D	-4.26	103.33	106.31
14	B	1221	CLA	C1D-ND-C4D	-4.26	103.33	106.31
18	b	4013	BCR	C3-C4-C5	-4.26	106.47	114.06
14	a	1114	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	b	1214	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	B	1201	CLA	C1D-ND-C4D	-4.25	103.33	106.31
14	B	1213	CLA	C1D-ND-C4D	-4.25	103.33	106.31
18	b	4017	BCR	C3-C4-C5	-4.25	106.47	114.06
14	H	1220	CLA	O2A-CGA-CBA	4.25	124.80	111.83
14	G	1127	CLA	O2A-CGA-CBA	4.25	124.80	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1127	CLA	O2A-CGA-CBA	4.25	124.80	111.83
14	G	1113	CLA	C2B-C1B-NB	4.25	114.73	110.33
14	H	1208	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
15	G	1121	F6C	C2D-C1D-ND	4.25	114.44	109.98
14	A	1113	CLA	C2B-C1B-NB	4.25	114.73	110.33
14	H	1219	CLA	C2B-C1B-NB	4.25	114.73	110.33
14	a	1116	CLA	O2A-C1-C2	4.25	124.46	108.11
14	G	1114	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	G	1116	CLA	O2A-C1-C2	4.25	124.45	108.11
14	G	1140	CLA	O2A-CGA-CBA	4.24	124.77	111.83
14	A	1116	CLA	O2A-C1-C2	4.24	124.43	108.11
14	G	1115	CLA	C1D-ND-C4D	-4.24	103.34	106.31
18	A	4011	BCR	C33-C5-C6	-4.24	119.86	124.48
14	A	1111	CLA	C4A-NA-C1A	4.24	108.61	106.68
14	A	1122	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
14	G	1114	CLA	C2D-C1D-ND	4.24	114.32	110.13
14	b	1023	CLA	C2B-C1B-NB	4.24	114.72	110.33
18	H	4013	BCR	C3-C4-C5	-4.24	106.50	114.06
14	B	1208	CLA	C1D-ND-C4D	-4.24	103.34	106.31
14	A	1107	CLA	C2D-C1D-ND	4.24	114.32	110.13
18	I	4020	BCR	C7-C8-C9	-4.23	119.97	126.23
18	i	4020	BCR	C7-C8-C9	-4.23	119.97	126.23
18	R	4020	BCR	C7-C8-C9	-4.23	119.97	126.23
14	B	1227	CLA	C4A-NA-C1A	4.23	108.61	106.68
14	A	1115	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	H	1233	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	L	1502	CLA	O2A-C1-C2	4.23	124.38	108.11
14	H	1222	CLA	CAA-C2A-C3A	-4.23	101.58	113.00
14	G	1126	CLA	O2A-CGA-CBA	4.22	124.72	111.83
13	G	1011	CL0	O2A-C1-C2	4.22	124.36	108.11
18	B	4013	BCR	C3-C4-C5	-4.22	106.53	114.06
13	A	1011	CL0	O2A-C1-C2	4.22	124.36	108.11
14	a	1107	CLA	C2D-C1D-ND	4.22	114.31	110.13
14	b	1222	CLA	CAA-C2A-C3A	-4.22	101.59	113.00
14	U	1502	CLA	O2A-C1-C2	4.22	124.35	108.11
19	A	5001	LHG	O7-C7-C8	4.22	120.61	111.48
13	a	1011	CL0	O2A-C1-C2	4.22	124.34	108.11
14	G	1107	CLA	C2D-C1D-ND	4.22	114.30	110.13
14	l	1502	CLA	O2A-C1-C2	4.22	124.34	108.11
14	G	1105	CLA	C2B-C1B-NB	4.22	114.70	110.33
14	b	1208	CLA	C1D-ND-C4D	-4.21	103.36	106.31
14	H	1208	CLA	C1D-ND-C4D	-4.21	103.36	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	4001	BCR	C24-C23-C22	-4.21	120.01	126.23
14	b	1238	CLA	C2B-C1B-NB	4.21	114.69	110.33
14	B	1222	CLA	CAA-C2A-C3A	-4.21	101.63	113.00
14	G	1118	CLA	C1D-ND-C4D	-4.20	103.36	106.31
14	A	1114	CLA	C2D-C1D-ND	4.20	114.29	110.13
14	A	1126	CLA	O2A-CGA-CBA	4.20	124.65	111.83
15	A	1120	F6C	C4A-NA-C1A	4.20	109.26	106.31
14	b	1226	CLA	O2A-C1-C2	4.20	124.27	108.11
14	B	1238	CLA	C2B-C1B-NB	4.20	114.68	110.33
14	a	1114	CLA	C2D-C1D-ND	4.20	114.28	110.13
14	B	1217	CLA	O2A-CGA-CBA	4.20	124.64	111.83
14	a	1126	CLA	O2A-CGA-CBA	4.20	124.64	111.83
14	B	1211	CLA	C2B-C1B-NB	4.20	114.68	110.33
14	H	1210	CLA	C2B-C1B-NB	4.20	114.68	110.33
14	b	1221	CLA	C1D-ND-C4D	-4.20	103.37	106.31
14	G	1112	CLA	C2B-C1B-NB	4.20	114.68	110.33
19	G	5001	LHG	O7-C7-C8	4.20	120.56	111.48
14	b	1201	CLA	C1D-ND-C4D	-4.20	103.37	106.31
14	b	1211	CLA	C2B-C1B-NB	4.20	114.68	110.33
14	H	1226	CLA	O2A-C1-C2	4.19	124.25	108.11
14	H	1211	CLA	C2B-C1B-NB	4.19	114.67	110.33
14	H	1238	CLA	C2B-C1B-NB	4.19	114.67	110.33
14	B	1226	CLA	O2A-C1-C2	4.19	124.24	108.11
14	a	1125	CLA	C1D-ND-C4D	-4.19	103.37	106.31
14	b	1217	CLA	O2A-CGA-CBA	4.18	124.59	111.83
14	a	1118	CLA	C1D-ND-C4D	-4.18	103.38	106.31
14	H	1201	CLA	C1D-ND-C4D	-4.18	103.38	106.31
14	H	1217	CLA	O2A-CGA-CBA	4.18	124.58	111.83
18	G	4003	BCR	C15-C14-C13	-4.18	121.42	127.28
14	b	1215	CLA	C2B-C1B-NB	4.18	114.66	110.33
19	a	5001	LHG	O7-C7-C8	4.18	120.51	111.48
14	G	1115	CLA	O2A-CGA-CBA	4.17	124.56	111.83
14	A	1115	CLA	O2A-CGA-CBA	4.17	124.56	111.83
14	G	1111	CLA	C4A-NA-C1A	4.17	108.58	106.68
18	A	4001	BCR	C24-C23-C22	-4.17	120.06	126.23
18	a	4001	BCR	C24-C23-C22	-4.17	120.06	126.23
14	G	1130	CLA	C2B-C1B-NB	4.17	114.65	110.33
14	a	1115	CLA	O2A-CGA-CBA	4.17	124.56	111.83
15	A	1121	F6C	C3A-C4A-NA	4.17	114.25	110.13
18	A	4003	BCR	C15-C14-C13	-4.17	121.43	127.28
14	B	1022	CLA	C1D-ND-C4D	-4.17	103.39	106.31
18	H	4012	BCR	C24-C23-C22	-4.17	120.07	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	i	4018	BCR	C33-C5-C6	-4.17	119.94	124.48
14	b	1231	CLA	O2A-CGA-CBA	4.16	124.53	111.83
14	A	1105	CLA	C2B-C1B-NB	4.16	114.64	110.33
18	b	4012	BCR	C24-C23-C22	-4.16	120.08	126.23
15	a	1120	F6C	C4A-NA-C1A	4.16	109.23	106.31
14	a	1135	CLA	O2A-CGA-CBA	4.16	124.52	111.83
19	b	5004	LHG	O7-C7-C8	4.16	120.48	111.48
14	G	1137	CLA	C1D-ND-C4D	-4.16	103.39	106.31
18	a	4003	BCR	C15-C14-C13	-4.16	121.45	127.28
15	G	1121	F6C	C3A-C4A-NA	4.16	114.24	110.13
19	B	5004	LHG	O7-C7-C8	4.16	120.47	111.48
14	B	1231	CLA	O2A-CGA-CBA	4.16	124.51	111.83
14	A	1118	CLA	C1D-ND-C4D	-4.16	103.40	106.31
14	a	1105	CLA	C2B-C1B-NB	4.15	114.63	110.33
15	a	1121	F6C	C3A-C4A-NA	4.15	114.24	110.13
14	A	1112	CLA	C2B-C1B-NB	4.15	114.63	110.33
19	H	5004	LHG	O7-C7-C8	4.15	120.46	111.48
15	G	1120	F6C	C4A-NA-C1A	4.15	109.22	106.31
18	G	4008	BCR	C24-C23-C22	-4.15	120.10	126.23
14	H	1231	CLA	O2A-CGA-CBA	4.15	124.48	111.83
14	H	1215	CLA	C2B-C1B-NB	4.15	114.62	110.33
14	G	1132	CLA	O2A-CGA-CBA	4.14	124.47	111.83
18	U	4022	BCR	C33-C5-C6	-4.14	119.96	124.48
14	a	1112	CLA	C2B-C1B-NB	4.14	114.62	110.33
14	A	1135	CLA	O2A-CGA-CBA	4.14	124.46	111.83
14	G	1135	CLA	O2A-CGA-CBA	4.14	124.46	111.83
18	L	4022	BCR	C33-C5-C6	-4.14	119.97	124.48
14	a	1132	CLA	O2A-CGA-CBA	4.14	124.45	111.83
14	a	1130	CLA	C2B-C1B-NB	4.14	114.62	110.33
14	H	1203	CLA	O2D-CGD-CBD	4.14	118.46	111.23
18	B	4012	BCR	C24-C23-C22	-4.13	120.12	126.23
14	A	1125	CLA	C1D-ND-C4D	-4.13	103.41	106.31
14	A	1130	CLA	C2B-C1B-NB	4.13	114.61	110.33
14	b	1203	CLA	O2D-CGD-CBD	4.13	118.45	111.23
14	A	1132	CLA	O2A-CGA-CBA	4.13	124.42	111.83
14	B	1215	CLA	C2B-C1B-NB	4.13	114.61	110.33
14	b	1210	CLA	C2B-C1B-NB	4.13	114.61	110.33
14	G	1125	CLA	C1D-ND-C4D	-4.13	103.42	106.31
14	b	1022	CLA	C1D-ND-C4D	-4.12	103.42	106.31
14	a	1116	CLA	O2A-CGA-CBA	4.12	124.41	111.83
14	B	1210	CLA	C2B-C1B-NB	4.12	114.60	110.33
14	b	1229	CLA	C2B-C1B-NB	4.12	114.60	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4008	BCR	C24-C23-C22	-4.12	120.14	126.23
14	a	1137	CLA	C1D-ND-C4D	-4.12	103.42	106.31
14	B	1203	CLA	O2D-CGD-CBD	4.12	118.43	111.23
14	a	1127	CLA	C1D-ND-C4D	-4.12	103.42	106.31
14	A	1112	CLA	C1D-ND-C4D	-4.12	103.42	106.31
14	a	1111	CLA	C1D-ND-C4D	-4.12	103.42	106.31
14	H	1229	CLA	C2B-C1B-NB	4.12	114.59	110.33
14	G	1133	CLA	O2A-CGA-CBA	4.11	124.38	111.83
14	G	1119	CLA	C2B-C1B-NB	4.11	114.59	110.33
14	A	1131	CLA	O2A-CGA-CBA	4.11	124.38	111.83
18	A	4008	BCR	C24-C23-C22	-4.11	120.15	126.23
14	b	1220	CLA	CAA-C2A-C3A	-4.11	101.89	113.00
14	a	1119	CLA	C2B-C1B-NB	4.11	114.59	110.33
14	A	1116	CLA	O2A-CGA-CBA	4.11	124.37	111.83
18	R	4018	BCR	C33-C5-C6	-4.11	120.00	124.48
14	H	1216	CLA	O2A-C1-C2	4.11	123.91	108.11
14	A	1137	CLA	C1D-ND-C4D	-4.11	103.43	106.31
14	H	1202	CLA	C1D-ND-C4D	-4.11	103.43	106.31
14	b	1216	CLA	O2A-C1-C2	4.11	123.91	108.11
14	G	1127	CLA	C1D-ND-C4D	-4.10	103.43	106.31
14	B	1229	CLA	C2B-C1B-NB	4.10	114.58	110.33
14	H	1012	CLA	C1D-ND-C4D	-4.10	103.43	106.31
14	G	1116	CLA	O2A-CGA-CBA	4.10	124.35	111.83
18	I	4018	BCR	C33-C5-C6	-4.10	120.01	124.48
14	a	1133	CLA	O2A-CGA-CBA	4.10	124.34	111.83
14	B	1220	CLA	CAA-C2A-C3A	-4.10	101.92	113.00
18	l	4022	BCR	C33-C5-C6	-4.10	120.01	124.48
15	G	1120	F6C	C3A-C4A-NA	4.10	114.18	110.13
14	G	1131	CLA	O2A-CGA-CBA	4.10	124.33	111.83
14	G	1111	CLA	CAC-C3C-C4C	4.09	130.12	124.79
14	A	1133	CLA	O2A-CGA-CBA	4.09	124.32	111.83
14	A	1127	CLA	C1D-ND-C4D	-4.09	103.44	106.31
14	a	1103	CLA	O2A-CGA-CBA	4.09	124.31	111.83
14	G	1104	CLA	O2A-CGA-CBA	4.09	124.31	111.83
14	a	1131	CLA	O2A-CGA-CBA	4.09	124.31	111.83
14	B	1227	CLA	C3D-C2D-C1D	-4.09	100.26	105.83
14	B	1216	CLA	O2A-C1-C2	4.09	123.83	108.11
14	A	1111	CLA	C2B-C1B-NB	4.08	114.56	110.33
18	B	4006	BCR	C4-C5-C6	-4.08	117.19	122.70
14	A	1111	CLA	CAC-C3C-C4C	4.08	130.10	124.79
14	H	1220	CLA	CAA-C2A-C3A	-4.08	101.97	113.00
14	A	1103	CLA	O2A-CGA-CBA	4.08	124.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	1120	F6C	C3A-C4A-NA	4.08	114.17	110.13
14	H	1214	CLA	C2D-C1D-ND	4.08	114.16	110.13
14	A	1104	CLA	O2A-CGA-CBA	4.08	124.27	111.83
18	a	4007	BCR	C33-C5-C6	-4.08	120.04	124.48
14	L	1502	CLA	CHD-C1D-ND	-4.07	119.07	124.80
14	H	1227	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
18	G	4001	BCR	C19-C18-C17	4.07	125.42	119.01
14	a	1104	CLA	O2A-CGA-CBA	4.07	124.25	111.83
14	A	1119	CLA	C2B-C1B-NB	4.07	114.55	110.33
18	H	4006	BCR	C4-C5-C6	-4.07	117.20	122.70
14	l	1502	CLA	CHD-C1D-ND	-4.07	119.08	124.80
14	G	1112	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	G	1114	CLA	C2B-C1B-NB	4.07	114.54	110.33
18	G	4007	BCR	C33-C5-C6	-4.07	120.05	124.48
15	A	1120	F6C	C3A-C4A-NA	4.06	114.15	110.13
14	a	1114	CLA	C2B-C1B-NB	4.06	114.54	110.33
18	A	4007	BCR	C33-C5-C6	-4.06	120.05	124.48
14	G	1103	CLA	O2A-CGA-CBA	4.06	124.21	111.83
14	G	1111	CLA	C2B-C1B-NB	4.06	114.53	110.33
14	b	1227	CLA	C3D-C2D-C1D	-4.06	100.29	105.83
14	A	1111	CLA	C1D-ND-C4D	-4.06	103.47	106.31
14	a	1112	CLA	C1D-ND-C4D	-4.06	103.47	106.31
14	K	1401	CLA	O2D-CGD-CBD	4.06	118.32	111.23
14	G	1117	CLA	O2A-CGA-CBA	4.06	124.21	111.83
14	G	1012	CLA	O2A-C1-C2	4.05	123.71	108.11
14	B	1214	CLA	C2D-C1D-ND	4.05	114.14	110.13
14	a	1111	CLA	C2B-C1B-NB	4.05	114.53	110.33
14	A	1012	CLA	O2A-C1-C2	4.05	123.69	108.11
14	a	1012	CLA	O2A-C1-C2	4.05	123.68	108.11
18	b	4006	BCR	C4-C5-C6	-4.05	117.24	122.70
14	b	1202	CLA	C1D-ND-C4D	-4.05	103.47	106.31
14	A	1116	CLA	C1D-ND-C4D	-4.04	103.47	106.31
14	G	1119	CLA	C1D-ND-C4D	-4.04	103.47	106.31
14	A	1119	CLA	O2A-C1-C2	4.04	123.67	108.11
18	A	4001	BCR	C19-C18-C17	4.04	125.37	119.01
14	T	1401	CLA	O2D-CGD-CBD	4.04	118.30	111.23
14	b	1214	CLA	C2D-C1D-ND	4.04	114.12	110.13
14	a	1119	CLA	C1D-ND-C4D	-4.04	103.48	106.31
14	A	1114	CLA	C2B-C1B-NB	4.04	114.52	110.33
14	a	1119	CLA	O2A-C1-C2	4.04	123.65	108.11
14	a	1111	CLA	CAC-C3C-C4C	4.04	130.04	124.79
18	a	4001	BCR	C19-C18-C17	4.04	125.36	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1129	CLA	O2D-CGD-O1D	-4.04	115.99	123.85
14	a	1117	CLA	O2A-CGA-CBA	4.04	124.14	111.83
14	A	1117	CLA	O2A-CGA-CBA	4.03	124.13	111.83
14	B	1238	CLA	C1D-ND-C4D	-4.03	103.48	106.31
14	a	1116	CLA	C1D-ND-C4D	-4.03	103.48	106.31
14	G	1119	CLA	O2A-C1-C2	4.03	123.62	108.11
14	a	1125	CLA	O2A-C1-C2	4.03	123.62	108.11
14	B	1204	CLA	C2B-C1B-NB	4.03	114.51	110.33
14	b	1224	CLA	C2B-C1B-NB	4.03	114.50	110.33
14	b	1228	CLA	C2B-C1B-NB	4.03	114.50	110.33
15	B	1230	F6C	C4A-C3A-C2A	-4.03	101.00	106.97
14	A	1129	CLA	O2D-CGD-O1D	-4.03	116.01	123.85
14	b	1225	CLA	O2A-CGA-CBA	4.03	124.11	111.83
14	G	1125	CLA	O2A-C1-C2	4.03	123.60	108.11
18	A	4002	BCR	C19-C18-C17	4.02	125.34	119.01
14	A	1119	CLA	C1D-ND-C4D	-4.02	103.49	106.31
14	a	1129	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
14	b	1204	CLA	C2B-C1B-NB	4.02	114.50	110.33
14	b	1023	CLA	O2A-C1-C2	4.02	123.58	108.11
15	H	1230	F6C	C4A-C3A-C2A	-4.02	101.01	106.97
14	H	1225	CLA	O2A-CGA-CBA	4.02	124.08	111.83
14	A	1109	CLA	CHD-C1D-ND	-4.02	119.15	124.80
14	A	1125	CLA	O2A-C1-C2	4.02	123.57	108.11
14	G	1111	CLA	C1D-ND-C4D	-4.02	103.49	106.31
14	k	1401	CLA	O2D-CGD-CBD	4.02	118.25	111.23
14	B	1202	CLA	C1D-ND-C4D	-4.01	103.50	106.31
14	H	1204	CLA	C2B-C1B-NB	4.01	114.49	110.33
18	a	4002	BCR	C19-C18-C17	4.01	125.32	119.01
14	H	1023	CLA	O2A-C1-C2	4.01	123.55	108.11
14	U	1502	CLA	CHD-C1D-ND	-4.01	119.16	124.80
14	H	1021	CLA	CAA-C2A-C3A	-4.01	102.17	113.00
14	a	1111	CLA	C4A-NA-C1A	4.01	108.51	106.68
14	G	1116	CLA	C1D-ND-C4D	-4.01	103.50	106.31
14	B	1225	CLA	O2A-CGA-CBA	4.01	124.05	111.83
14	B	1023	CLA	O2A-C1-C2	4.01	123.53	108.11
14	B	1228	CLA	C2B-C1B-NB	4.00	114.47	110.33
14	b	1021	CLA	CAA-C2A-C3A	-4.00	102.20	113.00
14	H	1228	CLA	C2B-C1B-NB	4.00	114.47	110.33
18	H	4016	BCR	C15-C14-C13	-4.00	121.67	127.28
14	B	1216	CLA	O2A-CGA-CBA	3.99	124.02	111.83
14	G	1109	CLA	CHD-C1D-ND	-3.99	119.18	124.80
14	L	1501	CLA	C2B-C1B-NB	3.99	114.47	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1021	CLA	CAA-C2A-C3A	-3.99	102.21	113.00
14	B	1022	CLA	O2A-CGA-CBA	3.99	124.01	111.83
18	B	4005	BCR	C34-C9-C10	-3.99	116.35	122.82
14	H	1224	CLA	C2B-C1B-NB	3.99	114.47	110.33
14	a	1133	CLA	C1D-ND-C4D	-3.99	103.51	106.31
14	H	1220	CLA	O2A-C1-C2	3.99	123.46	108.11
14	b	1216	CLA	O2A-CGA-CBA	3.99	123.99	111.83
14	b	1220	CLA	O2A-C1-C2	3.99	123.45	108.11
14	b	1022	CLA	O2A-CGA-CBA	3.98	123.98	111.83
14	H	1216	CLA	O2A-CGA-CBA	3.98	123.98	111.83
18	G	4002	BCR	C19-C18-C17	3.98	125.27	119.01
14	B	1220	CLA	O2A-C1-C2	3.98	123.43	108.11
14	H	1012	CLA	O2A-CGA-CBA	3.98	123.98	111.83
18	R	4020	BCR	C19-C18-C17	3.98	125.27	119.01
14	b	1226	CLA	C2D-C1D-ND	3.98	114.07	110.13
14	B	1224	CLA	C2B-C1B-NB	3.98	114.45	110.33
18	b	4016	BCR	C15-C14-C13	-3.98	121.70	127.28
14	a	1109	CLA	CHD-C1D-ND	-3.98	119.21	124.80
18	H	4005	BCR	C34-C9-C10	-3.97	116.38	122.82
14	a	1013	CLA	O2A-CGA-CBA	3.97	123.95	111.83
14	b	1214	CLA	O2A-CGA-CBA	3.97	123.94	111.83
14	a	1132	CLA	C2B-C1B-NB	3.97	114.44	110.33
14	B	1214	CLA	O2A-CGA-CBA	3.97	123.94	111.83
14	G	1132	CLA	C2B-C1B-NB	3.97	114.44	110.33
14	l	1501	CLA	C2B-C1B-NB	3.97	114.44	110.33
18	I	4020	BCR	C19-C18-C17	3.97	125.25	119.01
14	H	1214	CLA	O2A-CGA-CBA	3.96	123.92	111.83
15	b	1230	F6C	C4A-C3A-C2A	-3.96	101.09	106.97
14	A	1013	CLA	O2A-CGA-CBA	3.96	123.92	111.83
14	a	1117	CLA	C2B-C1B-NB	3.96	114.43	110.33
14	A	1133	CLA	C1D-ND-C4D	-3.96	103.53	106.31
14	B	1221	CLA	C2B-C1B-NB	3.96	114.43	110.33
14	b	1204	CLA	C4A-NA-C1A	3.96	108.48	106.68
18	i	4020	BCR	C19-C18-C17	3.96	125.23	119.01
14	b	1238	CLA	C1D-ND-C4D	-3.95	103.54	106.31
14	G	1013	CLA	O2A-CGA-CBA	3.95	123.89	111.83
14	H	1226	CLA	C2D-C1D-ND	3.95	114.03	110.13
18	B	4016	BCR	C15-C14-C13	-3.95	121.74	127.28
14	H	1213	CLA	C2B-C1B-NB	3.95	114.42	110.33
14	H	1229	CLA	C4-C3-C5	3.95	122.08	115.23
14	A	1122	CLA	O2A-CGA-CBA	3.94	123.86	111.83
14	H	1213	CLA	O2A-C1-C2	3.94	123.28	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b	4005	BCR	C34-C9-C10	-3.94	116.43	122.82
14	B	1213	CLA	O2A-C1-C2	3.94	123.27	108.11
14	B	1226	CLA	C2D-C1D-ND	3.94	114.02	110.13
14	A	1132	CLA	C2B-C1B-NB	3.94	114.41	110.33
14	U	1501	CLA	C2B-C1B-NB	3.94	114.41	110.33
14	b	1213	CLA	O2A-C1-C2	3.93	123.24	108.11
18	b	4005	BCR	C7-C8-C9	-3.93	120.42	126.23
14	a	1122	CLA	O2A-CGA-CBA	3.93	123.82	111.83
14	H	1221	CLA	C2B-C1B-NB	3.93	114.40	110.33
14	b	1224	CLA	O2A-CGA-CBA	3.93	123.81	111.83
14	H	1228	CLA	CHD-C1D-ND	-3.93	119.28	124.80
14	G	1117	CLA	C2B-C1B-NB	3.93	114.40	110.33
14	G	1133	CLA	C1D-ND-C4D	-3.93	103.56	106.31
14	H	1224	CLA	O2A-CGA-CBA	3.92	123.80	111.83
14	G	1122	CLA	C2B-C1B-NB	3.92	114.39	110.33
14	H	1238	CLA	C1D-ND-C4D	-3.92	103.56	106.31
18	G	4007	BCR	C3-C4-C5	-3.92	107.06	114.06
14	b	1221	CLA	C2B-C1B-NB	3.92	114.39	110.33
14	B	1225	CLA	O2A-C1-C2	3.92	123.19	108.11
18	H	4005	BCR	C7-C8-C9	-3.92	120.44	126.23
18	A	4007	BCR	C3-C4-C5	-3.92	107.07	114.06
14	B	1204	CLA	C4A-NA-C1A	3.92	108.47	106.68
20	l	5007	LMG	O7-C10-C11	3.92	119.95	111.48
18	a	4007	BCR	C3-C4-C5	-3.92	107.07	114.06
14	B	1228	CLA	CHD-C1D-ND	-3.91	119.29	124.80
14	B	1224	CLA	O2A-CGA-CBA	3.91	123.77	111.83
14	b	1225	CLA	O2A-C1-C2	3.91	123.17	108.11
14	B	1206	CLA	C1D-ND-C4D	-3.91	103.57	106.31
20	L	5007	LMG	O7-C10-C11	3.91	119.94	111.48
14	b	1210	CLA	O2A-CGA-O1A	-3.91	113.85	123.63
20	U	5007	LMG	O7-C10-C11	3.91	119.94	111.48
14	H	1223	CLA	O2A-CGA-CBA	3.91	123.75	111.83
18	B	4005	BCR	C7-C8-C9	-3.91	120.45	126.23
18	b	4009	BCR	C38-C26-C25	-3.91	120.22	124.48
14	B	1229	CLA	C4-C3-C5	3.91	122.01	115.23
18	G	4007	BCR	C24-C23-C22	-3.91	120.46	126.23
14	H	1225	CLA	O2A-C1-C2	3.91	123.14	108.11
18	B	4009	BCR	C38-C26-C25	-3.91	120.22	124.48
14	H	1206	CLA	C1D-ND-C4D	-3.91	103.57	106.31
14	G	1122	CLA	O2A-CGA-CBA	3.90	123.74	111.83
14	b	1229	CLA	C4-C3-C5	3.90	122.00	115.23
14	H	1210	CLA	O2A-CGA-O1A	-3.90	113.87	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1213	CLA	C2B-C1B-NB	3.90	114.37	110.33
15	A	1120	F6C	C4A-C3A-C2A	-3.90	101.19	106.97
18	b	4016	BCR	C24-C23-C22	-3.90	120.47	126.23
18	A	4007	BCR	C24-C23-C22	-3.89	120.47	126.23
14	b	1223	CLA	O2A-CGA-CBA	3.89	123.71	111.83
15	G	1120	F6C	C4A-C3A-C2A	-3.89	101.19	106.97
15	a	1120	F6C	C4A-C3A-C2A	-3.89	101.19	106.97
14	B	1223	CLA	O2A-CGA-CBA	3.89	123.70	111.83
14	B	1210	CLA	O2A-CGA-O1A	-3.89	113.89	123.63
14	H	1207	CLA	C1D-ND-C4D	-3.89	103.58	106.31
18	H	4009	BCR	C38-C26-C25	-3.89	120.24	124.48
14	B	1204	CLA	O2A-C1-C2	3.89	123.07	108.11
14	A	1117	CLA	C2B-C1B-NB	3.89	114.36	110.33
14	b	1229	CLA	CHD-C1D-ND	-3.88	119.34	124.80
14	B	1209	CLA	C2B-C1B-NB	3.88	114.35	110.33
14	b	1213	CLA	C2B-C1B-NB	3.88	114.35	110.33
18	B	4016	BCR	C24-C23-C22	-3.88	120.49	126.23
14	H	1209	CLA	C2B-C1B-NB	3.88	114.35	110.33
18	G	4008	BCR	C7-C8-C9	-3.88	120.49	126.23
14	A	1122	CLA	C2B-C1B-NB	3.88	114.35	110.33
14	H	1204	CLA	O2A-C1-C2	3.88	123.04	108.11
14	a	1118	CLA	O2A-C1-C2	3.88	123.04	108.11
14	b	1228	CLA	CHD-C1D-ND	-3.88	119.34	124.80
14	A	1103	CLA	C2B-C1B-NB	3.88	114.35	110.33
14	B	1229	CLA	CHD-C1D-ND	-3.88	119.34	124.80
14	a	1122	CLA	O2D-CGD-CBD	3.88	118.01	111.23
14	G	1118	CLA	O2A-C1-C2	3.88	123.03	108.11
14	b	1204	CLA	O2A-C1-C2	3.88	123.03	108.11
14	A	1118	CLA	O2A-C1-C2	3.88	123.02	108.11
14	a	1118	CLA	O2A-CGA-CBA	3.87	123.65	111.83
14	a	1104	CLA	C2B-C1B-NB	3.87	114.34	110.33
18	R	4020	BCR	C35-C13-C12	3.87	124.00	118.09
14	a	1122	CLA	C2B-C1B-NB	3.87	114.34	110.33
18	A	4008	BCR	C7-C8-C9	-3.87	120.51	126.23
14	a	1102	CLA	C1D-ND-C4D	-3.87	103.60	106.31
14	a	1115	CLA	C2B-C1B-NB	3.87	114.34	110.33
14	G	1102	CLA	C1D-ND-C4D	-3.87	103.60	106.31
14	G	1104	CLA	C2B-C1B-NB	3.86	114.33	110.33
14	B	1239	CLA	C1-C2-C3	-3.86	119.86	126.20
14	H	1238	CLA	C4A-NA-C1A	3.86	108.44	106.68
18	I	4020	BCR	C35-C13-C12	3.86	123.99	118.09
14	H	1023	CLA	CAA-C2A-C3A	-3.86	102.57	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1207	CLA	C1D-ND-C4D	-3.86	103.61	106.31
14	G	1103	CLA	C2B-C1B-NB	3.86	114.33	110.33
14	b	1023	CLA	CAA-C2A-C3A	-3.86	102.58	113.00
14	A	1118	CLA	O2A-CGA-CBA	3.86	123.59	111.83
18	i	4020	BCR	C35-C13-C12	3.86	123.98	118.09
14	H	1229	CLA	CHD-C1D-ND	-3.86	119.38	124.80
18	a	4007	BCR	C24-C23-C22	-3.85	120.53	126.23
14	A	1102	CLA	C1D-ND-C4D	-3.85	103.61	106.31
14	H	1239	CLA	C1D-ND-C4D	-3.85	103.61	106.31
18	B	4009	BCR	C33-C5-C6	-3.85	120.28	124.48
18	a	4008	BCR	C7-C8-C9	-3.85	120.54	126.23
14	B	1023	CLA	CAA-C2A-C3A	-3.85	102.60	113.00
14	b	1239	CLA	C1-C2-C3	-3.85	119.89	126.20
14	b	1209	CLA	C2B-C1B-NB	3.85	114.32	110.33
14	a	1103	CLA	C2B-C1B-NB	3.85	114.31	110.33
14	G	1118	CLA	O2A-CGA-CBA	3.85	123.56	111.83
14	A	1123	CLA	C1D-ND-C4D	-3.85	103.61	106.31
18	H	4016	BCR	C24-C23-C22	-3.84	120.55	126.23
14	b	1226	CLA	O2D-CGD-O1D	-3.84	116.37	123.85
14	G	1122	CLA	O2D-CGD-CBD	3.84	117.95	111.23
14	B	1226	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
14	G	1132	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
14	b	1238	CLA	O2A-C1-C2	3.84	122.87	108.11
14	H	1204	CLA	C4A-NA-C1A	3.84	108.43	106.68
14	a	1128	CLA	O2A-C1-C2	3.84	122.87	108.11
14	a	1132	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
14	H	1238	CLA	O2A-C1-C2	3.83	122.86	108.11
14	G	1128	CLA	O2A-C1-C2	3.83	122.86	108.11
18	B	4013	BCR	C7-C8-C9	-3.83	120.57	126.23
14	A	1128	CLA	O2A-C1-C2	3.83	122.85	108.11
18	B	4012	BCR	C33-C5-C6	-3.83	120.30	124.48
14	A	1102	CLA	O2A-CGA-CBA	3.83	123.52	111.83
14	G	1115	CLA	C2B-C1B-NB	3.83	114.30	110.33
14	B	1239	CLA	C1D-ND-C4D	-3.83	103.62	106.31
14	G	1123	CLA	O2A-CGA-CBA	3.83	123.51	111.83
14	H	1226	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
14	A	1122	CLA	O2D-CGD-CBD	3.83	117.92	111.23
14	A	1110	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
18	b	4013	BCR	C7-C8-C9	-3.83	120.57	126.23
14	A	1104	CLA	C2B-C1B-NB	3.83	114.30	110.33
14	A	1132	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
14	b	1206	CLA	C1D-ND-C4D	-3.83	103.63	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	l	4019	BCR	C38-C26-C25	-3.83	120.31	124.48
18	H	4006	BCR	C7-C8-C9	3.82	131.89	126.23
14	B	1238	CLA	O2A-C1-C2	3.82	122.81	108.11
14	a	1102	CLA	O2A-CGA-CBA	3.82	123.49	111.83
18	H	4012	BCR	C33-C5-C6	-3.82	120.31	124.48
14	B	1023	CLA	C4C-C3C-C2C	-3.82	101.33	106.89
14	a	1110	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
14	A	1123	CLA	O2A-CGA-CBA	3.82	123.48	111.83
14	H	1204	CLA	CHD-C1D-ND	-3.82	119.43	124.80
20	H	5002	LMG	O7-C10-C11	3.82	119.74	111.48
20	b	5002	LMG	O7-C10-C11	3.82	119.74	111.48
14	H	1239	CLA	C1-C2-C3	-3.82	119.95	126.20
20	B	5002	LMG	O7-C10-C11	3.81	119.73	111.48
18	H	4013	BCR	C7-C8-C9	-3.81	120.59	126.23
15	B	1230	F6C	C3A-C4A-NA	3.81	113.90	110.13
14	a	1115	CLA	CHD-C1D-ND	-3.81	119.44	124.80
18	b	4012	BCR	C38-C26-C25	-3.81	120.33	124.48
14	a	1123	CLA	O2A-CGA-CBA	3.81	123.45	111.83
14	G	1102	CLA	O2A-CGA-CBA	3.81	123.44	111.83
14	G	1110	CLA	O2D-CGD-O1D	-3.81	116.44	123.85
14	A	1115	CLA	C2B-C1B-NB	3.81	114.27	110.33
18	b	4012	BCR	C33-C5-C6	-3.81	120.33	124.48
18	b	4006	BCR	C7-C8-C9	3.80	131.86	126.23
18	B	4012	BCR	C38-C26-C25	-3.80	120.33	124.48
18	U	4019	BCR	C38-C26-C25	-3.80	120.33	124.48
14	L	1501	CLA	CBA-CAA-C2A	3.80	125.11	113.79
14	b	1204	CLA	CHD-C1D-ND	-3.80	119.45	124.80
14	b	1023	CLA	C4C-C3C-C2C	-3.80	101.36	106.89
15	H	1230	F6C	C3A-C4A-NA	3.80	113.89	110.13
18	B	4006	BCR	C7-C8-C9	3.80	131.85	126.23
14	U	1501	CLA	CBA-CAA-C2A	3.80	125.09	113.79
14	b	1216	CLA	C2B-C1B-NB	3.80	114.26	110.33
14	G	1012	CLA	CHD-C1D-ND	-3.80	119.46	124.80
14	B	1207	CLA	C1D-ND-C4D	-3.80	103.65	106.31
14	A	1115	CLA	CHD-C1D-ND	-3.80	119.46	124.80
18	H	4009	BCR	C33-C5-C6	-3.80	120.34	124.48
18	b	4009	BCR	C33-C5-C6	-3.80	120.34	124.48
14	H	1023	CLA	C4C-C3C-C2C	-3.79	101.37	106.89
14	A	1124	CLA	O2A-CGA-CBA	3.79	123.40	111.83
14	G	1124	CLA	O2A-CGA-CBA	3.79	123.40	111.83
14	a	1119	CLA	O2A-CGA-CBA	3.79	123.40	111.83
18	b	4017	BCR	C15-C14-C13	-3.79	121.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1013	CLA	CMB-C2B-C3B	3.79	135.47	126.55
18	b	4005	BCR	C33-C5-C6	-3.79	120.35	124.48
14	B	1204	CLA	CHD-C1D-ND	-3.79	119.47	124.80
14	G	1115	CLA	CHD-C1D-ND	-3.79	119.47	124.80
14	B	1216	CLA	C2B-C1B-NB	3.79	114.25	110.33
14	a	1124	CLA	O2A-CGA-CBA	3.79	123.38	111.83
14	a	1111	CLA	O2A-C1-C2	3.79	122.68	108.11
14	a	1013	CLA	CMB-C2B-C3B	3.79	135.46	126.55
14	A	1119	CLA	O2A-CGA-CBA	3.79	123.38	111.83
18	l	4022	BCR	C28-C27-C26	-3.78	107.31	114.06
14	b	1235	CLA	CAA-C2A-C3A	-3.78	102.77	113.00
18	M	4021	BCR	C19-C18-C17	3.78	124.96	119.01
14	A	1118	CLA	C4-C3-C5	3.78	121.80	115.23
14	G	1013	CLA	CMB-C2B-C3B	3.78	135.45	126.55
14	A	1135	CLA	C2B-C1B-NB	3.78	114.25	110.33
14	a	1118	CLA	C4-C3-C5	3.78	121.79	115.23
14	H	1235	CLA	CAA-C2A-C3A	-3.78	102.78	113.00
14	G	1119	CLA	O2A-CGA-CBA	3.78	123.36	111.83
14	G	1123	CLA	C1D-ND-C4D	-3.78	103.66	106.31
14	a	1135	CLA	C2B-C1B-NB	3.78	114.25	110.33
14	b	1239	CLA	C1D-ND-C4D	-3.78	103.66	106.31
14	l	1501	CLA	CBA-CAA-C2A	3.78	125.04	113.79
14	G	1118	CLA	C4-C3-C5	3.78	121.79	115.23
14	A	1012	CLA	CHD-C1D-ND	-3.78	119.49	124.80
18	U	4022	BCR	C28-C27-C26	-3.77	107.33	114.06
14	A	1012	CLA	C1D-ND-C4D	-3.77	103.67	106.31
14	G	1111	CLA	O2A-C1-C2	3.77	122.61	108.11
18	H	4005	BCR	C33-C5-C6	-3.77	120.37	124.48
14	G	1132	CLA	CAA-C2A-C3A	-3.77	102.82	113.00
14	A	1111	CLA	O2A-C1-C2	3.77	122.60	108.11
18	H	4017	BCR	C7-C8-C9	-3.77	120.67	126.23
14	A	1132	CLA	CAA-C2A-C3A	-3.76	102.83	113.00
14	B	1235	CLA	CAA-C2A-C3A	-3.76	102.83	113.00
14	a	1012	CLA	CHD-C1D-ND	-3.76	119.50	124.80
14	b	1021	CLA	CAA-CBA-CGA	-3.76	102.52	113.21
14	a	1136	CLA	O2A-C1-C2	3.76	122.59	108.11
14	b	1238	CLA	C4A-NA-C1A	3.76	108.39	106.68
18	B	4005	BCR	C33-C5-C6	-3.76	120.38	124.48
14	H	1021	CLA	CAA-CBA-CGA	-3.76	102.53	113.21
14	A	1136	CLA	O2A-C1-C2	3.76	122.58	108.11
14	a	1123	CLA	C1D-ND-C4D	-3.76	103.67	106.31
14	A	1125	CLA	O2D-CGD-O1D	-3.76	116.53	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1136	CLA	O2A-C1-C2	3.76	122.58	108.11
18	B	4017	BCR	C15-C14-C13	-3.76	122.01	127.28
14	a	1132	CLA	CAA-C2A-C3A	-3.76	102.84	113.00
14	G	1135	CLA	C2B-C1B-NB	3.76	114.22	110.33
14	G	1105	CLA	CHD-C1D-ND	-3.76	119.52	124.80
18	m	4021	BCR	C19-C18-C17	3.76	124.92	119.01
14	B	1238	CLA	C4A-NA-C1A	3.75	108.39	106.68
18	H	4012	BCR	C38-C26-C25	-3.75	120.39	124.48
18	b	4017	BCR	C7-C8-C9	-3.75	120.68	126.23
18	b	4006	BCR	C34-C9-C8	3.75	123.82	118.09
14	A	1130	CLA	OBD-CAD-C3D	-3.75	119.65	128.42
14	b	1206	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
14	B	1021	CLA	CAA-CBA-CGA	-3.75	102.56	113.21
18	L	4019	BCR	C38-C26-C25	-3.75	120.39	124.48
18	B	4017	BCR	C7-C8-C9	-3.75	120.69	126.23
14	B	1208	CLA	CAA-C2A-C3A	-3.75	102.88	113.00
18	B	4006	BCR	C34-C9-C8	3.75	123.81	118.09
14	H	1216	CLA	C2B-C1B-NB	3.75	114.21	110.33
14	a	1105	CLA	CHD-C1D-ND	-3.74	119.53	124.80
14	A	1106	CLA	C2B-C1B-NB	3.74	114.21	110.33
14	G	1125	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
18	L	4022	BCR	C28-C27-C26	-3.74	107.38	114.06
18	V	4021	BCR	C19-C18-C17	3.74	124.89	119.01
14	G	1130	CLA	OBD-CAD-C3D	-3.74	119.67	128.42
14	B	1227	CLA	C2D-C1D-ND	3.74	113.83	110.13
14	a	1130	CLA	OBD-CAD-C3D	-3.74	119.68	128.42
14	b	1203	CLA	O2A-C1-C2	3.74	122.49	108.11
14	G	1138	CLA	O2A-CGA-CBA	3.74	123.23	111.83
14	H	1234	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
14	H	1221	CLA	O2A-C1-C2	3.74	122.49	108.11
14	A	1107	CLA	C1D-ND-C4D	-3.74	103.69	106.31
14	H	1208	CLA	CAA-C2A-C3A	-3.73	102.91	113.00
14	B	1221	CLA	O2A-C1-C2	3.73	122.48	108.11
14	a	1107	CLA	C1D-ND-C4D	-3.73	103.69	106.31
14	H	1227	CLA	C2D-C1D-ND	3.73	113.82	110.13
14	l	1501	CLA	C1-C2-C3	-3.73	120.08	126.20
14	B	1206	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
14	b	1221	CLA	O2A-C1-C2	3.73	122.46	108.11
14	A	1105	CLA	CHD-C1D-ND	-3.73	119.55	124.80
14	b	1208	CLA	CAA-C2A-C3A	-3.73	102.92	113.00
18	H	4006	BCR	C34-C9-C8	3.73	123.78	118.09
14	H	1206	CLA	C3B-C2B-C1B	-3.73	102.78	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	U	1503	CLA	CAA-C2A-C3A	-3.73	102.93	113.00
14	H	1203	CLA	O2A-C1-C2	3.73	122.45	108.11
18	H	4004	BCR	C19-C18-C17	3.73	124.87	119.01
14	l	1503	CLA	CAA-C2A-C3A	-3.73	102.93	113.00
14	a	1138	CLA	O2A-CGA-CBA	3.73	123.20	111.83
14	B	1203	CLA	O2A-C1-C2	3.73	122.45	108.11
14	A	1138	CLA	O2A-CGA-CBA	3.73	123.19	111.83
15	b	1230	F6C	C3A-C4A-NA	3.72	113.81	110.13
14	G	1012	CLA	C1D-ND-C4D	-3.72	103.70	106.31
14	b	1234	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
14	L	1503	CLA	CAA-C2A-C3A	-3.72	102.94	113.00
14	A	1139	CLA	CAA-C2A-C3A	-3.72	102.94	113.00
14	a	1125	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
14	B	1214	CLA	O2A-C1-C2	3.72	122.42	108.11
14	B	1234	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
18	A	4001	BCR	C36-C18-C17	-3.72	116.79	122.82
14	B	1222	CLA	CHD-C1D-ND	-3.72	119.57	124.80
18	G	4001	BCR	C36-C18-C17	-3.72	116.80	122.82
14	G	1132	CLA	O2A-C1-C2	3.71	122.40	108.11
14	B	1211	CLA	O2A-CGA-CBA	3.71	123.16	111.83
14	l	1501	CLA	O2A-CGA-CBA	3.71	123.16	111.83
14	G	1106	CLA	C2B-C1B-NB	3.71	114.18	110.33
14	a	1130	CLA	O2A-CGA-CBA	3.71	123.15	111.83
14	A	1012	CLA	CMB-C2B-C1B	3.71	131.07	125.42
14	A	1130	CLA	O2A-CGA-CBA	3.71	123.15	111.83
14	a	1138	CLA	C1D-ND-C4D	-3.71	103.71	106.31
14	A	1132	CLA	O2A-C1-C2	3.71	122.38	108.11
18	a	4001	BCR	C36-C18-C17	-3.71	116.81	122.82
18	B	4004	BCR	C19-C18-C17	3.71	124.84	119.01
14	H	1214	CLA	O2A-C1-C2	3.71	122.37	108.11
14	B	1226	CLA	C2B-C1B-NB	3.71	114.17	110.33
14	G	1139	CLA	CAA-C2A-C3A	-3.70	102.99	113.00
14	H	1211	CLA	O2A-CGA-CBA	3.70	123.13	111.83
14	a	1139	CLA	CAA-C2A-C3A	-3.70	102.99	113.00
18	b	4004	BCR	C19-C18-C17	3.70	124.83	119.01
14	b	1214	CLA	O2A-C1-C2	3.70	122.35	108.11
14	G	1107	CLA	C1D-ND-C4D	-3.70	103.72	106.31
14	b	1211	CLA	O2A-CGA-CBA	3.70	123.12	111.83
14	a	1104	CLA	CHD-C1D-ND	-3.70	119.60	124.80
14	U	1501	CLA	O2A-CGA-CBA	3.70	123.11	111.83
14	a	1103	CLA	O2A-C1-C2	3.70	122.33	108.11
14	a	1132	CLA	O2A-C1-C2	3.69	122.33	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1222	CLA	CHD-C1D-ND	-3.69	119.60	124.80
14	G	1130	CLA	O2A-CGA-CBA	3.69	123.09	111.83
14	b	1226	CLA	C2B-C1B-NB	3.69	114.15	110.33
14	a	1012	CLA	CMB-C2B-C1B	3.69	131.04	125.42
14	L	1501	CLA	C1-C2-C3	-3.69	120.15	126.20
14	L	1501	CLA	O2A-CGA-CBA	3.69	123.08	111.83
14	b	1223	CLA	C2B-C1B-NB	3.69	114.15	110.33
14	b	1227	CLA	C2D-C1D-ND	3.69	113.78	110.13
14	U	1501	CLA	C1-C2-C3	-3.69	120.16	126.20
14	H	1223	CLA	C1D-ND-C4D	-3.69	103.72	106.31
14	a	1108	CLA	CHD-C1D-ND	-3.69	119.61	124.80
18	H	4017	BCR	C15-C14-C13	-3.69	122.11	127.28
14	a	1012	CLA	C1D-ND-C4D	-3.69	103.73	106.31
14	B	1218	CLA	C2B-C1B-NB	3.68	114.15	110.33
18	A	4002	BCR	C38-C26-C25	-3.68	120.47	124.48
14	H	1223	CLA	C2B-C1B-NB	3.68	114.14	110.33
14	A	1103	CLA	O2A-C1-C2	3.68	122.27	108.11
14	A	1124	CLA	CHD-C1D-ND	-3.68	119.62	124.80
14	a	1139	CLA	C2B-C1B-NB	3.68	114.14	110.33
14	G	1103	CLA	O2A-C1-C2	3.68	122.25	108.11
14	H	1235	CLA	CHD-C1D-ND	-3.68	119.63	124.80
14	A	1139	CLA	C2B-C1B-NB	3.68	114.14	110.33
14	A	1108	CLA	CHD-C1D-ND	-3.67	119.63	124.80
14	G	1108	CLA	CHD-C1D-ND	-3.67	119.63	124.80
14	b	1222	CLA	CHD-C1D-ND	-3.67	119.63	124.80
14	B	1216	CLA	C1D-ND-C4D	-3.67	103.74	106.31
14	B	1225	CLA	C1D-ND-C4D	-3.67	103.74	106.31
14	A	1104	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	G	1104	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	A	1104	CLA	O2A-C1-C2	3.67	122.23	108.11
14	G	1126	CLA	C1D-ND-C4D	-3.67	103.74	106.31
14	H	1213	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	L	1502	CLA	O2A-CGA-CBA	3.67	123.01	111.83
14	G	1104	CLA	O2A-C1-C2	3.66	122.21	108.11
18	G	4011	BCR	C34-C9-C10	-3.66	116.88	122.82
14	b	1235	CLA	CHD-C1D-ND	-3.66	119.65	124.80
13	A	1011	CL0	C1C-CHC-C4B	3.66	129.18	116.07
13	G	1011	CL0	C1C-CHC-C4B	3.66	129.18	116.07
18	B	4010	BCR	C15-C14-C13	-3.66	122.14	127.28
14	H	1225	CLA	C1D-ND-C4D	-3.66	103.74	106.31
14	G	1109	CLA	CAA-C2A-C3A	-3.66	103.11	113.00
14	a	1113	CLA	C1D-ND-C4D	-3.66	103.74	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	1011	CL0	C1C-CHC-C4B	3.66	129.16	116.07
14	A	1109	CLA	CAA-C2A-C3A	-3.66	103.11	113.00
14	a	1126	CLA	C1D-ND-C4D	-3.66	103.75	106.31
14	B	1235	CLA	CHD-C1D-ND	-3.66	119.65	124.80
19	b	5004	LHG	C5-O7-C7	-3.66	109.04	117.80
14	a	1138	CLA	CHD-C1D-ND	-3.66	119.66	124.80
14	G	1012	CLA	CMB-C2B-C1B	3.66	130.99	125.42
14	U	1502	CLA	O2A-CGA-CBA	3.66	122.98	111.83
14	a	1104	CLA	O2A-C1-C2	3.66	122.18	108.11
14	b	1212	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
14	b	1225	CLA	C1D-ND-C4D	-3.66	103.75	106.31
19	B	5004	LHG	C5-O7-C7	-3.66	109.05	117.80
18	G	4002	BCR	C38-C26-C25	-3.65	120.50	124.48
14	a	1106	CLA	C2B-C1B-NB	3.65	114.11	110.33
14	l	1502	CLA	O2A-CGA-CBA	3.65	122.97	111.83
14	a	1109	CLA	CAA-C2A-C3A	-3.65	103.13	113.00
14	a	1125	CLA	C2B-C1B-NB	3.65	114.11	110.33
14	B	1223	CLA	C2B-C1B-NB	3.65	114.11	110.33
14	G	1139	CLA	C2B-C1B-NB	3.65	114.11	110.33
18	b	4010	BCR	C15-C14-C13	-3.65	122.16	127.28
14	G	1137	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
14	a	1132	CLA	C1D-ND-C4D	-3.65	103.75	106.31
19	H	5004	LHG	C5-O7-C7	-3.65	109.06	117.80
14	H	1012	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
14	G	1124	CLA	CHD-C1D-ND	-3.65	119.67	124.80
18	A	4011	BCR	C34-C9-C10	-3.65	116.91	122.82
14	G	1113	CLA	C1D-ND-C4D	-3.65	103.75	106.31
14	H	1217	CLA	O2A-C1-C2	3.65	122.14	108.11
14	G	1138	CLA	C1D-ND-C4D	-3.65	103.75	106.31
14	b	1218	CLA	C2B-C1B-NB	3.65	114.11	110.33
14	B	1208	CLA	CHD-C1D-ND	-3.64	119.67	124.80
14	B	1217	CLA	O2A-C1-C2	3.64	122.13	108.11
14	A	1132	CLA	C1D-ND-C4D	-3.64	103.76	106.31
14	G	1132	CLA	C1D-ND-C4D	-3.64	103.76	106.31
14	b	1022	CLA	C2B-C1B-NB	3.64	114.10	110.33
18	H	4010	BCR	C15-C14-C13	-3.64	122.17	127.28
14	b	1236	CLA	C2B-C1B-NB	3.64	114.10	110.33
14	a	1124	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	G	1125	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
14	b	1208	CLA	O2A-C1-C2	3.64	122.11	108.11
14	G	1131	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	a	1131	CLA	CHD-C1D-ND	-3.64	119.68	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1208	CLA	O2A-C1-C2	3.64	122.11	108.11
14	H	1208	CLA	O2A-C1-C2	3.64	122.11	108.11
14	H	1236	CLA	C2B-C1B-NB	3.64	114.10	110.33
14	A	1126	CLA	C1D-ND-C4D	-3.64	103.76	106.31
18	H	4005	BCR	C38-C26-C25	-3.64	120.52	124.48
14	b	1213	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	b	1217	CLA	O2A-C1-C2	3.63	122.09	108.11
14	A	1138	CLA	C1D-ND-C4D	-3.63	103.76	106.31
14	H	1212	CLA	O2D-CGD-O1D	-3.63	116.77	123.85
14	H	1218	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	B	1213	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	G	1138	CLA	CAA-C2A-C3A	-3.63	103.18	113.00
14	H	1216	CLA	C1D-ND-C4D	-3.63	103.76	106.31
14	A	1138	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	G	1108	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	A	1138	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
14	a	1138	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
14	b	1216	CLA	C1D-ND-C4D	-3.63	103.77	106.31
14	b	1223	CLA	C1D-ND-C4D	-3.63	103.77	106.31
14	B	1236	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	G	1135	CLA	O2A-C1-C2	3.63	122.07	108.11
14	A	1136	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	a	1132	CLA	CMB-C2B-C1B	3.63	130.94	125.42
14	A	1137	CLA	O2D-CGD-O1D	-3.62	116.79	123.85
14	A	1113	CLA	C1D-ND-C4D	-3.62	103.77	106.31
14	G	1109	CLA	C2B-C1B-NB	3.62	114.08	110.33
14	B	1212	CLA	O2D-CGD-O1D	-3.62	116.80	123.85
14	G	1125	CLA	C2B-C1B-NB	3.62	114.08	110.33
14	a	1108	CLA	C2B-C1B-NB	3.62	114.08	110.33
14	B	1223	CLA	C1D-ND-C4D	-3.62	103.77	106.31
14	A	1135	CLA	O2A-C1-C2	3.62	122.03	108.11
14	A	1110	CLA	C2B-C1B-NB	3.62	114.08	110.33
14	G	1138	CLA	CHD-C1D-ND	-3.62	119.71	124.80
14	a	1135	CLA	O2A-C1-C2	3.62	122.03	108.11
14	b	1210	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
18	m	4021	BCR	C7-C8-C9	3.62	131.58	126.23
18	a	4002	BCR	C38-C26-C25	-3.62	120.54	124.48
14	a	1137	CLA	O2D-CGD-O1D	-3.61	116.81	123.85
14	A	1125	CLA	C2B-C1B-NB	3.61	114.07	110.33
18	a	4011	BCR	C34-C9-C10	-3.61	116.96	122.82
14	B	1022	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
14	A	1133	CLA	O2A-C1-C2	3.61	122.01	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1208	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	H	1012	CLA	C2B-C1B-NB	3.61	114.07	110.33
14	b	1236	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	G	1133	CLA	O2A-C1-C2	3.61	122.00	108.11
14	b	1022	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
14	H	1210	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
18	V	4021	BCR	C7-C8-C9	3.61	131.57	126.23
14	G	1110	CLA	C2B-C1B-NB	3.61	114.07	110.33
14	G	1136	CLA	C2B-C1B-NB	3.61	114.06	110.33
14	a	1133	CLA	O2A-C1-C2	3.61	121.98	108.11
14	B	1236	CLA	CHD-C1D-ND	-3.60	119.73	124.80
14	b	1231	CLA	CMC-C2C-C1C	3.60	130.67	125.03
14	A	1109	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	H	1226	CLA	C2B-C1B-NB	3.60	114.06	110.33
15	b	1237	F6C	CMA-C3A-C4A	-3.60	118.38	124.73
18	b	4009	BCR	C3-C4-C5	-3.60	107.63	114.06
14	a	1110	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	a	1136	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	G	1102	CLA	CHD-C1D-ND	-3.60	119.73	124.80
18	b	4005	BCR	C38-C26-C25	-3.60	120.56	124.48
14	H	1236	CLA	CHD-C1D-ND	-3.60	119.74	124.80
18	M	4021	BCR	C8-C7-C6	3.60	136.61	127.00
14	B	1232	CLA	C2B-C1B-NB	3.60	114.06	110.33
18	i	4018	BCR	C37-C22-C21	-3.60	116.99	122.82
15	B	1237	F6C	CMA-C3A-C4A	-3.60	118.39	124.73
18	R	4018	BCR	C37-C22-C21	-3.60	116.99	122.82
18	V	4021	BCR	C8-C7-C6	3.59	136.60	127.00
14	b	1232	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	b	1208	CLA	CHD-C1D-ND	-3.59	119.75	124.80
18	B	4005	BCR	C38-C26-C25	-3.59	120.56	124.48
18	m	4021	BCR	C8-C7-C6	3.59	136.59	127.00
14	G	1101	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	a	1109	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	A	1133	CLA	CHD-C1D-ND	-3.59	119.75	124.80
14	A	1125	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
14	G	1132	CLA	CMB-C2B-C1B	3.59	130.88	125.42
14	L	1503	CLA	O2A-CGA-CBA	3.59	122.78	111.83
14	A	1131	CLA	CHD-C1D-ND	-3.59	119.75	124.80
14	U	1503	CLA	O2A-CGA-CBA	3.59	122.77	111.83
18	R	4020	BCR	C3-C4-C5	-3.59	107.66	114.06
18	B	4009	BCR	C3-C4-C5	-3.59	107.66	114.06
18	b	4006	BCR	C3-C4-C5	-3.59	107.66	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1132	CLA	CMB-C2B-C1B	3.58	130.88	125.42
15	H	1237	F6C	CMA-C3A-C4A	-3.58	118.42	124.73
14	B	1210	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
14	A	1140	CLA	C2B-C1B-NB	3.58	114.04	110.33
14	A	1101	CLA	C2B-C1B-NB	3.58	114.04	110.33
14	a	1012	CLA	C4A-NA-C1A	3.58	108.31	106.68
14	B	1231	CLA	CMC-C2C-C1C	3.58	130.63	125.03
15	A	1121	F6C	CMA-C3A-C2A	-3.58	116.47	126.15
14	B	1022	CLA	C2B-C1B-NB	3.58	114.04	110.33
14	B	1212	CLA	C2B-C1B-NB	3.58	114.04	110.33
14	a	1102	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	a	1133	CLA	CHD-C1D-ND	-3.58	119.77	124.80
18	H	4006	BCR	C3-C4-C5	-3.58	107.68	114.06
14	l	1503	CLA	O2A-CGA-CBA	3.58	122.74	111.83
14	A	1012	CLA	C2B-C1B-NB	3.58	114.03	110.33
14	a	1101	CLA	CAA-C2A-C3A	-3.58	103.34	113.00
18	I	4018	BCR	C37-C22-C21	-3.57	117.03	122.82
14	l	1503	CLA	CHD-C1D-ND	-3.57	119.78	124.80
18	H	4009	BCR	C3-C4-C5	-3.57	107.69	114.06
14	H	1232	CLA	C2B-C1B-NB	3.57	114.03	110.33
18	i	4020	BCR	C3-C4-C5	-3.57	107.69	114.06
18	M	4021	BCR	C7-C8-C9	3.57	131.51	126.23
14	H	1231	CLA	CMC-C2C-C1C	3.57	130.61	125.03
14	L	1503	CLA	CHD-C1D-ND	-3.57	119.78	124.80
14	B	1232	CLA	C1D-ND-C4D	-3.57	103.81	106.31
15	G	1121	F6C	CMA-C3A-C2A	-3.56	116.51	126.15
14	G	1012	CLA	CAA-C2A-C3A	-3.56	103.37	113.00
18	I	4020	BCR	C3-C4-C5	-3.56	107.70	114.06
14	A	1108	CLA	C2B-C1B-NB	3.56	114.02	110.33
15	a	1121	F6C	CMA-C3A-C2A	-3.56	116.51	126.15
14	A	1102	CLA	CHD-C1D-ND	-3.56	119.79	124.80
14	A	1101	CLA	CAA-C2A-C3A	-3.56	103.37	113.00
14	a	1125	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
14	A	1117	CLA	O2A-C1-C2	3.56	121.80	108.11
14	a	1012	CLA	CAA-C2A-C3A	-3.56	103.38	113.00
14	B	1022	CLA	CAA-C2A-C3A	-3.56	103.38	113.00
14	U	1503	CLA	CHD-C1D-ND	-3.56	119.80	124.80
14	b	1022	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
14	G	1133	CLA	CHD-C1D-ND	-3.56	119.80	124.80
18	G	4003	BCR	C28-C27-C26	-3.56	107.71	114.06
14	G	1117	CLA	O2A-C1-C2	3.56	121.79	108.11
21	a	6002	LMT	O5B-C5B-C4B	3.56	116.11	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1101	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
14	a	1117	CLA	O2A-C1-C2	3.56	121.79	108.11
14	a	1012	CLA	C2B-C1B-NB	3.55	114.01	110.33
14	H	1232	CLA	C1D-ND-C4D	-3.55	103.82	106.31
18	a	4003	BCR	C28-C27-C26	-3.55	107.72	114.06
14	a	1101	CLA	C2B-C1B-NB	3.55	114.01	110.33
18	B	4006	BCR	C3-C4-C5	-3.55	107.72	114.06
14	H	1212	CLA	C2B-C1B-NB	3.55	114.01	110.33
14	H	1203	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	G	1012	CLA	C4A-NA-C1A	3.55	108.30	106.68
14	H	1012	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
14	b	1232	CLA	C1D-ND-C4D	-3.55	103.82	106.31
14	H	1202	CLA	C2B-C1B-NB	3.55	114.00	110.33
14	a	1140	CLA	C2B-C1B-NB	3.55	114.00	110.33
14	a	1013	CLA	C1-C2-C3	-3.55	120.39	126.20
14	b	1212	CLA	C2B-C1B-NB	3.55	114.00	110.33
14	a	1109	CLA	O2A-CGA-CBA	3.54	125.19	114.00
14	A	1130	CLA	C4A-NA-C1A	3.54	108.30	106.68
18	A	4003	BCR	C28-C27-C26	-3.54	107.74	114.06
21	G	6002	LMT	O5B-C5B-C4B	3.54	116.08	109.70
14	G	1109	CLA	O2A-CGA-CBA	3.54	125.18	114.00
14	A	1013	CLA	C1-C2-C3	-3.54	120.40	126.20
14	A	1109	CLA	O2A-CGA-CBA	3.54	125.18	114.00
14	A	1012	CLA	CAA-C2A-C3A	-3.54	103.45	113.00
18	H	4012	BCR	C7-C8-C9	-3.53	121.01	126.23
14	a	1118	CLA	C2B-C1B-NB	3.53	113.99	110.33
14	A	1115	CLA	C4-C3-C5	3.53	121.36	115.23
14	A	1135	CLA	CAA-C2A-C3A	-3.53	103.46	113.00
14	G	1012	CLA	C2B-C1B-NB	3.53	113.98	110.33
18	M	4021	BCR	C36-C18-C17	-3.53	117.10	122.82
14	a	1135	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
14	B	1210	CLA	CHD-C1D-ND	-3.53	119.84	124.80
14	H	1210	CLA	CHD-C1D-ND	-3.53	119.84	124.80
21	A	6002	LMT	O5B-C5B-C4B	3.53	116.05	109.70
14	a	1130	CLA	C4A-NA-C1A	3.52	108.29	106.68
14	b	1203	CLA	CHD-C1D-ND	-3.52	119.84	124.80
14	B	1202	CLA	C2B-C1B-NB	3.52	113.98	110.33
14	b	1202	CLA	C2B-C1B-NB	3.52	113.98	110.33
18	B	4012	BCR	C7-C8-C9	-3.52	121.02	126.23
14	G	1130	CLA	C4A-NA-C1A	3.52	108.28	106.68
14	b	1210	CLA	CHD-C1D-ND	-3.52	119.85	124.80
14	H	1227	CLA	C1D-ND-C4D	-3.52	103.84	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1231	CLA	CHD-C1D-ND	-3.52	119.85	124.80
14	k	1401	CLA	C2B-C1B-NB	3.52	113.97	110.33
18	b	4012	BCR	C7-C8-C9	-3.52	121.03	126.23
14	b	1227	CLA	CAA-C2A-C3A	-3.52	103.50	113.00
14	a	1105	CLA	CAA-C2A-C3A	-3.52	103.50	113.00
18	H	4006	BCR	C1-C6-C5	-3.51	117.84	122.64
14	G	1013	CLA	C1-C2-C3	-3.51	120.44	126.20
18	b	4006	BCR	C1-C6-C5	-3.51	117.84	122.64
14	G	1135	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
14	B	1203	CLA	CHD-C1D-ND	-3.51	119.86	124.80
14	G	1140	CLA	C2B-C1B-NB	3.51	113.97	110.33
18	a	4003	BCR	C3-C4-C5	-3.51	107.80	114.06
14	G	1115	CLA	C4-C3-C5	3.51	121.32	115.23
18	A	4003	BCR	C3-C4-C5	-3.51	107.80	114.06
15	a	1121	F6C	C4A-C3A-C2A	-3.51	101.77	106.97
14	G	1128	CLA	CMB-C2B-C3B	3.51	134.80	126.55
18	m	4021	BCR	C36-C18-C17	-3.51	117.13	122.82
14	a	1128	CLA	CMB-C2B-C3B	3.51	134.80	126.55
14	G	1118	CLA	C2B-C1B-NB	3.51	113.96	110.33
14	b	1226	CLA	CHD-C1D-ND	-3.51	119.87	124.80
14	A	1118	CLA	C2B-C1B-NB	3.51	113.96	110.33
14	G	1105	CLA	CAA-C2A-C3A	-3.50	103.53	113.00
14	a	1137	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	B	1227	CLA	CAA-C2A-C3A	-3.50	103.53	113.00
14	A	1128	CLA	CMB-C2B-C3B	3.50	134.79	126.55
14	A	1105	CLA	CAA-C2A-C3A	-3.50	103.53	113.00
14	a	1103	CLA	CHD-C1D-ND	-3.50	119.88	124.80
14	B	1207	CLA	C2B-C1B-NB	3.50	113.95	110.33
15	G	1121	F6C	C4A-C3A-C2A	-3.50	101.78	106.97
14	G	1103	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	a	1115	CLA	C4-C3-C5	3.49	121.29	115.23
18	V	4021	BCR	C36-C18-C17	-3.49	117.16	122.82
18	G	4003	BCR	C3-C4-C5	-3.49	107.83	114.06
14	G	1135	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	L	1503	CLA	C2B-C1B-NB	3.49	113.95	110.33
14	A	1107	CLA	CMB-C2B-C1B	3.49	130.73	125.42
14	G	1137	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	H	1227	CLA	CAA-C2A-C3A	-3.49	103.57	113.00
14	a	1122	CLA	CAC-C3C-C4C	3.49	129.33	124.79
14	k	1401	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	l	1503	CLA	C2B-C1B-NB	3.49	113.94	110.33
14	H	1231	CLA	CHD-C1D-ND	-3.49	119.89	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1136	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
14	G	1122	CLA	CAC-C3C-C4C	3.49	129.32	124.79
14	H	1202	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	A	1012	CLA	C4A-NA-C1A	3.48	108.27	106.68
15	A	1121	F6C	C4A-C3A-C2A	-3.48	101.81	106.97
14	A	1135	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	T	1401	CLA	C2B-C1B-NB	3.48	113.94	110.33
14	a	1136	CLA	CHD-C1D-ND	-3.48	119.91	124.80
18	B	4006	BCR	C1-C6-C5	-3.48	117.88	122.64
14	G	1127	CLA	C2B-C1B-NB	3.48	113.93	110.33
14	G	1136	CLA	CHD-C1D-ND	-3.48	119.91	124.80
14	K	1401	CLA	C2B-C1B-NB	3.48	113.93	110.33
14	H	1207	CLA	C2B-C1B-NB	3.48	113.93	110.33
14	G	1130	CLA	CHD-C1D-ND	-3.47	119.91	124.80
14	U	1503	CLA	C2B-C1B-NB	3.47	113.93	110.33
14	H	1226	CLA	CHD-C1D-ND	-3.47	119.91	124.80
14	H	1213	CLA	CAA-C2A-C3A	-3.47	103.61	113.00
14	b	1214	CLA	C2B-C1B-NB	3.47	113.93	110.33
14	B	1227	CLA	C1D-ND-C4D	-3.47	103.88	106.31
14	G	1130	CLA	C1D-ND-C4D	-3.47	103.88	106.31
14	H	1214	CLA	C2B-C1B-NB	3.47	113.93	110.33
14	x	1701	CLA	C2B-C1B-NB	3.47	113.92	110.33
14	G	1115	CLA	CAA-C2A-C3A	-3.47	103.63	113.00
14	A	1137	CLA	CHD-C1D-ND	-3.47	119.92	124.80
14	a	1135	CLA	CHD-C1D-ND	-3.47	119.92	124.80
14	b	1231	CLA	CMB-C2B-C3B	3.47	134.70	126.55
18	G	4007	BCR	C15-C14-C13	-3.47	122.42	127.28
19	a	5001	LHG	O8-C23-C24	3.47	122.40	111.83
14	a	1127	CLA	C2B-C1B-NB	3.46	113.92	110.33
14	G	1013	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
14	K	1401	CLA	CHD-C1D-ND	-3.46	119.93	124.80
14	A	1115	CLA	CAA-C2A-C3A	-3.46	103.65	113.00
14	G	1123	CLA	O2A-C1-C2	3.46	121.42	108.11
14	b	1227	CLA	C1D-ND-C4D	-3.46	103.89	106.31
18	a	4008	BCR	C34-C9-C10	-3.46	117.22	122.82
18	A	4008	BCR	C34-C9-C10	-3.46	117.22	122.82
14	A	1122	CLA	CAC-C3C-C4C	3.46	129.29	124.79
14	H	1223	CLA	O2A-C1-C2	3.46	121.41	108.11
14	a	1118	CLA	CAA-C2A-C3A	-3.46	103.66	113.00
14	B	1226	CLA	CHD-C1D-ND	-3.46	119.94	124.80
14	a	1123	CLA	O2A-C1-C2	3.45	121.40	108.11
14	G	1107	CLA	CMB-C2B-C1B	3.45	130.68	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1213	CLA	CAA-C2A-C3A	-3.45	103.67	113.00
14	H	1231	CLA	CMB-C2B-C3B	3.45	134.67	126.55
18	A	4007	BCR	C15-C14-C13	-3.45	122.44	127.28
14	B	1223	CLA	O2A-C1-C2	3.45	121.39	108.11
14	B	1231	CLA	CMB-C2B-C3B	3.45	134.67	126.55
14	A	1123	CLA	O2A-C1-C2	3.45	121.39	108.11
14	a	1107	CLA	CMB-C2B-C1B	3.45	130.67	125.42
14	a	1115	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
14	A	1136	CLA	O2D-CGD-O1D	-3.45	117.14	123.85
14	A	1103	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	G	1118	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
14	A	1118	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
14	b	1213	CLA	CAA-C2A-C3A	-3.45	103.68	113.00
14	A	1136	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	X	1701	CLA	C2B-C1B-NB	3.45	113.90	110.33
19	A	5001	LHG	O8-C23-C24	3.45	122.34	111.83
14	A	1130	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	B	1231	CLA	CHD-C1D-ND	-3.45	119.95	124.80
18	B	4009	BCR	C34-C9-C8	3.44	123.35	118.09
14	b	1223	CLA	O2A-C1-C2	3.44	121.36	108.11
14	a	1130	CLA	CHD-C1D-ND	-3.44	119.96	124.80
14	T	1401	CLA	CHD-C1D-ND	-3.44	119.96	124.80
14	B	1220	CLA	C2B-C1B-NB	3.44	113.90	110.33
14	b	1207	CLA	C2B-C1B-NB	3.44	113.89	110.33
14	a	1116	CLA	CHD-C1D-ND	-3.44	119.96	124.80
19	G	5001	LHG	O8-C23-C24	3.44	122.33	111.83
14	B	1206	CLA	O2A-CGA-CBA	3.44	124.87	114.00
14	H	1207	CLA	O2A-CGA-CBA	3.44	124.86	114.00
14	b	1207	CLA	O2A-CGA-CBA	3.44	124.86	114.00
14	B	1202	CLA	CHD-C1D-ND	-3.44	119.97	124.80
14	b	1202	CLA	CHD-C1D-ND	-3.44	119.97	124.80
14	b	1218	CLA	CHD-C1D-ND	-3.44	119.97	124.80
14	A	1114	CLA	C1D-ND-C4D	-3.43	103.90	106.31
18	a	4007	BCR	C15-C14-C13	-3.43	122.46	127.28
14	B	1220	CLA	CMA-C3A-C4A	3.43	121.00	111.77
18	G	4008	BCR	C34-C9-C10	-3.43	117.25	122.82
14	H	1220	CLA	CMA-C3A-C4A	3.43	121.00	111.77
14	G	1115	CLA	O2A-C1-C2	3.43	121.32	108.11
14	b	1209	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	G	1103	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
14	a	1115	CLA	O2A-C1-C2	3.43	121.31	108.11
14	W	1701	CLA	C2B-C1B-NB	3.43	113.88	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1206	CLA	O2A-CGA-CBA	3.43	124.84	114.00
14	A	1129	CLA	O2A-CGA-CBA	3.43	124.83	114.00
14	G	1102	CLA	C1-C2-C3	-3.43	120.58	126.20
14	G	1129	CLA	O2A-CGA-CBA	3.43	124.83	114.00
14	H	1205	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
14	a	1136	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
14	B	1214	CLA	C2B-C1B-NB	3.43	113.88	110.33
14	A	1112	CLA	CHD-C1D-ND	-3.43	119.98	124.80
14	A	1115	CLA	O2A-C1-C2	3.43	121.29	108.11
14	b	1220	CLA	CMA-C3A-C4A	3.43	120.98	111.77
14	A	1102	CLA	C1-C2-C3	-3.42	120.59	126.20
14	G	1116	CLA	CHD-C1D-ND	-3.42	119.98	124.80
14	B	1209	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	A	1113	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	H	1218	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	a	1104	CLA	C1-C2-C3	-3.42	120.59	126.20
14	a	1102	CLA	C1-C2-C3	-3.42	120.59	126.20
14	A	1116	CLA	C2B-C1B-NB	3.42	113.87	110.33
14	a	1116	CLA	C2B-C1B-NB	3.42	113.87	110.33
14	a	1113	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	H	1210	CLA	C4-C3-C5	3.42	121.16	115.23
14	B	1226	CLA	C3B-C2B-C1B	-3.42	103.14	107.17
14	B	1205	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
14	B	1207	CLA	O2A-CGA-CBA	3.42	124.79	114.00
14	H	1206	CLA	O2A-CGA-CBA	3.41	124.79	114.00
14	A	1127	CLA	C2B-C1B-NB	3.41	113.87	110.33
14	b	1210	CLA	C4-C3-C5	3.41	121.15	115.23
14	H	1209	CLA	CHD-C1D-ND	-3.41	120.00	124.80
14	G	1112	CLA	CHD-C1D-ND	-3.41	120.00	124.80
14	H	1220	CLA	C2B-C1B-NB	3.41	113.86	110.33
14	a	1013	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
14	A	1104	CLA	C1-C2-C3	-3.41	120.61	126.20
14	A	1103	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
14	b	1226	CLA	C3B-C2B-C1B	-3.41	103.15	107.17
18	G	4011	BCR	C33-C5-C4	3.41	120.86	113.60
14	B	1220	CLA	C1-C2-C3	-3.41	120.61	126.20
14	A	1114	CLA	CHD-C1D-ND	-3.41	120.01	124.80
14	A	1116	CLA	CHD-C1D-ND	-3.41	120.01	124.80
14	G	1126	CLA	CHD-C1D-ND	-3.41	120.01	124.80
14	a	1129	CLA	O2A-CGA-CBA	3.41	124.76	114.00
14	B	1210	CLA	C4-C3-C5	3.41	121.14	115.23
14	B	1216	CLA	CHD-C1D-ND	-3.40	120.01	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1114	CLA	CHD-C1D-ND	-3.40	120.01	124.80
14	G	1104	CLA	C1-C2-C3	-3.40	120.62	126.20
14	a	1126	CLA	CHD-C1D-ND	-3.40	120.01	124.80
14	B	1218	CLA	CHD-C1D-ND	-3.40	120.01	124.80
14	H	1216	CLA	CHD-C1D-ND	-3.40	120.01	124.80
14	A	1130	CLA	C1D-ND-C4D	-3.40	103.92	106.31
14	G	1113	CLA	CHD-C1D-ND	-3.40	120.02	124.80
18	G	4003	BCR	C27-C26-C25	-3.40	118.11	122.70
14	G	1116	CLA	C2B-C1B-NB	3.40	113.85	110.33
14	b	1217	CLA	C2B-C1B-NB	3.40	113.85	110.33
14	a	1101	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
18	b	4009	BCR	C34-C9-C8	3.40	123.28	118.09
14	l	1501	CLA	C1-O2A-CGA	3.40	124.88	116.65
14	H	1220	CLA	C1-C2-C3	-3.40	120.63	126.20
14	B	1233	CLA	CHD-C1D-ND	-3.40	120.02	124.80
18	a	4011	BCR	C33-C5-C4	3.40	120.84	113.60
14	G	1013	CLA	C2C-C1C-NC	3.40	113.55	109.98
14	b	1220	CLA	C1-C2-C3	-3.40	120.63	126.20
18	H	4009	BCR	C34-C9-C8	3.39	123.27	118.09
14	a	1103	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
14	b	1204	CLA	CAA-C2A-C3A	-3.39	103.83	113.00
14	B	1223	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
14	G	1118	CLA	CHD-C1D-ND	-3.39	120.03	124.80
14	G	1101	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
14	U	1503	CLA	C1-C2-C3	-3.39	120.64	126.20
14	b	1215	CLA	C1D-ND-C4D	-3.39	103.93	106.31
14	B	1215	CLA	C4-C3-C5	3.39	121.11	115.23
14	a	1112	CLA	CHD-C1D-ND	-3.39	120.03	124.80
14	G	1112	CLA	O2A-CGA-CBA	3.39	124.70	114.00
14	a	1112	CLA	O2A-CGA-CBA	3.39	124.70	114.00
14	B	1204	CLA	CAA-C2A-C3A	-3.39	103.85	113.00
14	U	1501	CLA	C1-O2A-CGA	3.39	124.84	116.65
14	A	1126	CLA	CHD-C1D-ND	-3.38	120.04	124.80
14	b	1205	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
14	H	1204	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
14	A	1101	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
14	b	1233	CLA	CHD-C1D-ND	-3.38	120.04	124.80
14	A	1118	CLA	CHD-C1D-ND	-3.38	120.04	124.80
14	A	1112	CLA	O2A-CGA-CBA	3.38	124.68	114.00
14	G	1139	CLA	O2A-CGA-CBA	3.38	124.68	114.00
14	a	1139	CLA	O2A-CGA-CBA	3.38	124.68	114.00
14	H	1233	CLA	CHD-C1D-ND	-3.38	120.05	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1114	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	b	1216	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	A	1013	CLA	C1C-C2C-C3C	-3.38	103.43	106.98
14	G	1114	CLA	C1D-ND-C4D	-3.38	103.94	106.31
14	b	1208	CLA	C2B-C1B-NB	3.38	113.83	110.33
14	L	1503	CLA	C1-C2-C3	-3.38	120.67	126.20
18	A	4011	BCR	C33-C5-C4	3.38	120.79	113.60
14	B	1212	CLA	O2A-CGA-CBA	3.38	124.67	114.00
14	H	1226	CLA	C3B-C2B-C1B	-3.37	103.19	107.17
14	a	1126	CLA	C1-C2-C3	-3.37	120.67	126.20
14	l	1503	CLA	C1-C2-C3	-3.37	120.67	126.20
13	a	1011	CL0	C4-C3-C5	3.37	121.08	115.23
14	B	1217	CLA	C2B-C1B-NB	3.37	113.82	110.33
14	b	1212	CLA	O2A-CGA-CBA	3.37	124.65	114.00
14	a	1114	CLA	C1D-ND-C4D	-3.37	103.95	106.31
14	A	1139	CLA	O2A-CGA-CBA	3.37	124.65	114.00
14	a	1130	CLA	C1D-ND-C4D	-3.37	103.95	106.31
14	b	1220	CLA	C2B-C1B-NB	3.37	113.82	110.33
14	L	1501	CLA	C1-O2A-CGA	3.37	124.80	116.65
18	a	4003	BCR	C27-C26-C25	-3.37	118.16	122.70
14	a	1013	CLA	CHD-C1D-ND	-3.37	120.07	124.80
14	G	1131	CLA	C1D-ND-C4D	-3.36	103.95	106.31
13	A	1011	CL0	CAA-CBA-CGA	-3.36	103.65	113.21
18	A	4003	BCR	C27-C26-C25	-3.36	118.16	122.70
14	H	1215	CLA	C4-C3-C5	3.36	121.07	115.23
13	G	1011	CL0	C4-C3-C5	3.36	121.06	115.23
14	a	1118	CLA	CHD-C1D-ND	-3.36	120.07	124.80
14	b	1232	CLA	CHD-C1D-ND	-3.36	120.07	124.80
14	b	1223	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
14	A	1013	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	b	1228	CLA	O2A-CGA-CBA	3.36	124.61	114.00
14	a	1111	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	B	1228	CLA	O2A-CGA-CBA	3.36	124.60	114.00
14	H	1212	CLA	O2A-CGA-CBA	3.36	124.60	114.00
14	b	1215	CLA	C4-C3-C5	3.35	121.05	115.23
14	H	1215	CLA	C1D-ND-C4D	-3.35	103.96	106.31
13	G	1011	CL0	CAA-CBA-CGA	-3.35	103.69	113.21
14	a	1140	CLA	O2A-C1-C2	3.35	121.01	108.11
14	H	1228	CLA	O2A-CGA-CBA	3.35	124.59	114.00
14	a	1013	CLA	C2C-C1C-NC	3.35	113.50	109.98
14	H	1232	CLA	CHD-C1D-ND	-3.35	120.09	124.80
14	A	1106	CLA	O2D-CGD-O1D	-3.35	117.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1223	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
14	G	1106	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
15	a	1120	F6C	O2D-CGD-O1D	-3.34	117.34	123.85
14	A	1126	CLA	C1-C2-C3	-3.34	120.72	126.20
14	B	1236	CLA	O2A-CGA-CBA	3.34	124.56	114.00
13	A	1011	CL0	C4-C3-C5	3.34	121.03	115.23
14	A	1140	CLA	O2A-C1-C2	3.34	120.97	108.11
14	b	1204	CLA	CMB-C2B-C1B	3.34	130.51	125.42
14	G	1111	CLA	CHD-C1D-ND	-3.34	120.10	124.80
14	B	1208	CLA	C2B-C1B-NB	3.34	113.79	110.33
14	a	1106	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
15	A	1120	F6C	O2D-CGD-O1D	-3.34	117.34	123.85
14	H	1208	CLA	C2B-C1B-NB	3.34	113.79	110.33
14	G	1140	CLA	O2A-C1-C2	3.34	120.97	108.11
14	A	1111	CLA	CHD-C1D-ND	-3.34	120.10	124.80
13	a	1011	CL0	CAA-CBA-CGA	-3.34	103.73	113.21
18	a	4007	BCR	C38-C26-C25	-3.34	120.84	124.48
14	G	1117	CLA	CHD-C1D-ND	-3.34	120.11	124.80
14	A	1013	CLA	C2C-C1C-NC	3.34	113.49	109.98
14	B	1023	CLA	CHD-C1D-ND	-3.34	120.11	124.80
15	G	1120	F6C	O2D-CGD-O1D	-3.34	117.36	123.85
18	A	4007	BCR	C38-C26-C25	-3.33	120.84	124.48
18	B	4009	BCR	C34-C9-C10	-3.33	117.41	122.82
15	A	1121	F6C	CHA-C4D-ND	3.33	136.24	133.05
18	H	4009	BCR	C34-C9-C10	-3.33	117.42	122.82
14	H	1236	CLA	O2A-CGA-CBA	3.33	124.53	114.00
14	H	1234	CLA	C3C-C4C-NC	3.33	114.70	110.43
14	B	1204	CLA	CMB-C2B-C1B	3.33	130.49	125.42
14	H	1205	CLA	C1-C2-C3	-3.33	120.74	126.20
18	b	4009	BCR	C34-C9-C10	-3.33	117.42	122.82
14	G	1126	CLA	O2A-C1-C2	3.33	120.92	108.11
14	A	1117	CLA	CBA-CAA-C2A	3.33	123.69	113.79
14	H	1217	CLA	C2B-C1B-NB	3.33	113.78	110.33
14	a	1117	CLA	CBA-CAA-C2A	3.33	123.69	113.79
14	a	1126	CLA	O2A-C1-C2	3.33	120.90	108.11
14	B	1232	CLA	CHD-C1D-ND	-3.33	120.12	124.80
14	B	1218	CLA	O2A-CGA-CBA	3.32	124.50	114.00
14	b	1218	CLA	O2A-CGA-CBA	3.32	124.50	114.00
14	a	1130	CLA	CAA-C2A-C3A	-3.32	104.02	113.00
14	G	1130	CLA	CAA-C2A-C3A	-3.32	104.03	113.00
14	a	1132	CLA	CHD-C1D-ND	-3.32	120.13	124.80
14	b	1236	CLA	O2A-CGA-CBA	3.32	124.49	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1234	CLA	C3C-C4C-NC	3.32	114.68	110.43
14	G	1117	CLA	CBA-CAA-C2A	3.32	123.67	113.79
14	B	1215	CLA	C1D-ND-C4D	-3.32	103.98	106.31
14	B	1211	CLA	O2A-C1-C2	3.32	120.88	108.11
14	b	1209	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
14	G	1126	CLA	C1-C2-C3	-3.32	120.76	126.20
14	a	1110	CLA	CHD-C1D-ND	-3.32	120.13	124.80
14	H	1218	CLA	O2A-CGA-CBA	3.32	124.48	114.00
14	B	1209	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
14	H	1023	CLA	CHD-C1D-ND	-3.32	120.14	124.80
15	G	1121	F6C	CHA-C4D-ND	3.32	136.22	133.05
14	H	1211	CLA	CHD-C1D-ND	-3.32	120.14	124.80
14	B	1022	CLA	CMB-C2B-C1B	3.31	130.47	125.42
14	A	1110	CLA	CHD-C1D-ND	-3.31	120.14	124.80
14	B	1205	CLA	C1-C2-C3	-3.31	120.77	126.20
14	b	1203	CLA	C2B-C1B-NB	3.31	113.76	110.33
14	b	1211	CLA	O2A-C1-C2	3.31	120.86	108.11
15	H	1237	F6C	CHA-C4D-ND	3.31	136.22	133.05
14	A	1132	CLA	CHD-C1D-ND	-3.31	120.14	124.80
14	H	1227	CLA	C2B-C1B-NB	3.31	113.76	110.33
14	b	1023	CLA	CHD-C1D-ND	-3.31	120.14	124.80
14	H	1012	CLA	CMB-C2B-C1B	3.31	130.46	125.42
14	b	1238	CLA	C4D-C3D-CAD	3.31	111.70	108.11
14	B	1234	CLA	C3C-C4C-NC	3.31	114.67	110.43
14	B	1239	CLA	CHD-C1D-ND	-3.31	120.15	124.80
14	A	1104	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
14	A	1126	CLA	O2A-C1-C2	3.31	120.84	108.11
14	G	1110	CLA	CHD-C1D-ND	-3.31	120.15	124.80
15	a	1121	F6C	O2A-CGA-CBA	3.31	124.45	114.00
14	H	1204	CLA	CMB-C2B-C1B	3.31	130.46	125.42
14	l	1502	CLA	C2B-C1B-NB	3.31	113.75	110.33
14	G	1117	CLA	C1D-ND-C4D	-3.31	103.99	106.31
15	A	1121	F6C	O2A-CGA-CBA	3.31	124.45	114.00
18	b	4010	BCR	C7-C8-C9	-3.30	121.35	126.23
14	G	1123	CLA	CMA-C3A-C4A	3.30	120.65	111.77
15	b	1237	F6C	CHA-C4D-ND	3.30	136.21	133.05
14	U	1502	CLA	C2B-C1B-NB	3.30	113.75	110.33
14	G	1104	CLA	CAA-C2A-C3A	-3.30	104.07	113.00
14	a	1117	CLA	CHD-C1D-ND	-3.30	120.15	124.80
14	a	1123	CLA	CMA-C3A-C4A	3.30	120.65	111.77
14	G	1013	CLA	CHD-C1D-ND	-3.30	120.16	124.80
15	B	1237	F6C	CHA-C4D-ND	3.30	136.21	133.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1123	CLA	C2B-C1B-NB	3.30	113.75	110.33
15	G	1121	F6C	O2A-CGA-CBA	3.30	124.43	114.00
14	a	1128	CLA	C3B-C2B-C1B	-3.30	103.28	107.17
14	b	1222	CLA	CAA-CBA-CGA	-3.30	103.84	113.21
14	H	1209	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
14	B	1232	CLA	O2A-CGA-CBA	3.30	124.43	114.00
14	b	1022	CLA	CMB-C2B-C1B	3.30	130.44	125.42
14	G	1132	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	H	1211	CLA	O2A-C1-C2	3.30	120.80	108.11
18	G	4007	BCR	C38-C26-C25	-3.30	120.89	124.48
14	A	1117	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	A	1130	CLA	CAA-C2A-C3A	-3.30	104.09	113.00
14	H	1222	CLA	CAA-CBA-CGA	-3.30	103.84	113.21
14	a	1104	CLA	CAA-C2A-C3A	-3.30	104.09	113.00
14	H	1203	CLA	C2B-C1B-NB	3.30	113.75	110.33
14	A	1128	CLA	C3B-C2B-C1B	-3.30	103.28	107.17
14	b	1211	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	B	1238	CLA	C4-C3-C5	3.30	120.95	115.23
14	H	1201	CLA	C4-C3-C5	3.30	120.95	115.23
14	B	1226	CLA	CMB-C2B-C3B	3.30	134.30	126.55
14	G	1128	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	B	1223	CLA	C3C-C4C-NC	3.29	114.65	110.43
15	a	1121	F6C	CHA-C4D-ND	3.29	136.20	133.05
14	G	1123	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	a	1123	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	b	1232	CLA	O2A-CGA-CBA	3.29	124.40	114.00
14	b	1226	CLA	CMB-C2B-C3B	3.29	134.29	126.55
14	a	1131	CLA	C1D-ND-C4D	-3.29	104.00	106.31
14	b	1205	CLA	C1-C2-C3	-3.29	120.80	126.20
14	b	1227	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	A	1123	CLA	CMA-C3A-C4A	3.29	120.62	111.77
18	H	4010	BCR	C7-C8-C9	-3.29	121.36	126.23
14	W	1701	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
14	b	1224	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
14	G	1119	CLA	CHD-C1D-ND	-3.29	120.17	124.80
14	x	1701	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
14	A	1131	CLA	C1D-ND-C4D	-3.29	104.00	106.31
14	H	1232	CLA	O2A-CGA-CBA	3.29	124.40	114.00
14	B	1222	CLA	CAA-CBA-CGA	-3.29	103.87	113.21
14	A	1102	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
15	a	1121	F6C	C4A-NA-C1A	3.29	108.62	106.31
14	B	1021	CLA	O2A-C1-C2	3.29	120.76	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1226	CLA	CMB-C2B-C3B	3.29	134.28	126.55
14	b	1214	CLA	C1-C2-C3	-3.29	120.81	126.20
14	B	1203	CLA	C2B-C1B-NB	3.29	113.73	110.33
14	B	1238	CLA	C4D-C3D-CAD	3.29	111.68	108.11
18	B	4010	BCR	C7-C8-C9	-3.29	121.37	126.23
14	A	1137	CLA	C2B-C1B-NB	3.29	113.73	110.33
14	B	1022	CLA	C1-C2-C3	-3.29	120.81	126.20
14	A	1119	CLA	CHD-C1D-ND	-3.29	120.18	124.80
14	H	1223	CLA	C3C-C4C-NC	3.29	114.64	110.43
14	B	1227	CLA	C2B-C1B-NB	3.29	113.73	110.33
14	b	1238	CLA	C4-C3-C5	3.28	120.93	115.23
14	H	1239	CLA	CHD-C1D-ND	-3.28	120.18	124.80
14	G	1128	CLA	C3B-C2B-C1B	-3.28	103.30	107.17
14	H	1224	CLA	CAA-C2A-C3A	-3.28	104.13	113.00
14	a	1137	CLA	C2B-C1B-NB	3.28	113.73	110.33
14	B	1211	CLA	C1-C2-C3	-3.28	120.82	126.20
14	X	1701	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
15	a	1120	F6C	CMA-C3A-C4A	-3.28	118.95	124.73
14	H	1021	CLA	CMC-C2C-C1C	3.28	130.16	125.03
14	G	1102	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
14	B	1224	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
14	b	1201	CLA	C4-C3-C5	3.28	120.92	115.23
14	H	1238	CLA	C4-C3-C5	3.28	120.92	115.23
14	b	1214	CLA	CHD-C1D-ND	-3.28	120.19	124.80
14	b	1021	CLA	O2A-C1-C2	3.28	120.72	108.11
15	G	1120	F6C	CMA-C3A-C4A	-3.28	118.96	124.73
14	H	1238	CLA	C4D-C3D-CAD	3.28	111.66	108.11
18	b	4013	BCR	C28-C27-C26	-3.27	108.22	114.06
14	L	1502	CLA	C2B-C1B-NB	3.27	113.72	110.33
15	A	1120	F6C	CMA-C3A-C4A	-3.27	118.96	124.73
14	a	1119	CLA	CHD-C1D-ND	-3.27	120.19	124.80
14	B	1211	CLA	CHD-C1D-ND	-3.27	120.20	124.80
14	A	1107	CLA	O2A-CGA-CBA	3.27	124.34	114.00
14	G	1137	CLA	C2B-C1B-NB	3.27	113.72	110.33
14	W	1701	CLA	O2A-CGA-CBA	3.27	124.34	114.00
14	A	1128	CLA	CHD-C1D-ND	-3.27	120.20	124.80
14	a	1102	CLA	CAA-C2A-C3A	-3.27	104.16	113.00
14	B	1214	CLA	C1-C2-C3	-3.27	120.84	126.20
14	H	1021	CLA	O2A-C1-C2	3.27	120.69	108.11
14	H	1211	CLA	C1-C2-C3	-3.27	120.84	126.20
14	b	1022	CLA	C1-C2-C3	-3.27	120.84	126.20
18	B	4013	BCR	C28-C27-C26	-3.27	108.23	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1012	CLA	C1-C2-C3	-3.27	120.84	126.20
14	H	1214	CLA	C1-C2-C3	-3.27	120.84	126.20
14	x	1701	CLA	O2A-CGA-CBA	3.27	124.32	114.00
14	B	1201	CLA	C4-C3-C5	3.27	120.90	115.23
14	B	1021	CLA	CMC-C2C-C1C	3.27	130.14	125.03
18	H	4013	BCR	C28-C27-C26	-3.26	108.23	114.06
14	X	1701	CLA	O2A-CGA-CBA	3.26	124.31	114.00
14	a	1117	CLA	C1D-ND-C4D	-3.26	104.02	106.31
14	A	1124	CLA	CAA-C2A-C3A	-3.26	104.19	113.00
14	B	1214	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	b	1021	CLA	CMC-C2C-C1C	3.26	130.13	125.03
14	H	1214	CLA	CHD-C1D-ND	-3.26	120.22	124.80
15	H	1230	F6C	C4A-NA-C1A	3.26	108.60	106.31
14	H	1224	CLA	O1D-CGD-CBD	-3.26	118.10	124.52
14	b	1223	CLA	C3C-C4C-NC	3.25	114.60	110.43
14	B	1224	CLA	O1D-CGD-CBD	-3.25	118.10	124.52
14	a	1128	CLA	CHD-C1D-ND	-3.25	120.23	124.80
14	b	1239	CLA	CHD-C1D-ND	-3.25	120.23	124.80
14	b	1234	CLA	O2A-CGA-CBA	3.25	121.75	111.83
15	G	1121	F6C	C4A-NA-C1A	3.25	108.59	106.31
14	B	1201	CLA	CHD-C1D-ND	-3.25	120.23	124.80
14	a	1107	CLA	O2A-CGA-CBA	3.25	124.26	114.00
14	B	1234	CLA	O2A-CGA-CBA	3.25	121.74	111.83
14	B	1234	CLA	C2B-C1B-NB	3.25	113.69	110.33
14	a	1136	CLA	C4-C3-C5	3.25	120.86	115.23
14	b	1211	CLA	C1-C2-C3	-3.25	120.88	126.20
14	a	1129	CLA	C2B-C1B-NB	3.25	113.69	110.33
14	a	1124	CLA	CAA-C2A-C3A	-3.25	104.23	113.00
14	G	1124	CLA	CAA-C2A-C3A	-3.25	104.23	113.00
14	H	1012	CLA	C3C-C4C-NC	3.24	114.59	110.43
14	H	1202	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
15	A	1121	F6C	CHB-C4A-C3A	-3.24	118.74	125.49
14	A	1129	CLA	C2B-C1B-NB	3.24	113.69	110.33
14	B	1202	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
15	G	1121	F6C	CHB-C4A-C3A	-3.24	118.74	125.49
13	a	1011	CL0	O2D-CGD-O1D	-3.24	117.54	123.85
14	G	1114	CLA	O2A-CGA-CBA	3.24	124.24	114.00
14	a	1114	CLA	O2A-CGA-CBA	3.24	124.24	114.00
14	b	1224	CLA	O1D-CGD-CBD	-3.24	118.12	124.52
14	A	1114	CLA	O2A-CGA-CBA	3.24	124.24	114.00
15	a	1121	F6C	CHB-C4A-C3A	-3.24	118.75	125.49
15	B	1230	F6C	C4A-NA-C1A	3.24	108.59	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1205	CLA	CBA-CAA-C2A	3.24	123.43	113.79
14	b	1239	CLA	CMB-C2B-C1B	3.24	130.35	125.42
14	b	1233	CLA	O2A-CGA-CBA	3.24	124.23	114.00
14	G	1107	CLA	O2A-CGA-CBA	3.24	124.23	114.00
18	a	4002	BCR	C36-C18-C17	-3.24	117.57	122.82
18	G	4002	BCR	C28-C27-C26	-3.24	108.28	114.06
14	G	1138	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
20	B	5002	LMG	O8-C28-C29	3.24	121.70	111.83
16	G	2001	PQN	C14-C13-C15	3.24	120.84	115.23
15	G	1120	F6C	O2A-CGA-CBA	3.24	124.22	114.00
14	G	1122	CLA	CHD-C1D-ND	-3.23	120.25	124.80
15	A	1120	F6C	O2A-CGA-CBA	3.23	124.22	114.00
15	a	1120	F6C	O2A-CGA-CBA	3.23	124.22	114.00
14	A	1101	CLA	CHD-C1D-ND	-3.23	120.25	124.80
14	H	1201	CLA	CHD-C1D-ND	-3.23	120.25	124.80
14	b	1234	CLA	CHD-C1D-ND	-3.23	120.25	124.80
18	V	4021	BCR	C34-C9-C10	-3.23	117.58	122.82
14	B	1235	CLA	CMB-C2B-C3B	3.23	134.15	126.55
14	H	1234	CLA	O2A-CGA-CBA	3.23	121.68	111.83
14	A	1117	CLA	C1D-ND-C4D	-3.23	104.05	106.31
18	A	4002	BCR	C36-C18-C17	-3.23	117.58	122.82
18	A	4002	BCR	C28-C27-C26	-3.23	108.30	114.06
14	b	1222	CLA	CAA-C2A-C1A	-3.23	101.40	111.97
20	b	5002	LMG	O8-C28-C29	3.23	121.68	111.83
15	b	1230	F6C	C4A-NA-C1A	3.23	108.58	106.31
14	G	1136	CLA	C4-C3-C5	3.23	120.83	115.23
18	a	4002	BCR	C28-C27-C26	-3.23	108.30	114.06
14	H	1205	CLA	CBA-CAA-C2A	3.23	123.39	113.79
14	b	1205	CLA	CBA-CAA-C2A	3.23	123.39	113.79
20	H	5002	LMG	O8-C28-C29	3.23	121.67	111.83
14	H	1222	CLA	CAA-C2A-C1A	-3.22	101.41	111.97
14	b	1201	CLA	CHD-C1D-ND	-3.22	120.26	124.80
14	b	1022	CLA	C3C-C4C-NC	3.22	114.56	110.43
14	B	1233	CLA	O2A-CGA-CBA	3.22	124.19	114.00
14	H	1205	CLA	CHD-C1D-ND	-3.22	120.27	124.80
18	G	4002	BCR	C36-C18-C17	-3.22	117.59	122.82
13	A	1011	CL0	O2D-CGD-O1D	-3.22	117.57	123.85
14	A	1138	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	G	1129	CLA	C2B-C1B-NB	3.22	113.67	110.33
14	B	1224	CLA	CMC-C2C-C1C	3.22	130.07	125.03
14	b	1224	CLA	CMC-C2C-C1C	3.22	130.07	125.03
18	m	4021	BCR	C34-C9-C10	-3.22	117.60	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1137	CLA	O2A-CGA-CBA	3.22	124.18	114.00
14	H	1233	CLA	O2A-CGA-CBA	3.22	124.18	114.00
16	a	2001	PQN	C14-C13-C15	3.22	120.82	115.23
14	b	1234	CLA	C2B-C1B-NB	3.22	113.67	110.33
14	a	1138	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	B	1203	CLA	C1-C2-C3	-3.22	120.92	126.20
14	B	1222	CLA	CAA-C2A-C1A	-3.22	101.42	111.97
14	G	1101	CLA	CHD-C1D-ND	-3.22	120.27	124.80
16	A	2001	PQN	C14-C13-C15	3.22	120.81	115.23
14	b	1215	CLA	CHD-C1D-ND	-3.22	120.27	124.80
14	b	1205	CLA	CHD-C1D-ND	-3.22	120.27	124.80
14	H	1239	CLA	CMB-C2B-C1B	3.22	130.32	125.42
14	b	1202	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	a	1122	CLA	CHD-C1D-ND	-3.21	120.28	124.80
15	H	1237	F6C	C3A-C4A-NA	3.21	113.31	110.13
14	a	1137	CLA	O2A-CGA-CBA	3.21	124.16	114.00
18	m	4021	BCR	C3-C4-C5	-3.21	108.33	114.06
14	H	1234	CLA	C2B-C1B-NB	3.21	113.66	110.33
14	H	1215	CLA	CHD-C1D-ND	-3.21	120.28	124.80
14	B	1234	CLA	CHD-C1D-ND	-3.21	120.28	124.80
14	H	1224	CLA	CMC-C2C-C1C	3.21	130.05	125.03
14	b	1023	CLA	CBC-CAC-C3C	3.21	121.12	112.42
14	b	1210	CLA	O2A-CGA-CBA	3.21	121.62	111.83
14	b	1235	CLA	CMB-C2B-C3B	3.21	134.10	126.55
13	G	1011	CL0	O2D-CGD-O1D	-3.21	117.60	123.85
14	H	1207	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
14	G	1137	CLA	O2A-CGA-CBA	3.21	124.14	114.00
14	B	1021	CLA	C4-C3-C5	3.21	120.80	115.23
14	H	1023	CLA	CBC-CAC-C3C	3.21	121.11	112.42
14	B	1023	CLA	CBC-CAC-C3C	3.21	121.11	112.42
14	A	1122	CLA	CHD-C1D-ND	-3.21	120.29	124.80
14	B	1215	CLA	CHD-C1D-ND	-3.21	120.29	124.80
14	H	1203	CLA	C1-C2-C3	-3.20	120.95	126.20
14	a	1101	CLA	CHD-C1D-ND	-3.20	120.29	124.80
14	B	1210	CLA	O2A-CGA-CBA	3.20	121.61	111.83
18	M	4021	BCR	C34-C9-C10	-3.20	117.63	122.82
14	H	1021	CLA	C4-C3-C5	3.20	120.79	115.23
18	M	4021	BCR	C3-C4-C5	-3.20	108.34	114.06
18	A	4003	BCR	C30-C25-C26	-3.20	118.26	122.64
14	b	1207	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
14	B	1239	CLA	CMB-C2B-C1B	3.20	130.29	125.42
14	b	1225	CLA	C2B-C1B-NB	3.20	113.65	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	V	4021	BCR	C3-C4-C5	-3.20	108.35	114.06
14	H	1235	CLA	CMB-C2B-C3B	3.20	134.08	126.55
15	A	1121	F6C	C4A-NA-C1A	3.20	108.56	106.31
18	i	4018	BCR	C34-C9-C10	-3.20	117.63	122.82
14	B	1022	CLA	C3C-C4C-NC	3.20	114.53	110.43
14	H	1210	CLA	O2A-CGA-CBA	3.20	121.58	111.83
14	H	1234	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	A	1136	CLA	C4-C3-C5	3.20	120.78	115.23
14	a	1113	CLA	O2A-CGA-CBA	3.19	124.09	114.00
14	A	1135	CLA	C1-C2-C3	-3.19	121.59	126.76
14	A	1113	CLA	O2A-CGA-CBA	3.19	124.09	114.00
14	A	1136	CLA	CMA-C3A-C4A	3.19	120.36	111.77
14	a	1122	CLA	O2A-C1-C2	3.19	120.40	108.11
14	G	1122	CLA	O2A-C1-C2	3.19	120.39	108.11
14	a	1136	CLA	CMA-C3A-C4A	3.19	120.35	111.77
18	I	4018	BCR	C34-C9-C10	-3.19	117.65	122.82
14	a	1140	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
13	a	1011	CL0	C1-O2A-CGA	3.19	124.37	116.65
14	A	1122	CLA	O2A-C1-C2	3.19	120.37	108.11
14	G	1136	CLA	CMA-C3A-C4A	3.19	120.34	111.77
14	A	1140	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
15	H	1230	F6C	CHA-C4D-ND	3.18	136.10	133.05
14	H	1225	CLA	C2B-C1B-NB	3.18	113.63	110.33
14	G	1113	CLA	O2A-CGA-CBA	3.18	124.05	114.00
14	B	1225	CLA	C2B-C1B-NB	3.18	113.62	110.33
14	b	1203	CLA	C1-C2-C3	-3.18	120.98	126.20
18	G	4003	BCR	C30-C25-C26	-3.18	118.29	122.64
14	G	1140	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
14	B	1022	CLA	OBD-CAD-C3D	-3.18	120.99	128.42
14	b	1021	CLA	C4-C3-C5	3.18	120.74	115.23
18	R	4018	BCR	C34-C9-C10	-3.18	117.67	122.82
14	B	1207	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
14	B	1227	CLA	O2A-CGA-CBA	3.18	124.04	114.00
18	a	4008	BCR	C38-C26-C25	-3.18	121.02	124.48
14	B	1205	CLA	CHD-C1D-ND	-3.17	120.33	124.80
14	H	1227	CLA	O2A-CGA-CBA	3.17	124.03	114.00
14	a	1106	CLA	O2A-CGA-CBA	3.17	124.03	114.00
15	b	1230	F6C	OMB-CMB-C2B	-3.17	118.46	125.62
14	G	1135	CLA	C1-C2-C3	-3.17	121.63	126.76
14	a	1135	CLA	C1-C2-C3	-3.17	121.63	126.76
18	G	4001	BCR	C3-C4-C5	-3.17	108.40	114.06
15	B	1230	F6C	O2A-CGA-CBA	3.17	124.01	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1106	CLA	O2A-CGA-CBA	3.17	124.01	114.00
15	B	1237	F6C	C3A-C4A-NA	3.17	113.26	110.13
14	A	1129	CLA	CHD-C1D-ND	-3.17	120.34	124.80
13	G	1011	CL0	C1-O2A-CGA	3.17	124.32	116.65
14	b	1227	CLA	O2A-CGA-CBA	3.17	124.01	114.00
18	A	4001	BCR	C3-C4-C5	-3.17	108.41	114.06
18	I	4020	BCR	C34-C9-C8	3.17	122.92	118.09
14	B	1210	CLA	O2A-C1-C2	3.16	120.29	108.11
15	a	1120	F6C	CHD-C1D-ND	-3.16	119.55	124.31
15	H	1230	F6C	CHA-C1A-C2A	-3.16	121.90	130.41
14	A	1106	CLA	O2A-CGA-CBA	3.16	124.00	114.00
14	b	1022	CLA	OBD-CAD-C3D	-3.16	121.02	128.42
15	b	1237	F6C	C3A-C4A-NA	3.16	113.26	110.13
13	A	1011	CL0	C1-O2A-CGA	3.16	124.31	116.65
14	G	1128	CLA	C2B-C1B-NB	3.16	113.60	110.33
14	G	1106	CLA	CHD-C1D-ND	-3.16	120.35	124.80
14	H	1012	CLA	OBD-CAD-C3D	-3.16	121.03	128.42
14	b	1210	CLA	O2A-C1-C2	3.16	120.27	108.11
14	b	1219	CLA	O2A-CGA-CBA	3.16	123.98	114.00
18	a	4003	BCR	C30-C25-C26	-3.16	118.32	122.64
14	H	1209	CLA	O2A-CGA-CBA	3.16	123.97	114.00
15	B	1230	F6C	CHA-C1A-C2A	-3.16	121.92	130.41
14	B	1219	CLA	O2A-CGA-CBA	3.16	123.97	114.00
14	a	1106	CLA	CHD-C1D-ND	-3.16	120.36	124.80
14	B	1226	CLA	C1-C2-C3	-3.15	121.03	126.20
15	G	1120	F6C	CHD-C1D-ND	-3.15	119.56	124.31
14	A	1110	CLA	O2A-CGA-CBA	3.15	123.96	114.00
14	A	1105	CLA	O2A-CGA-CBA	3.15	123.96	114.00
14	G	1110	CLA	O2A-CGA-CBA	3.15	123.96	114.00
14	H	1023	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
14	H	1210	CLA	O2A-C1-C2	3.15	120.23	108.11
14	G	1129	CLA	CHD-C1D-ND	-3.15	120.37	124.80
15	H	1230	F6C	O2A-CGA-CBA	3.15	123.95	114.00
15	A	1120	F6C	CHD-C1D-ND	-3.15	119.57	124.31
14	a	1128	CLA	C2B-C1B-NB	3.15	113.59	110.33
18	i	4020	BCR	C34-C9-C8	3.15	122.90	118.09
14	B	1234	CLA	CMB-C2B-C1B	3.15	130.21	125.42
18	R	4020	BCR	C34-C9-C8	3.15	122.90	118.09
14	B	1209	CLA	O2A-CGA-CBA	3.15	123.94	114.00
14	a	1105	CLA	O2A-CGA-CBA	3.15	123.94	114.00
14	G	1139	CLA	CHD-C1D-ND	-3.15	120.38	124.80
14	H	1219	CLA	O2A-CGA-CBA	3.15	123.94	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	I	4020	BCR	C24-C23-C22	-3.15	121.58	126.23
14	b	1226	CLA	C1-C2-C3	-3.15	121.04	126.20
14	b	1209	CLA	O2A-CGA-CBA	3.15	123.94	114.00
18	B	4005	BCR	C37-C22-C21	-3.14	117.72	122.82
15	B	1230	F6C	C3D-C4D-ND	3.14	115.11	109.93
15	b	1230	F6C	C3D-C4D-ND	3.14	115.11	109.93
14	G	1135	CLA	CAC-C3C-C4C	3.14	128.88	124.79
14	b	1023	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
14	a	1129	CLA	CHD-C1D-ND	-3.14	120.38	124.80
14	H	1226	CLA	C1-C2-C3	-3.14	121.05	126.20
14	T	1401	CLA	O2A-CGA-CBA	3.14	123.92	114.00
14	G	1105	CLA	O2A-CGA-CBA	3.14	123.92	114.00
14	A	1106	CLA	CHD-C1D-ND	-3.14	120.39	124.80
14	H	1238	CLA	CAC-C3C-C4C	3.14	128.87	124.79
14	B	1220	CLA	CHD-C1D-ND	-3.14	120.39	124.80
18	a	4001	BCR	C3-C4-C5	-3.14	108.46	114.06
14	H	1215	CLA	O2A-CGA-O1A	-3.14	115.78	123.63
14	a	1110	CLA	O2A-CGA-CBA	3.14	123.91	114.00
14	a	1108	CLA	O2A-CGA-CBA	3.14	123.91	114.00
14	b	1207	CLA	CHD-C1D-ND	-3.13	120.39	124.80
14	b	1238	CLA	CAC-C3C-C4C	3.13	128.87	124.79
14	A	1128	CLA	C2B-C1B-NB	3.13	113.58	110.33
15	b	1230	F6C	CHA-C1A-C2A	-3.13	121.98	130.41
14	k	1401	CLA	O2A-CGA-CBA	3.13	123.90	114.00
14	b	1224	CLA	CHD-C1D-ND	-3.13	120.39	124.80
14	H	1224	CLA	CHD-C1D-ND	-3.13	120.40	124.80
14	b	1220	CLA	CHD-C1D-ND	-3.13	120.40	124.80
18	b	4014	BCR	C7-C8-C9	-3.13	121.60	126.23
18	H	4014	BCR	C7-C8-C9	-3.13	121.61	126.23
14	G	1108	CLA	O2A-CGA-CBA	3.13	123.89	114.00
18	R	4020	BCR	C24-C23-C22	-3.13	121.61	126.23
18	i	4020	BCR	C24-C23-C22	-3.13	121.61	126.23
14	G	1102	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
14	G	1123	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
14	a	1123	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
18	H	4005	BCR	C37-C22-C21	-3.13	117.75	122.82
14	B	1023	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
15	b	1230	F6C	O2A-CGA-CBA	3.13	123.87	114.00
14	a	1139	CLA	CHD-C1D-ND	-3.12	120.41	124.80
14	b	1208	CLA	CMB-C2B-C1B	3.12	130.18	125.42
14	B	1215	CLA	O2A-CGA-O1A	-3.12	115.81	123.63
14	H	1219	CLA	CHD-C1D-ND	-3.12	120.41	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1123	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	K	1401	CLA	O2A-CGA-CBA	3.12	123.86	114.00
14	a	1123	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	a	1135	CLA	CAC-C3C-C4C	3.12	128.85	124.79
14	A	1123	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
14	a	1102	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	H	1220	CLA	CHD-C1D-ND	-3.12	120.41	124.80
14	A	1108	CLA	O2A-CGA-CBA	3.12	123.85	114.00
14	a	1128	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	G	1123	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	a	1125	CLA	C4C-C3C-C2C	-3.12	102.36	106.89
14	B	1224	CLA	CHD-C1D-ND	-3.12	120.42	124.80
14	l	1501	CLA	O2D-CGD-O1D	-3.11	117.78	123.85
14	H	1207	CLA	CHD-C1D-ND	-3.11	120.42	124.80
18	b	4005	BCR	C37-C22-C21	-3.11	117.77	122.82
18	B	4014	BCR	C7-C8-C9	-3.11	121.63	126.23
14	A	1139	CLA	CHD-C1D-ND	-3.11	120.42	124.80
14	A	1129	CLA	CMC-C2C-C1C	3.11	129.90	125.03
14	A	1107	CLA	C2B-C1B-NB	3.11	113.55	110.33
14	A	1116	CLA	CMC-C2C-C1C	3.11	129.90	125.03
14	A	1135	CLA	CAC-C3C-C4C	3.11	128.84	124.79
14	B	1238	CLA	CAC-C3C-C4C	3.11	128.84	124.79
14	G	1111	CLA	C1-O2A-CGA	3.11	124.18	116.65
14	B	1207	CLA	CHD-C1D-ND	-3.11	120.42	124.80
14	b	1234	CLA	CMB-C2B-C1B	3.11	130.16	125.42
14	b	1219	CLA	CHD-C1D-ND	-3.11	120.43	124.80
14	a	1116	CLA	CMC-C2C-C1C	3.11	129.89	125.03
14	H	1208	CLA	CMB-C2B-C1B	3.11	130.15	125.42
14	b	1215	CLA	O2A-CGA-O1A	-3.11	115.85	123.63
18	I	4020	BCR	C12-C13-C14	-3.11	114.12	119.01
14	a	1140	CLA	C4-C3-C5	3.11	120.62	115.23
14	H	1234	CLA	CMB-C2B-C1B	3.11	130.15	125.42
14	G	1125	CLA	C3C-C4C-NC	3.11	114.41	110.43
14	L	1501	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
18	i	4020	BCR	C12-C13-C14	-3.11	114.12	119.01
14	A	1111	CLA	C1-O2A-CGA	3.11	124.17	116.65
18	R	4020	BCR	C12-C13-C14	-3.10	114.13	119.01
14	H	1231	CLA	C1-C2-C3	-3.10	121.11	126.20
14	b	1231	CLA	C1-C2-C3	-3.10	121.11	126.20
14	L	1502	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	H	1210	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
13	A	1011	CL0	CMA-C3A-C4A	-3.10	107.93	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1125	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
14	B	1231	CLA	C1-C2-C3	-3.10	121.12	126.20
14	b	1208	CLA	C1-C2-C3	-3.10	121.12	126.20
14	B	1219	CLA	CHD-C1D-ND	-3.10	120.44	124.80
14	a	1125	CLA	C3C-C4C-NC	3.10	114.40	110.43
14	G	1116	CLA	CMC-C2C-C1C	3.10	129.87	125.03
15	H	1230	F6C	C3D-C4D-ND	3.09	115.03	109.93
14	A	1102	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	a	1118	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
13	a	1011	CL0	CMA-C3A-C4A	-3.09	107.95	114.61
14	a	1126	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
14	b	1210	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
13	G	1011	CL0	CMA-C3A-C4A	-3.09	107.95	114.61
14	k	1401	CLA	CMA-C3A-C4A	3.09	120.08	111.77
14	l	1502	CLA	C1-C2-C3	-3.09	121.13	126.20
14	A	1128	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	A	1125	CLA	C3C-C4C-NC	3.09	114.39	110.43
14	G	1140	CLA	C4-C3-C5	3.09	120.59	115.23
14	H	1236	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	U	1501	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	T	1401	CLA	CMA-C3A-C4A	3.09	120.07	111.77
14	G	1126	CLA	CAA-C2A-C3A	-3.09	104.66	113.00
14	G	1128	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	G	1129	CLA	CMC-C2C-C1C	3.09	129.86	125.03
14	A	1140	CLA	C4-C3-C5	3.08	120.58	115.23
14	a	1130	CLA	O2A-C1-C2	3.08	119.97	108.11
14	l	1502	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
14	k	1401	CLA	CMB-C2B-C1B	3.08	130.11	125.42
14	U	1502	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
14	A	1125	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
14	a	1107	CLA	C2B-C1B-NB	3.08	113.52	110.33
14	a	1111	CLA	C1-O2A-CGA	3.08	124.11	116.65
14	K	1401	CLA	CMA-C3A-C4A	3.08	120.06	111.77
14	B	1210	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
14	G	1107	CLA	C2B-C1B-NB	3.08	113.52	110.33
14	G	1130	CLA	O2A-C1-C2	3.08	119.96	108.11
14	B	1222	CLA	O2A-C1-C2	3.08	119.96	108.11
14	U	1502	CLA	C1-C2-C3	-3.08	121.15	126.20
14	B	1231	CLA	O2A-C1-C2	3.08	119.95	108.11
14	G	1118	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
14	U	1502	CLA	CAA-C2A-C3A	-3.08	104.68	113.00
14	A	1130	CLA	O2A-C1-C2	3.08	119.95	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1208	CLA	C1-C2-C3	-3.08	121.16	126.20
14	L	1502	CLA	C1-C2-C3	-3.08	121.16	126.20
14	b	1236	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
14	a	1129	CLA	CMC-C2C-C1C	3.07	129.84	125.03
14	B	1236	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	b	1222	CLA	O2A-C1-C2	3.07	119.94	108.11
14	A	1126	CLA	CAA-C2A-C3A	-3.07	104.69	113.00
14	H	1215	CLA	CMB-C2B-C3B	3.07	133.78	126.55
14	a	1113	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
18	A	4008	BCR	C38-C26-C25	-3.07	121.13	124.48
14	B	1235	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	H	1222	CLA	O2A-C1-C2	3.07	119.92	108.11
14	b	1215	CLA	CMB-C2B-C3B	3.07	133.77	126.55
14	b	1231	CLA	O2A-C1-C2	3.07	119.92	108.11
14	B	1236	CLA	C3D-C4D-ND	3.07	114.97	109.99
14	H	1231	CLA	O2A-C1-C2	3.07	119.92	108.11
14	B	1225	CLA	C3C-C4C-NC	3.07	114.36	110.43
18	R	4018	BCR	C34-C9-C8	3.07	122.77	118.09
14	B	1208	CLA	C1-C2-C3	-3.07	121.17	126.20
14	L	1502	CLA	CAA-C2A-C3A	-3.06	104.72	113.00
14	B	1215	CLA	CMB-C2B-C3B	3.06	133.76	126.55
14	H	1236	CLA	C3D-C4D-ND	3.06	114.97	109.99
14	B	1206	CLA	CHD-C1D-ND	-3.06	120.49	124.80
14	b	1225	CLA	C3C-C4C-NC	3.06	114.35	110.43
15	H	1230	F6C	OMB-CMB-C2B	-3.06	118.71	125.62
18	B	4004	BCR	C2-C1-C6	3.06	114.89	110.44
18	l	4019	BCR	C36-C18-C17	-3.06	117.86	122.82
14	A	1125	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
14	H	1207	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
14	G	1125	CLA	CAA-C2A-C3A	-3.06	104.73	113.00
14	b	1236	CLA	C3D-C4D-ND	3.06	114.96	109.99
18	G	4008	BCR	C38-C26-C25	-3.06	121.15	124.48
14	A	1113	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	a	1125	CLA	CAA-C2A-C3A	-3.06	104.74	113.00
14	H	1225	CLA	C3C-C4C-NC	3.06	114.34	110.43
14	T	1401	CLA	CMB-C2B-C1B	3.05	130.07	125.42
14	B	1208	CLA	CMB-C2B-C1B	3.05	130.07	125.42
14	l	1502	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
18	L	4019	BCR	C36-C18-C17	-3.05	117.87	122.82
15	A	1120	F6C	CHB-C4A-C3A	-3.05	119.14	125.49
14	b	1233	CLA	C2B-C1B-NB	3.05	113.49	110.33
14	B	1207	CLA	CAA-C2A-C3A	-3.05	104.76	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1013	CLA	CMC-C2C-C1C	3.05	129.80	125.03
14	a	1013	CLA	CMC-C2C-C1C	3.05	129.80	125.03
14	B	1228	CLA	CAC-C3C-C4C	3.05	128.76	124.79
14	b	1229	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	A	1113	CLA	CMB-C2B-C3B	3.05	133.71	126.55
14	b	1207	CLA	CAA-C2A-C3A	-3.05	104.77	113.00
14	a	1013	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	b	1228	CLA	CAC-C3C-C4C	3.04	128.75	124.79
18	i	4018	BCR	C34-C9-C8	3.04	122.74	118.09
14	H	1202	CLA	O2A-C1-C2	3.04	119.82	108.11
14	A	1118	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
14	b	1202	CLA	O2A-C1-C2	3.04	119.81	108.11
14	b	1235	CLA	CMA-C3A-C4A	3.04	119.94	111.77
14	b	1235	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	H	1228	CLA	CAC-C3C-C4C	3.04	128.75	124.79
18	I	4018	BCR	C34-C9-C8	3.04	122.73	118.09
14	H	1235	CLA	CMA-C3A-C4A	3.04	119.94	111.77
14	B	1202	CLA	O2A-C1-C2	3.04	119.80	108.11
18	H	4004	BCR	C2-C1-C6	3.04	114.85	110.44
15	G	1120	F6C	CHB-C4A-C3A	-3.03	119.18	125.49
14	B	1235	CLA	CMA-C3A-C4A	3.03	119.93	111.77
15	b	1230	F6C	CHA-C4D-ND	3.03	135.95	133.05
14	K	1401	CLA	CMB-C2B-C1B	3.03	130.04	125.42
18	b	4004	BCR	C2-C1-C6	3.03	114.84	110.44
14	b	1234	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
14	A	1013	CLA	CMC-C2C-C1C	3.03	129.77	125.03
14	H	1206	CLA	CHD-C1D-ND	-3.03	120.54	124.80
14	A	1124	CLA	C1-C2-C3	-3.03	121.24	126.20
14	G	1113	CLA	CMB-C2B-C3B	3.03	133.67	126.55
14	G	1113	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
14	B	1233	CLA	C2B-C1B-NB	3.03	113.46	110.33
14	B	1229	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
14	H	1233	CLA	C2B-C1B-NB	3.02	113.46	110.33
14	G	1101	CLA	O2A-CGA-CBA	3.02	123.56	114.00
15	B	1237	F6C	C4-C3-C5	3.02	120.48	115.23
14	a	1111	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
15	a	1120	F6C	CHB-C4A-C3A	-3.02	119.20	125.49
14	a	1113	CLA	CMB-C2B-C3B	3.02	133.65	126.55
14	H	1235	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	b	1227	CLA	C4D-C3D-CAD	3.02	111.38	108.11
14	b	1239	CLA	CAA-CBA-CGA	-3.02	104.64	113.21
14	A	1013	CLA	O2D-CGD-O1D	-3.02	117.97	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1230	F6C	OMB-CMB-C2B	-3.02	118.81	125.62
14	B	1233	CLA	CMB-C2B-C1B	3.02	130.01	125.42
14	b	1201	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
15	b	1237	F6C	C4-C3-C5	3.02	120.46	115.23
14	H	1239	CLA	CAA-CBA-CGA	-3.02	104.65	113.21
18	U	4019	BCR	C36-C18-C17	-3.01	117.93	122.82
14	G	1124	CLA	C1-C2-C3	-3.01	121.26	126.20
14	B	1234	CLA	C4C-C3C-C2C	-3.01	102.50	106.89
14	A	1101	CLA	O2A-CGA-CBA	3.01	123.52	114.00
14	a	1130	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	A	1131	CLA	C1-C2-C3	-3.01	121.26	126.20
14	B	1239	CLA	CAA-CBA-CGA	-3.01	104.66	113.21
14	A	1106	CLA	CMB-C2B-C1B	3.01	130.00	125.42
14	H	1229	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
14	G	1140	CLA	C3C-C4C-NC	3.01	114.28	110.43
13	A	1011	CL0	CMA-C3A-C2A	-3.01	102.51	114.13
14	B	1204	CLA	C1-O2A-CGA	3.01	123.93	116.65
14	A	1140	CLA	C3C-C4C-NC	3.01	114.28	110.43
14	b	1204	CLA	C1-O2A-CGA	3.01	123.93	116.65
14	a	1101	CLA	O2A-CGA-CBA	3.01	123.50	114.00
14	A	1102	CLA	CMB-C2B-C3B	3.01	133.62	126.55
14	B	1231	CLA	C4D-C3D-CAD	3.01	111.37	108.11
14	H	1227	CLA	C4D-C3D-CAD	3.01	111.37	108.11
15	H	1237	F6C	C4-C3-C5	3.01	120.44	115.23
18	b	4013	BCR	C38-C26-C25	-3.01	121.20	124.48
14	B	1201	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	H	1201	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	G	1111	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	G	1013	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	H	1233	CLA	CMB-C2B-C1B	3.00	129.99	125.42
14	B	1227	CLA	C4D-C3D-CAD	3.00	111.37	108.11
14	H	1217	CLA	CHD-C1D-ND	-3.00	120.58	124.80
20	A	5005	LMG	O8-C28-C29	3.00	120.99	111.83
14	a	1102	CLA	CMB-C2B-C3B	3.00	133.61	126.55
14	b	1233	CLA	CMB-C2B-C1B	3.00	129.99	125.42
14	a	1108	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
20	a	5005	LMG	O8-C28-C29	3.00	120.98	111.83
14	G	1108	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
14	A	1108	CLA	CAA-C2A-C3A	-3.00	104.90	113.00
14	b	1206	CLA	CHD-C1D-ND	-3.00	120.58	124.80
14	B	1233	CLA	CMA-C3A-C4A	3.00	119.83	111.77
14	H	1234	CLA	C4C-C3C-C2C	-3.00	102.53	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4017	BCR	C34-C9-C8	3.00	122.67	118.09
13	G	1011	CL0	CMA-C3A-C2A	-3.00	102.56	114.13
20	G	5005	LMG	O8-C28-C29	3.00	120.97	111.83
14	A	1130	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
14	B	1205	CLA	C1-O2A-CGA	2.99	123.90	116.65
14	G	1106	CLA	CMB-C2B-C1B	2.99	129.98	125.42
13	a	1011	CL0	CMA-C3A-C2A	-2.99	102.57	114.13
18	a	4008	BCR	C39-C30-C25	-2.99	105.55	110.24
14	A	1111	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	G	1130	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	b	1229	CLA	CMB-C2B-C3B	2.99	133.58	126.55
14	b	1235	CLA	O2A-C1-C2	2.99	119.61	108.11
14	G	1116	CLA	C1-C2-C3	-2.99	121.30	126.20
15	B	1230	F6C	CHA-C4D-ND	2.99	135.91	133.05
14	H	1235	CLA	O2A-C1-C2	2.99	119.60	108.11
14	B	1222	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
14	a	1131	CLA	C1-C2-C3	-2.99	121.31	126.20
18	b	4017	BCR	C34-C9-C8	2.99	122.65	118.09
14	A	1131	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
14	b	1205	CLA	C1-O2A-CGA	2.98	123.88	116.65
14	G	1102	CLA	CMB-C2B-C3B	2.98	133.57	126.55
14	a	1131	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
14	A	1013	CLA	C3C-C4C-NC	2.98	114.25	110.43
14	G	1131	CLA	C1-C2-C3	-2.98	121.31	126.20
14	a	1124	CLA	C1-C2-C3	-2.98	121.31	126.20
14	B	1221	CLA	CAA-C2A-C3A	-2.98	104.94	113.00
14	b	1217	CLA	CHD-C1D-ND	-2.98	120.61	124.80
14	H	1233	CLA	CMA-C3A-C4A	2.98	119.79	111.77
14	B	1212	CLA	CHD-C1D-ND	-2.98	120.61	124.80
18	H	4005	BCR	C40-C30-C25	-2.98	105.57	110.24
14	B	1235	CLA	O2A-C1-C2	2.98	119.58	108.11
18	G	4008	BCR	C39-C30-C25	-2.98	105.57	110.24
14	H	1205	CLA	C1-O2A-CGA	2.98	123.86	116.65
14	H	1212	CLA	CHD-C1D-ND	-2.98	120.61	124.80
14	H	1229	CLA	CMB-C2B-C3B	2.98	133.56	126.55
14	H	1222	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	b	1222	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	A	1125	CLA	C1-C2-C3	-2.98	121.32	126.20
18	A	4008	BCR	C39-C30-C25	-2.98	105.58	110.24
18	H	4017	BCR	C34-C9-C8	2.98	122.64	118.09
14	G	1135	CLA	C4D-C3D-CAD	2.98	111.34	108.11
15	b	1237	F6C	C4A-C3A-C2A	-2.98	102.56	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1113	CLA	CAA-C2A-C3A	-2.98	104.96	113.00
14	b	1231	CLA	C4D-C3D-CAD	2.97	111.34	108.11
14	b	1221	CLA	CAA-C2A-C3A	-2.97	104.96	113.00
14	b	1233	CLA	CMA-C3A-C4A	2.97	119.76	111.77
14	a	1115	CLA	CMC-C2C-C1C	2.97	129.68	125.03
14	a	1106	CLA	CMB-C2B-C1B	2.97	129.94	125.42
18	H	4013	BCR	C38-C26-C25	-2.97	121.24	124.48
14	a	1113	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
14	G	1117	CLA	CMB-C2B-C3B	2.97	133.54	126.55
14	L	1501	CLA	CHD-C1D-ND	-2.97	120.62	124.80
18	B	4013	BCR	C38-C26-C25	-2.97	121.24	124.48
18	b	4010	BCR	C19-C18-C17	2.97	123.68	119.01
14	A	1115	CLA	CMC-C2C-C1C	2.97	129.68	125.03
14	b	1218	CLA	CMA-C3A-C4A	2.97	119.75	111.77
20	I	5006	LMG	O8-C28-C29	2.97	120.89	111.83
14	H	1224	CLA	C3C-C4C-NC	2.97	114.23	110.43
14	b	1021	CLA	C3C-C4C-NC	2.97	114.23	110.43
14	H	1204	CLA	C1-O2A-CGA	2.97	123.84	116.65
14	A	1116	CLA	C1-C2-C3	-2.97	121.33	126.20
14	B	1202	CLA	C4-C3-C5	2.97	120.38	115.23
14	H	1234	CLA	CAC-C3C-C4C	2.97	128.65	124.79
15	H	1237	F6C	C3C-C4C-NC	2.97	113.57	110.32
14	B	1229	CLA	CMB-C2B-C3B	2.97	133.53	126.55
18	b	4005	BCR	C40-C30-C25	-2.97	105.59	110.24
14	B	1212	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
15	H	1230	F6C	C3C-C4C-NC	2.97	113.57	110.32
14	H	1221	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
15	B	1237	F6C	C4A-C3A-C2A	-2.97	102.57	106.97
18	a	4008	BCR	C34-C9-C8	2.97	122.62	118.09
14	H	1212	CLA	CAA-C2A-C3A	-2.97	104.98	113.00
14	a	1140	CLA	C3C-C4C-NC	2.97	114.23	110.43
14	G	1115	CLA	CMC-C2C-C1C	2.96	129.66	125.03
14	a	1013	CLA	C3C-C4C-NC	2.96	114.22	110.43
14	B	1218	CLA	CMA-C3A-C4A	2.96	119.73	111.77
14	G	1113	CLA	CAA-C2A-C3A	-2.96	105.00	113.00
14	B	1217	CLA	CHD-C1D-ND	-2.96	120.64	124.80
20	l	5007	LMG	O8-C28-C29	2.96	120.86	111.83
14	A	1135	CLA	C4D-C3D-CAD	2.96	111.32	108.11
20	i	5006	LMG	O8-C28-C29	2.96	120.86	111.83
20	U	5007	LMG	O8-C28-C29	2.96	120.86	111.83
14	a	1116	CLA	C1-C2-C3	-2.96	121.35	126.20
14	b	1204	CLA	C1-C2-C3	-2.96	121.35	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1234	CLA	C1-C2-C3	-2.96	121.35	126.20
15	H	1237	F6C	C4A-C3A-C2A	-2.96	102.58	106.97
18	A	4008	BCR	C34-C9-C8	2.96	122.61	118.09
20	R	5006	LMG	O8-C28-C29	2.96	120.85	111.83
14	b	1212	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
14	G	1131	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	a	1126	CLA	O1D-CGD-CBD	-2.95	118.69	124.52
14	b	1234	CLA	C1-C2-C3	-2.95	121.36	126.20
14	b	1234	CLA	CAC-C3C-C4C	2.95	128.63	124.79
14	U	1501	CLA	C3C-C4C-NC	2.95	114.21	110.43
14	H	1231	CLA	C4D-C3D-CAD	2.95	111.31	108.11
18	b	4012	BCR	C30-C25-C24	2.95	123.65	115.65
14	G	1013	CLA	C3C-C4C-NC	2.95	114.21	110.43
14	a	1125	CLA	C1-C2-C3	-2.95	121.36	126.20
14	B	1224	CLA	C1-C2-C3	-2.95	121.37	126.20
18	G	4008	BCR	C34-C9-C8	2.95	122.59	118.09
18	H	4004	BCR	C38-C26-C25	-2.95	121.27	124.48
14	H	1202	CLA	C4-C3-C5	2.95	120.34	115.23
14	G	1128	CLA	C1-C2-C3	-2.94	121.37	126.20
14	A	1140	CLA	CHD-C1D-ND	-2.94	120.66	124.80
18	H	4010	BCR	C19-C18-C17	2.94	123.64	119.01
14	G	1126	CLA	O1D-CGD-CBD	-2.94	118.71	124.52
14	a	1137	CLA	O1D-CGD-CBD	-2.94	118.71	124.52
20	L	5007	LMG	O8-C28-C29	2.94	120.81	111.83
18	b	4004	BCR	C38-C26-C25	-2.94	121.27	124.48
18	B	4010	BCR	C19-C18-C17	2.94	123.64	119.01
14	U	1501	CLA	CHD-C1D-ND	-2.94	120.66	124.80
18	B	4012	BCR	C33-C5-C4	2.94	119.87	113.60
14	b	1202	CLA	C4-C3-C5	2.94	120.33	115.23
18	B	4012	BCR	C30-C25-C24	2.94	123.63	115.65
14	b	1224	CLA	C3C-C4C-NC	2.94	114.19	110.43
14	A	1128	CLA	C1-C2-C3	-2.94	121.38	126.20
14	a	1117	CLA	CMB-C2B-C3B	2.94	133.46	126.55
14	H	1204	CLA	C3D-C4D-ND	2.94	114.76	109.99
14	H	1224	CLA	C1-C2-C3	-2.94	121.38	126.20
14	B	1224	CLA	C3C-C4C-NC	2.94	114.19	110.43
18	B	4009	BCR	C33-C5-C4	2.94	119.86	113.60
18	b	4012	BCR	C33-C5-C4	2.94	119.86	113.60
18	H	4009	BCR	C33-C5-C4	2.94	119.86	113.60
18	B	4016	BCR	C27-C26-C25	-2.94	118.74	122.70
14	H	1218	CLA	CMA-C3A-C4A	2.94	119.67	111.77
14	b	1224	CLA	C1-C2-C3	-2.94	121.39	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1233	CLA	CAA-C2A-C3A	-2.93	105.07	113.00
18	B	4005	BCR	C40-C30-C25	-2.93	105.64	110.24
15	H	1237	F6C	CHB-C4A-C3A	-2.93	119.39	125.49
18	H	4010	BCR	C3-C4-C5	-2.93	108.83	114.06
15	b	1237	F6C	CHB-C4A-C3A	-2.93	119.39	125.49
14	b	1204	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	A	1126	CLA	O1D-CGD-CBD	-2.93	118.73	124.52
14	B	1023	CLA	CHB-C4A-NA	2.93	128.63	124.40
14	G	1133	CLA	C4D-C3D-CAD	2.93	111.29	108.11
14	a	1128	CLA	C1-C2-C3	-2.93	121.39	126.20
14	a	1132	CLA	C1-C2-C3	-2.93	121.39	126.20
14	B	1204	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	H	1023	CLA	CHB-C4A-NA	2.93	128.63	124.40
14	G	1127	CLA	CAA-C2A-C3A	-2.93	105.08	113.00
14	B	1234	CLA	CAC-C3C-C4C	2.93	128.60	124.79
14	b	1212	CLA	CHD-C1D-ND	-2.93	120.68	124.80
14	H	1234	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
18	H	4012	BCR	C30-C25-C24	2.93	123.60	115.65
14	B	1204	CLA	C1-C2-C3	-2.93	121.40	126.20
18	H	4012	BCR	C33-C5-C4	2.93	119.84	113.60
18	b	4016	BCR	C27-C26-C25	-2.93	118.75	122.70
14	a	1127	CLA	CAA-C2A-C3A	-2.93	105.08	113.00
14	B	1021	CLA	C3C-C4C-NC	2.93	114.18	110.43
15	b	1230	F6C	CHD-C1D-ND	-2.93	119.90	124.31
14	A	1117	CLA	CMB-C2B-C3B	2.93	133.44	126.55
14	l	1501	CLA	C3C-C4C-NC	2.93	114.18	110.43
19	B	5004	LHG	O8-C23-C24	2.93	120.76	111.83
18	b	4009	BCR	C33-C5-C4	2.93	119.84	113.60
14	B	1233	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
14	H	1221	CLA	CHD-C1D-ND	-2.93	120.69	124.80
14	b	1233	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
14	a	1135	CLA	CMA-C3A-C4A	2.93	119.64	111.77
15	B	1237	F6C	C3C-C4C-NC	2.93	113.53	110.32
18	A	4011	BCR	C38-C26-C25	-2.93	121.29	124.48
14	a	1135	CLA	C4D-C3D-CAD	2.92	111.28	108.11
14	H	1204	CLA	C1-C2-C3	-2.92	121.41	126.20
14	B	1234	CLA	C1-C2-C3	-2.92	121.41	126.20
14	G	1125	CLA	C1-C2-C3	-2.92	121.41	126.20
14	A	1129	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
14	A	1127	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
14	l	1501	CLA	CHD-C1D-ND	-2.92	120.69	124.80
14	G	1137	CLA	O1D-CGD-CBD	-2.92	118.76	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1237	F6C	CHB-C4A-C3A	-2.92	119.42	125.49
14	b	1023	CLA	CHB-C4A-NA	2.92	128.61	124.40
14	L	1501	CLA	C3C-C4C-NC	2.92	114.17	110.43
14	B	1222	CLA	C4-C3-C5	2.92	120.29	115.23
14	A	1132	CLA	C1-C2-C3	-2.92	121.42	126.20
14	H	1222	CLA	C4-C3-C5	2.92	120.29	115.23
14	A	1139	CLA	CAC-C3C-C4C	2.92	128.58	124.79
18	b	4010	BCR	C3-C4-C5	-2.92	108.86	114.06
14	b	1234	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	A	1137	CLA	O1D-CGD-CBD	-2.92	118.77	124.52
14	B	1234	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
14	B	1212	CLA	C3C-C4C-NC	2.91	114.16	110.43
14	G	1129	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
18	G	4008	BCR	C28-C27-C26	-2.91	108.86	114.06
14	H	1021	CLA	C3C-C4C-NC	2.91	114.16	110.43
19	H	5004	LHG	O8-C23-C24	2.91	120.71	111.83
14	B	1221	CLA	CHD-C1D-ND	-2.91	120.71	124.80
14	a	1129	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
19	b	5004	LHG	O8-C23-C24	2.91	120.70	111.83
18	B	4010	BCR	C3-C4-C5	-2.91	108.87	114.06
14	b	1023	CLA	CHD-C4C-NC	-2.91	119.72	124.23
18	A	4007	BCR	C34-C9-C8	2.91	122.53	118.09
18	B	4004	BCR	C38-C26-C25	-2.91	121.31	124.48
14	a	1012	CLA	C1-O2A-CGA	2.91	123.69	116.65
14	a	1140	CLA	CHD-C1D-ND	-2.90	120.72	124.80
14	a	1133	CLA	C4D-C3D-CAD	2.90	111.26	108.11
18	a	4008	BCR	C28-C27-C26	-2.90	108.88	114.06
14	a	1107	CLA	CAA-C2A-C3A	-2.90	105.15	113.00
14	A	1012	CLA	C1-O2A-CGA	2.90	123.68	116.65
14	G	1135	CLA	CMA-C3A-C4A	2.90	119.57	111.77
14	b	1221	CLA	CHD-C1D-ND	-2.90	120.72	124.80
14	a	1139	CLA	CAC-C3C-C4C	2.90	128.56	124.79
14	B	1022	CLA	CHD-C1D-ND	-2.90	120.72	124.80
18	B	4009	BCR	C7-C8-C9	-2.90	121.94	126.23
14	A	1107	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
14	G	1107	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
18	a	4007	BCR	C34-C9-C8	2.90	122.52	118.09
14	H	1203	CLA	C4-C3-C5	2.90	120.26	115.23
14	a	1103	CLA	C4-C3-C5	2.90	120.26	115.23
14	A	1135	CLA	CMA-C3A-C4A	2.90	119.56	111.77
15	b	1237	F6C	C3C-C4C-NC	2.90	113.50	110.32
14	G	1122	CLA	C1-C2-C3	-2.90	121.45	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1213	CLA	C1-C2-C3	-2.90	121.45	126.20
14	A	1122	CLA	C4-C3-C5	2.90	120.26	115.23
14	G	1103	CLA	C1-C2-C3	-2.90	121.45	126.20
14	G	1132	CLA	C1-C2-C3	-2.90	121.45	126.20
14	B	1232	CLA	CMA-C3A-C4A	2.90	119.55	111.77
18	A	4008	BCR	C28-C27-C26	-2.89	108.89	114.06
14	H	1201	CLA	O2A-C1-C2	2.89	119.25	108.11
14	A	1123	CLA	CHD-C1D-ND	-2.89	120.73	124.80
14	B	1203	CLA	C4-C3-C5	2.89	120.25	115.23
14	b	1222	CLA	C4-C3-C5	2.89	120.25	115.23
18	H	4016	BCR	C27-C26-C25	-2.89	118.79	122.70
14	G	1012	CLA	C1-O2A-CGA	2.89	123.65	116.65
14	H	1232	CLA	CMA-C3A-C4A	2.89	119.55	111.77
14	B	1204	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	G	1139	CLA	CAC-C3C-C4C	2.89	128.55	124.79
15	H	1237	F6C	C1-C2-C3	-2.89	121.46	126.20
18	B	4005	BCR	C38-C26-C27	2.89	119.76	113.60
18	H	4005	BCR	C38-C26-C27	2.89	119.76	113.60
14	B	1023	CLA	CHD-C4C-NC	-2.89	119.75	124.23
14	H	1023	CLA	CHD-C4C-NC	-2.89	119.75	124.23
18	b	4005	BCR	C38-C26-C27	2.89	119.76	113.60
18	a	4011	BCR	C38-C26-C25	-2.89	121.33	124.48
14	b	1215	CLA	CBA-CAA-C2A	2.89	122.39	113.79
14	b	1201	CLA	O2A-C1-C2	2.89	119.22	108.11
14	b	1204	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
14	A	1133	CLA	C4D-C3D-CAD	2.89	111.24	108.11
14	b	1217	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
18	b	4014	BCR	C34-C9-C8	2.88	122.49	118.09
14	G	1126	CLA	C4-C3-C5	2.88	120.23	115.23
14	B	1201	CLA	O2A-C1-C2	2.88	119.20	108.11
14	A	1103	CLA	C1-C2-C3	-2.88	121.47	126.20
13	a	1011	CL0	CMB-C2B-C3B	2.88	130.44	124.68
18	G	4003	BCR	C1-C6-C5	-2.88	118.70	122.64
18	b	4009	BCR	C7-C8-C9	-2.88	121.97	126.23
14	b	1216	CLA	CMB-C2B-C1B	2.88	129.81	125.42
14	b	1203	CLA	C4-C3-C5	2.88	120.23	115.23
14	B	1226	CLA	CAA-C2A-C3A	-2.88	105.21	113.00
14	H	1217	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
18	b	4017	BCR	C38-C26-C25	-2.88	121.34	124.48
14	W	1701	CLA	CHD-C1D-ND	-2.88	120.75	124.80
14	B	1216	CLA	CMB-C2B-C1B	2.88	129.80	125.42
18	G	4007	BCR	C34-C9-C8	2.88	122.48	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1215	CLA	CBA-CAA-C2A	2.88	122.35	113.79
18	H	4017	BCR	C38-C26-C25	-2.88	121.34	124.48
18	H	4005	BCR	C30-C25-C26	-2.88	118.70	122.64
14	b	1232	CLA	CMA-C3A-C4A	2.88	119.50	111.77
14	a	1122	CLA	C1-C2-C3	-2.88	121.49	126.20
14	H	1226	CLA	CAA-C2A-C3A	-2.87	105.23	113.00
14	H	1204	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
14	G	1140	CLA	CHD-C1D-ND	-2.87	120.76	124.80
14	b	1233	CLA	CMC-C2C-C1C	2.87	129.53	125.03
18	A	4003	BCR	C1-C6-C5	-2.87	118.71	122.64
21	A	6002	LMT	O1'-C1'-C2'	2.87	112.64	108.27
14	b	1226	CLA	CAA-C2A-C3A	-2.87	105.23	113.00
14	a	1126	CLA	C4-C3-C5	2.87	120.22	115.23
18	B	4016	BCR	C7-C8-C9	-2.87	121.98	126.23
14	G	1123	CLA	CHD-C1D-ND	-2.87	120.76	124.80
14	b	1022	CLA	CHD-C1D-ND	-2.87	120.76	124.80
14	x	1701	CLA	CHD-C1D-ND	-2.87	120.76	124.80
14	B	1215	CLA	CBA-CAA-C2A	2.87	122.33	113.79
14	b	1214	CLA	C1D-ND-C4D	-2.87	104.30	106.31
14	B	1233	CLA	CMC-C2C-C1C	2.87	129.52	125.03
18	B	4005	BCR	C30-C25-C26	-2.87	118.72	122.64
18	H	4014	BCR	C35-C13-C12	2.87	122.47	118.09
14	A	1128	CLA	C1D-ND-C4D	-2.87	104.30	106.31
14	A	1139	CLA	CMC-C2C-C1C	2.87	129.51	125.03
14	a	1111	CLA	C4-C3-C5	2.87	120.20	115.23
14	B	1213	CLA	C1-C2-C3	-2.87	121.50	126.20
15	B	1237	F6C	C1-C2-C3	-2.87	121.50	126.20
14	H	1213	CLA	CMC-C2C-C1C	2.87	129.51	125.03
14	A	1126	CLA	C4-C3-C5	2.87	120.20	115.23
18	H	4014	BCR	C34-C9-C8	2.87	122.47	118.09
21	a	6002	LMT	O1'-C1'-C2'	2.87	112.62	108.27
14	H	1224	CLA	CMA-C3A-C4A	2.86	119.47	111.77
18	G	4011	BCR	C38-C26-C25	-2.86	121.36	124.48
14	a	1122	CLA	C4-C3-C5	2.86	120.20	115.23
14	H	1216	CLA	CMB-C2B-C1B	2.86	129.78	125.42
14	G	1122	CLA	C4-C3-C5	2.86	120.20	115.23
14	a	1103	CLA	C1-C2-C3	-2.86	121.51	126.20
13	A	1011	CL0	CMB-C2B-C3B	2.86	130.40	124.68
18	L	4019	BCR	C33-C5-C4	2.86	119.69	113.60
14	G	1109	CLA	CMA-C3A-C4A	2.86	119.46	111.77
14	b	1021	CLA	C2B-C1B-NB	2.86	113.29	110.33
13	G	1011	CL0	CMB-C2B-C3B	2.86	130.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1123	CLA	C4D-C3D-CAD	2.86	111.21	108.11
14	B	1217	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
14	G	1139	CLA	CMC-C2C-C1C	2.86	129.50	125.03
14	H	1214	CLA	C1D-ND-C4D	-2.86	104.31	106.31
14	b	1224	CLA	CMA-C3A-C4A	2.86	119.45	111.77
14	G	1128	CLA	C1D-ND-C4D	-2.85	104.31	106.31
14	a	1109	CLA	CMA-C3A-C4A	2.85	119.44	111.77
18	b	4014	BCR	C35-C13-C12	2.85	122.45	118.09
14	B	1213	CLA	CMC-C2C-C1C	2.85	129.49	125.03
14	A	1122	CLA	C1-C2-C3	-2.85	121.52	126.20
14	A	1133	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
14	b	1213	CLA	CMC-C2C-C1C	2.85	129.49	125.03
14	a	1133	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
14	a	1139	CLA	CMC-C2C-C1C	2.85	129.49	125.03
18	H	4016	BCR	C7-C8-C9	-2.85	122.02	126.23
15	b	1237	F6C	C1-C2-C3	-2.85	121.53	126.20
14	a	1123	CLA	C4D-C3D-CAD	2.85	111.20	108.11
14	B	1224	CLA	CMA-C3A-C4A	2.85	119.43	111.77
14	A	1109	CLA	CMA-C3A-C4A	2.85	119.43	111.77
14	H	1233	CLA	CMC-C2C-C1C	2.85	129.49	125.03
14	A	1107	CLA	CHD-C1D-ND	-2.85	120.79	124.80
18	B	4014	BCR	C34-C9-C8	2.85	122.44	118.09
14	x	1701	CLA	C3C-C4C-NC	2.85	114.08	110.43
14	H	1213	CLA	C1-C2-C3	-2.85	121.53	126.20
14	H	1012	CLA	CHD-C1D-ND	-2.85	120.80	124.80
14	X	1701	CLA	C3C-C4C-NC	2.85	114.08	110.43
14	a	1122	CLA	CAA-C2A-C3A	-2.85	105.31	113.00
14	G	1115	CLA	CBA-CAA-C2A	2.85	122.26	113.79
14	A	1109	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
14	G	1133	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
18	b	4005	BCR	C30-C25-C26	-2.85	118.75	122.64
14	H	1209	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
21	G	6002	LMT	O1'-C1'-C2'	2.84	112.59	108.27
18	a	4003	BCR	C1-C6-C5	-2.84	118.75	122.64
14	G	1103	CLA	C4-C3-C5	2.84	120.17	115.23
14	A	1118	CLA	CBC-CAC-C3C	-2.84	104.71	112.42
14	G	1136	CLA	C4D-C3D-CAD	2.84	111.19	108.11
14	a	1115	CLA	CBA-CAA-C2A	2.84	122.25	113.79
14	a	1123	CLA	CHD-C1D-ND	-2.84	120.80	124.80
14	B	1205	CLA	CAA-C2A-C3A	-2.84	105.32	113.00
14	W	1701	CLA	C3C-C4C-NC	2.84	114.07	110.43
14	b	1227	CLA	CHD-C1D-ND	-2.84	120.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	l	1503	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
14	A	1111	CLA	C4-C3-C5	2.84	120.16	115.23
18	b	4016	BCR	C7-C8-C9	-2.84	122.03	126.23
14	G	1122	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
14	G	1111	CLA	C4-C3-C5	2.84	120.16	115.23
14	b	1212	CLA	C3C-C4C-NC	2.84	114.07	110.43
14	H	1205	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
18	l	4019	BCR	C33-C5-C4	2.84	119.65	113.60
14	H	1227	CLA	CHD-C1D-ND	-2.84	120.81	124.80
14	H	1222	CLA	CMB-C2B-C3B	2.84	133.22	126.55
14	B	1214	CLA	C1D-ND-C4D	-2.84	104.32	106.31
14	G	1128	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
14	A	1115	CLA	CBA-CAA-C2A	2.84	122.23	113.79
14	X	1701	CLA	CHD-C1D-ND	-2.84	120.81	124.80
14	A	1103	CLA	C4-C3-C5	2.84	120.15	115.23
14	H	1021	CLA	C2B-C1B-NB	2.84	113.27	110.33
14	b	1209	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
14	B	1222	CLA	CMB-C2B-C3B	2.83	133.22	126.55
14	B	1239	CLA	C4D-C3D-CAD	2.83	111.18	108.11
14	b	1222	CLA	CMB-C2B-C3B	2.83	133.21	126.55
14	a	1136	CLA	C4D-C3D-CAD	2.83	111.18	108.11
14	B	1209	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
18	H	4009	BCR	C7-C8-C9	-2.83	122.05	126.23
14	G	1107	CLA	CHD-C1D-ND	-2.83	120.82	124.80
14	H	1212	CLA	C3C-C4C-NC	2.83	114.06	110.43
18	U	4019	BCR	C33-C5-C4	2.83	119.63	113.60
14	A	1116	CLA	C4D-C3D-CAD	2.83	111.18	108.11
14	H	1211	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	a	1128	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
14	B	1021	CLA	C2B-C1B-NB	2.83	113.26	110.33
14	a	1107	CLA	CHD-C1D-ND	-2.83	120.82	124.80
14	H	1217	CLA	C4D-C3D-CAD	2.83	111.18	108.11
14	A	1127	CLA	C1-O2A-CGA	2.83	123.49	116.65
14	A	1013	CLA	CHB-C4A-NA	2.83	128.48	124.40
14	A	1128	CLA	CAA-C2A-C3A	-2.83	105.36	113.00
14	a	1013	CLA	CHB-C4A-NA	2.82	128.47	124.40
14	G	1116	CLA	C4D-C3D-CAD	2.82	111.17	108.11
14	b	1217	CLA	C4D-C3D-CAD	2.82	111.17	108.11
14	b	1205	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
14	G	1118	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
14	B	1023	CLA	C1-C2-C3	-2.82	121.58	126.20
18	B	4012	BCR	C39-C30-C25	2.82	114.67	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1230	F6C	CHD-C1D-ND	-2.82	120.06	124.31
14	b	1217	CLA	CMB-C2B-C1B	2.82	129.71	125.42
14	b	1211	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	B	1214	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	G	1127	CLA	C1-O2A-CGA	2.82	123.47	116.65
18	b	4010	BCR	C33-C5-C6	-2.82	121.41	124.48
14	A	1110	CLA	C3C-C4C-NC	2.82	114.04	110.43
18	H	4004	BCR	C38-C26-C27	2.82	119.60	113.60
15	H	1237	F6C	O2D-CGD-O1D	-2.82	118.36	123.85
18	l	4019	BCR	C19-C18-C17	2.82	123.44	119.01
14	a	1118	CLA	CBC-CAC-C3C	-2.82	104.78	112.42
14	H	1239	CLA	C4D-C3D-CAD	2.82	111.16	108.11
18	B	4014	BCR	C35-C13-C12	2.82	122.39	118.09
15	H	1230	F6C	CHD-C1D-ND	-2.82	120.07	124.31
14	H	1205	CLA	C4D-C3D-CAD	2.81	111.16	108.11
14	B	1227	CLA	CHD-C1D-ND	-2.81	120.84	124.80
14	b	1201	CLA	C4D-C3D-CAD	2.81	111.16	108.11
14	H	1214	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
18	R	4020	BCR	C36-C18-C17	-2.81	118.26	122.82
14	L	1503	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	B	1211	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	G	1109	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
18	b	4014	BCR	C33-C5-C6	-2.81	121.42	124.48
14	A	1122	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
18	b	4014	BCR	C28-C27-C26	-2.81	109.05	114.06
14	U	1503	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	H	1224	CLA	C4-C3-C5	2.81	120.10	115.23
18	i	4018	BCR	C38-C26-C25	-2.81	121.42	124.48
18	i	4020	BCR	C36-C18-C17	-2.81	118.27	122.82
15	b	1237	F6C	O2D-CGD-O1D	-2.81	118.38	123.85
14	b	1214	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
15	B	1237	F6C	O2D-CGD-O1D	-2.81	118.39	123.85
14	a	1113	CLA	CBC-CAC-C3C	-2.81	104.81	112.42
18	H	4012	BCR	C39-C30-C25	2.81	114.64	110.24
14	A	1136	CLA	C4D-C3D-CAD	2.81	111.15	108.11
15	G	1120	F6C	C3C-C4C-NC	2.81	113.39	110.32
14	a	1127	CLA	C1-O2A-CGA	2.81	123.44	116.65
14	B	1201	CLA	C4D-C3D-CAD	2.81	111.15	108.11
14	a	1116	CLA	C4D-C3D-CAD	2.81	111.15	108.11
18	I	4020	BCR	C36-C18-C17	-2.81	118.27	122.82
14	B	1238	CLA	CMB-C2B-C3B	2.80	133.15	126.55
18	b	4004	BCR	C38-C26-C27	2.80	119.58	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b	4009	BCR	C38-C26-C27	2.80	119.57	113.60
14	A	1138	CLA	C1-O2A-CGA	2.80	123.44	116.65
14	b	1201	CLA	CMC-C2C-C1C	2.80	129.41	125.03
18	B	4006	BCR	C33-C5-C4	2.80	119.57	113.60
14	G	1013	CLA	CHB-C4A-NA	2.80	128.44	124.40
14	a	1109	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
18	b	4012	BCR	C39-C30-C25	2.80	114.64	110.24
14	B	1235	CLA	C1-O2A-CGA	2.80	123.43	116.65
14	b	1235	CLA	C1-O2A-CGA	2.80	123.43	116.65
18	B	4017	BCR	C38-C26-C25	-2.80	121.43	124.48
14	b	1023	CLA	C1-C2-C3	-2.80	121.61	126.20
14	H	1239	CLA	CAA-C2A-C3A	-2.80	105.43	113.00
14	B	1205	CLA	C4D-C3D-CAD	2.80	111.15	108.11
18	B	4009	BCR	C38-C26-C27	2.80	119.57	113.60
14	A	1103	CLA	CAC-C3C-C4C	2.80	128.43	124.79
14	H	1235	CLA	C1-O2A-CGA	2.80	123.43	116.65
14	B	1239	CLA	CAA-C2A-C3A	-2.80	105.44	113.00
14	H	1217	CLA	CMB-C2B-C1B	2.80	129.68	125.42
14	b	1239	CLA	C4D-C3D-CAD	2.80	111.15	108.11
14	G	1123	CLA	C4D-C3D-CAD	2.80	111.14	108.11
18	B	4014	BCR	C33-C5-C6	-2.80	121.43	124.48
15	a	1121	F6C	CHD-C1D-ND	-2.80	120.10	124.31
14	G	1114	CLA	CMB-C2B-C3B	2.80	133.13	126.55
14	b	1238	CLA	CMB-C2B-C3B	2.80	133.13	126.55
18	U	4022	BCR	C33-C5-C4	2.80	119.56	113.60
14	H	1201	CLA	CMC-C2C-C1C	2.80	129.40	125.03
14	B	1217	CLA	C4D-C3D-CAD	2.80	111.14	108.11
14	X	1701	CLA	CMA-C3A-C4A	2.80	119.29	111.77
14	B	1224	CLA	C4-C3-C5	2.80	120.08	115.23
18	B	4010	BCR	C33-C5-C6	-2.80	121.43	124.48
14	H	1238	CLA	CMB-C2B-C3B	2.79	133.12	126.55
14	W	1701	CLA	CMA-C3A-C4A	2.79	119.28	111.77
14	b	1236	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
14	B	1217	CLA	CMB-C2B-C1B	2.79	129.67	125.42
14	G	1110	CLA	C3C-C4C-NC	2.79	114.01	110.43
14	A	1131	CLA	CMC-C2C-C1C	2.79	129.40	125.03
18	H	4006	BCR	C33-C5-C4	2.79	119.55	113.60
18	l	4022	BCR	C33-C5-C4	2.79	119.55	113.60
14	x	1701	CLA	CMA-C3A-C4A	2.79	119.28	111.77
14	A	1130	CLA	C4-C3-C5	2.79	120.07	115.23
14	A	1114	CLA	CMB-C2B-C3B	2.79	133.12	126.55
18	H	4014	BCR	C28-C27-C26	-2.79	109.08	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	4019	BCR	C19-C18-C17	2.79	123.40	119.01
14	H	1207	CLA	CMC-C2C-C1C	2.79	129.40	125.03
14	b	1239	CLA	CAA-C2A-C3A	-2.79	105.46	113.00
14	a	1130	CLA	C4-C3-C5	2.79	120.07	115.23
14	a	1138	CLA	C1-O2A-CGA	2.79	123.40	116.65
14	a	1012	CLA	OBD-CAD-C3D	-2.79	121.90	128.42
18	R	4018	BCR	C33-C5-C4	2.79	119.54	113.60
18	G	4008	BCR	C33-C5-C6	-2.79	121.44	124.48
18	H	4010	BCR	C33-C5-C6	-2.79	121.44	124.48
14	A	1013	CLA	CHB-C1B-C2B	-2.79	119.33	127.43
18	B	4004	BCR	C38-C26-C27	2.79	119.54	113.60
14	A	1113	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
15	A	1121	F6C	CHD-C1D-ND	-2.79	120.11	124.31
14	a	1013	CLA	CHB-C1B-C2B	-2.79	119.34	127.43
18	R	4018	BCR	C38-C26-C25	-2.79	121.44	124.48
14	B	1201	CLA	CMC-C2C-C1C	2.79	129.39	125.03
14	H	1217	CLA	C1-C2-C3	-2.79	121.63	126.20
14	H	1218	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
18	H	4009	BCR	C38-C26-C27	2.79	119.54	113.60
14	b	1225	CLA	CMB-C2B-C3B	2.79	133.10	126.55
14	A	1126	CLA	C3C-C4C-NC	2.79	114.00	110.43
14	B	1236	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
14	a	1114	CLA	CMB-C2B-C3B	2.78	133.10	126.55
14	G	1131	CLA	CMC-C2C-C1C	2.78	129.38	125.03
18	I	4018	BCR	C38-C26-C25	-2.78	121.45	124.48
14	a	1103	CLA	CAC-C3C-C4C	2.78	128.41	124.79
14	A	1115	CLA	C1-C2-C3	-2.78	121.64	126.20
14	H	1236	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
14	H	1222	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	B	1217	CLA	C1-C2-C3	-2.78	121.64	126.20
18	b	4006	BCR	C33-C5-C4	2.78	119.53	113.60
14	B	1222	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	B	1207	CLA	CMC-C2C-C1C	2.78	129.38	125.03
14	G	1109	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	G	1137	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	H	1201	CLA	C4D-C3D-CAD	2.78	111.13	108.11
14	b	1205	CLA	C4D-C3D-CAD	2.78	111.13	108.11
15	b	1230	F6C	C3C-C4C-NC	2.78	113.37	110.32
14	H	1225	CLA	CMB-C2B-C3B	2.78	133.09	126.55
18	L	4022	BCR	C33-C5-C4	2.78	119.52	113.60
14	A	1123	CLA	C3C-C4C-NC	2.78	113.99	110.43
15	A	1120	F6C	C3C-C4C-NC	2.78	113.37	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1108	CLA	CMA-C3A-C4A	2.78	119.24	111.77
14	b	1225	CLA	C1-C2-C3	-2.78	121.64	126.20
15	B	1230	F6C	C3C-C4C-NC	2.78	113.36	110.32
14	A	1012	CLA	OBD-CAD-C3D	-2.78	121.92	128.42
14	G	1012	CLA	OBD-CAD-C3D	-2.78	121.92	128.42
14	G	1123	CLA	C3C-C4C-NC	2.78	113.99	110.43
18	i	4018	BCR	C33-C5-C4	2.78	119.52	113.60
14	G	1127	CLA	C1-C2-C3	-2.78	121.65	126.20
14	B	1208	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	b	1222	CLA	C4D-C3D-CAD	2.78	111.12	108.11
14	B	1225	CLA	CMB-C2B-C3B	2.78	133.08	126.55
14	H	1023	CLA	C1-C2-C3	-2.78	121.65	126.20
14	b	1208	CLA	O2D-CGD-O1D	-2.78	118.45	123.85
15	a	1120	F6C	C3C-C4C-NC	2.77	113.36	110.32
14	G	1113	CLA	CBC-CAC-C3C	-2.77	104.90	112.42
18	B	4014	BCR	C28-C27-C26	-2.77	109.11	114.06
14	G	1108	CLA	CMA-C3A-C4A	2.77	119.23	111.77
14	b	1207	CLA	CMC-C2C-C1C	2.77	129.37	125.03
14	a	1122	CLA	CMA-C3A-C4A	2.77	119.23	111.77
14	a	1131	CLA	CMC-C2C-C1C	2.77	129.37	125.03
14	A	1122	CLA	CMA-C3A-C4A	2.77	119.22	111.77
14	a	1127	CLA	C1-C2-C3	-2.77	121.66	126.20
14	H	1225	CLA	C1-C2-C3	-2.77	121.66	126.20
14	G	1126	CLA	C3C-C4C-NC	2.77	113.98	110.43
14	b	1224	CLA	C4-C3-C5	2.77	120.04	115.23
14	G	1130	CLA	C4-C3-C5	2.77	120.04	115.23
14	G	1122	CLA	CMA-C3A-C4A	2.77	119.22	111.77
14	a	1129	CLA	C4D-C3D-CAD	2.77	111.11	108.11
18	H	4014	BCR	C33-C5-C6	-2.77	121.46	124.48
14	G	1111	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
14	a	1128	CLA	C1D-ND-C4D	-2.77	104.37	106.31
14	G	1115	CLA	C1-C2-C3	-2.77	121.66	126.20
14	B	1021	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
18	I	4018	BCR	C33-C5-C4	2.77	119.50	113.60
14	B	1225	CLA	C1-C2-C3	-2.77	121.66	126.20
14	G	1013	CLA	CHB-C1B-C2B	-2.77	119.39	127.43
14	b	1022	CLA	CMC-C2C-C1C	2.77	129.36	125.03
14	H	1208	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	b	1239	CLA	C3C-C4C-NC	2.77	113.97	110.43
14	G	1138	CLA	C1-O2A-CGA	2.77	123.34	116.65
14	a	1123	CLA	C3C-C4C-NC	2.76	113.97	110.43
14	B	1022	CLA	CMC-C2C-C1C	2.76	129.35	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1012	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	a	1127	CLA	CHD-C1D-ND	-2.76	120.91	124.80
14	H	1214	CLA	OBD-CAD-C3D	-2.76	121.95	128.42
18	U	4019	BCR	C19-C18-C17	2.76	123.36	119.01
15	B	1237	F6C	CMA-C3A-C2A	-2.76	118.67	126.15
14	A	1108	CLA	CMA-C3A-C4A	2.76	119.20	111.77
14	b	1214	CLA	C4-C3-C5	2.76	120.02	115.23
15	b	1237	F6C	CMA-C3A-C2A	-2.76	118.68	126.15
15	G	1121	F6C	CHD-C1D-ND	-2.76	120.15	124.31
14	A	1127	CLA	C1-C2-C3	-2.76	121.67	126.20
14	A	1111	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
14	a	1111	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
14	H	1214	CLA	C4-C3-C5	2.76	120.02	115.23
14	H	1232	CLA	C4D-C3D-CAD	2.76	111.10	108.11
14	G	1129	CLA	C3C-C4C-NC	2.76	113.97	110.43
14	a	1133	CLA	C2B-C1B-NB	2.76	113.19	110.33
14	H	1229	CLA	C3D-C4D-ND	2.76	114.47	109.99
14	H	1021	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	B	1214	CLA	OBD-CAD-C3D	-2.76	121.97	128.42
14	b	1217	CLA	C1-C2-C3	-2.76	121.68	126.20
14	H	1239	CLA	CMC-C2C-C3C	2.76	133.60	126.15
14	B	1214	CLA	C4-C3-C5	2.76	120.01	115.23
14	a	1115	CLA	C1-C2-C3	-2.76	121.68	126.20
14	K	1401	CLA	C4D-C3D-CAD	2.76	111.10	108.11
14	a	1109	CLA	C4D-C3D-CAD	2.76	111.10	108.11
14	H	1238	CLA	C3C-C4C-NC	2.76	113.96	110.43
14	b	1238	CLA	C3C-C4C-NC	2.76	113.96	110.43
14	G	1135	CLA	CMB-C2B-C3B	2.76	133.03	126.55
15	H	1237	F6C	CMA-C3A-C2A	-2.76	118.70	126.15
18	R	4020	BCR	C8-C9-C10	2.75	123.34	119.01
14	G	1103	CLA	CAC-C3C-C4C	2.75	128.37	124.79
14	A	1012	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
18	A	4011	BCR	C36-C18-C19	-2.75	113.88	118.09
14	a	1129	CLA	C3C-C4C-NC	2.75	113.96	110.43
14	B	1232	CLA	C4D-C3D-CAD	2.75	111.09	108.11
14	b	1214	CLA	OBD-CAD-C3D	-2.75	121.99	128.42
14	b	1229	CLA	C3D-C4D-ND	2.75	114.46	109.99
14	B	1239	CLA	CMC-C2C-C3C	2.75	133.59	126.15
14	b	1239	CLA	CMC-C2C-C3C	2.75	133.59	126.15
14	A	1129	CLA	C4D-C3D-CAD	2.75	111.09	108.11
18	b	4017	BCR	C34-C9-C10	-2.75	118.36	122.82
14	B	1238	CLA	C3C-C4C-NC	2.75	113.95	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	4011	BCR	C36-C18-C19	-2.75	113.89	118.09
14	a	1012	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	b	1021	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	H	1012	CLA	CMC-C2C-C1C	2.75	129.33	125.03
14	H	1207	CLA	CAC-C3C-C4C	2.75	128.36	124.79
14	a	1138	CLA	C4-C3-C5	2.75	119.99	115.23
14	A	1135	CLA	CMB-C2B-C3B	2.74	133.01	126.55
18	H	4016	BCR	C30-C25-C26	-2.74	118.89	122.64
14	b	1221	CLA	C3C-C4C-NC	2.74	113.95	110.43
18	B	4017	BCR	C34-C9-C10	-2.74	118.37	122.82
14	B	1218	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
14	k	1401	CLA	C4D-C3D-CAD	2.74	111.08	108.11
14	A	1133	CLA	C2B-C1B-NB	2.74	113.17	110.33
14	L	1501	CLA	OBD-CAD-C3D	-2.74	122.01	128.42
14	a	1110	CLA	C3C-C4C-NC	2.74	113.94	110.43
14	a	1127	CLA	C3C-C4C-NC	2.74	113.94	110.43
14	b	1215	CLA	O2A-C1-C2	2.74	118.65	108.11
14	b	1233	CLA	CAC-C3C-C4C	2.74	128.35	124.79
14	B	1021	CLA	C11-C12-C13	-2.74	106.87	115.97
14	l	1501	CLA	OBD-CAD-C3D	-2.74	122.02	128.42
14	H	1233	CLA	C4D-C3D-CAD	2.74	111.08	108.11
14	b	1021	CLA	C11-C12-C13	-2.73	106.88	115.97
14	H	1021	CLA	C11-C12-C13	-2.73	106.88	115.97
14	a	1126	CLA	C3C-C4C-NC	2.73	113.93	110.43
18	A	4008	BCR	C33-C5-C6	-2.73	121.50	124.48
14	a	1101	CLA	C3C-C4C-NC	2.73	113.93	110.43
14	a	1137	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	b	1233	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	b	1218	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
14	b	1211	CLA	CMB-C2B-C3B	2.73	132.98	126.55
18	a	4011	BCR	C36-C18-C19	-2.73	113.91	118.09
14	B	1215	CLA	O2A-C1-C2	2.73	118.62	108.11
14	U	1501	CLA	OBD-CAD-C3D	-2.73	122.03	128.42
14	a	1135	CLA	CMB-C2B-C3B	2.73	132.97	126.55
14	B	1233	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	B	1221	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
14	H	1215	CLA	O2A-C1-C2	2.73	118.61	108.11
14	b	1235	CLA	C3D-C4D-ND	2.73	114.42	109.99
14	B	1239	CLA	CMD-C2D-C3D	-2.73	121.43	127.69
14	G	1129	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	B	1239	CLA	C3C-C4C-NC	2.73	113.93	110.43
14	G	1101	CLA	C3C-C4C-NC	2.73	113.93	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4016	BCR	C30-C25-C26	-2.73	118.91	122.64
14	H	1221	CLA	CMC-C2C-C1C	2.73	129.30	125.03
14	b	1221	CLA	CMC-C2C-C1C	2.73	129.30	125.03
14	A	1013	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
18	R	4020	BCR	C38-C26-C25	-2.73	121.51	124.48
14	G	1133	CLA	C2B-C1B-NB	2.73	113.15	110.33
14	H	1211	CLA	CMB-C2B-C3B	2.73	132.96	126.55
14	H	1206	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
14	G	1109	CLA	C3D-C4D-ND	2.73	114.42	109.99
14	A	1109	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	B	1203	CLA	C4D-C3D-CAD	2.73	111.07	108.11
14	H	1239	CLA	C3C-C4C-NC	2.73	113.92	110.43
14	G	1138	CLA	C4-C3-C5	2.72	119.96	115.23
18	i	4020	BCR	C8-C9-C10	2.72	123.30	119.01
14	b	1207	CLA	CAC-C3C-C4C	2.72	128.34	124.79
14	G	1101	CLA	CMC-C2C-C1C	2.72	129.29	125.03
14	a	1107	CLA	CMC-C2C-C1C	2.72	129.29	125.03
14	b	1221	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
18	I	4020	BCR	C38-C26-C25	-2.72	121.51	124.48
14	H	1235	CLA	C4-C3-C5	2.72	119.95	115.23
18	b	4016	BCR	C30-C25-C26	-2.72	118.92	122.64
14	H	1239	CLA	CMD-C2D-C3D	-2.72	121.44	127.69
14	A	1106	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
14	A	1127	CLA	CHD-C1D-ND	-2.72	120.97	124.80
14	H	1221	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	G	1106	CLA	O1D-CGD-CBD	-2.72	119.15	124.52
14	H	1206	CLA	C2B-C1B-NB	2.72	113.15	110.33
14	a	1105	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	a	1101	CLA	CMC-C2C-C1C	2.72	129.28	125.03
14	A	1138	CLA	C4-C3-C5	2.72	119.95	115.23
14	A	1107	CLA	CMC-C2C-C1C	2.72	129.28	125.03
14	B	1229	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	a	1106	CLA	O1D-CGD-CBD	-2.72	119.16	124.52
14	B	1233	CLA	CAC-C3C-C4C	2.72	128.33	124.79
14	G	1127	CLA	CHD-C1D-ND	-2.72	120.98	124.80
14	T	1401	CLA	C4D-C3D-CAD	2.72	111.06	108.11
14	B	1226	CLA	CHB-C1B-C2B	-2.72	119.54	127.43
14	A	1129	CLA	C3C-C4C-NC	2.72	113.91	110.43
14	A	1101	CLA	CMC-C2C-C1C	2.71	129.28	125.03
14	G	1013	CLA	C3D-C4D-ND	2.71	114.40	109.99
14	B	1211	CLA	CMB-C2B-C3B	2.71	132.93	126.55
14	b	1239	CLA	CMD-C2D-C3D	-2.71	121.47	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1211	CLA	C4D-C3D-CAD	2.71	111.05	108.11
18	i	4018	BCR	C8-C7-C6	-2.71	119.75	127.00
13	A	1011	CL0	C4D-ND-C1D	-2.71	103.16	105.22
14	H	1012	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	a	1132	CLA	CBB-CAB-C3B	-2.71	113.97	127.53
18	a	4008	BCR	C33-C5-C6	-2.71	121.53	124.48
14	H	1233	CLA	CAC-C3C-C4C	2.71	128.32	124.79
14	H	1226	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
14	B	1235	CLA	C3D-C4D-ND	2.71	114.39	109.99
14	b	1211	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	b	1226	CLA	CHB-C1B-C2B	-2.71	119.56	127.43
18	a	4011	BCR	C1-C6-C5	-2.71	118.93	122.64
14	A	1101	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	G	1132	CLA	CBB-CAB-C3B	-2.71	113.98	127.53
14	A	1137	CLA	C4D-C3D-CAD	2.71	111.05	108.11
14	H	1235	CLA	C3D-C4D-ND	2.71	114.39	109.99
14	A	1127	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	B	1221	CLA	CMC-C2C-C1C	2.71	129.26	125.03
14	A	1136	CLA	CMC-C2C-C1C	2.71	129.26	125.03
14	a	1117	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	B	1211	CLA	CMC-C2C-C1C	2.71	129.26	125.03
18	H	4017	BCR	C34-C9-C10	-2.71	118.43	122.82
14	a	1109	CLA	C3D-C4D-ND	2.71	114.38	109.99
14	a	1137	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	A	1132	CLA	CBB-CAB-C3B	-2.70	114.01	127.53
14	G	1119	CLA	CAC-C3C-C4C	2.70	128.31	124.79
14	G	1113	CLA	OBD-CAD-C3D	-2.70	122.10	128.42
14	b	1211	CLA	CMC-C2C-C1C	2.70	129.26	125.03
14	b	1232	CLA	C4D-C3D-CAD	2.70	111.04	108.11
14	B	1216	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
18	b	4013	BCR	C2-C1-C6	2.70	114.36	110.44
14	b	1206	CLA	C2B-C1B-NB	2.70	113.13	110.33
18	I	4018	BCR	C8-C7-C6	-2.70	119.78	127.00
14	A	1117	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
18	R	4018	BCR	C8-C7-C6	-2.70	119.79	127.00
14	H	1226	CLA	CHB-C1B-C2B	-2.70	119.59	127.43
14	a	1119	CLA	CAC-C3C-C4C	2.70	128.30	124.79
14	A	1122	CLA	C4D-C3D-CAD	2.70	111.04	108.11
14	A	1119	CLA	CAC-C3C-C4C	2.70	128.30	124.79
14	G	1107	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	H	1211	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	L	1503	CLA	C3D-C4D-ND	2.70	114.37	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1234	CLA	O2A-C1-C2	2.70	118.49	108.11
14	H	1234	CLA	O2A-C1-C2	2.70	118.49	108.11
14	G	1117	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	b	1206	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
14	A	1113	CLA	OBD-CAD-C3D	-2.70	122.11	128.42
18	L	4019	BCR	C1-C6-C5	-2.70	118.95	122.64
14	b	1234	CLA	O2A-C1-C2	2.70	118.48	108.11
14	A	1109	CLA	C3D-C4D-ND	2.70	114.37	109.99
18	I	4020	BCR	C8-C9-C10	2.69	123.25	119.01
14	A	1013	CLA	C3D-C4D-ND	2.69	114.37	109.99
14	H	1221	CLA	C3C-C4C-NC	2.69	113.88	110.43
18	i	4020	BCR	C38-C26-C25	-2.69	121.54	124.48
18	L	4019	BCR	C7-C8-C9	-2.69	122.25	126.23
14	b	1216	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
14	b	1210	CLA	CAA-CBA-CGA	-2.69	105.56	113.21
14	B	1206	CLA	C2B-C1B-NB	2.69	113.12	110.33
14	a	1013	CLA	C4C-C3C-C2C	-2.69	102.97	106.89
14	A	1107	CLA	C4D-C3D-CAD	2.69	111.03	108.11
14	G	1127	CLA	C3C-C4C-NC	2.69	113.88	110.43
14	U	1503	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	a	1113	CLA	OBD-CAD-C3D	-2.69	122.12	128.42
14	H	1203	CLA	C4D-C3D-CAD	2.69	111.03	108.11
14	b	1234	CLA	C4-C3-C5	2.69	119.90	115.23
18	l	4019	BCR	C1-C6-C5	-2.69	118.96	122.64
14	G	1135	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
14	G	1105	CLA	C3D-C4D-ND	2.69	114.36	109.99
15	H	1230	F6C	O2D-CGD-O1D	-2.69	118.61	123.85
14	H	1222	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	B	1210	CLA	CAA-CBA-CGA	-2.69	105.57	113.21
18	B	4013	BCR	C2-C1-C6	2.69	114.35	110.44
18	b	4006	BCR	C38-C26-C25	-2.69	121.55	124.48
18	U	4019	BCR	C7-C8-C9	-2.69	122.26	126.23
14	b	1234	CLA	C4D-C3D-CAD	2.69	111.03	108.11
18	G	4011	BCR	C1-C6-C5	-2.69	118.96	122.64
14	a	1013	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	B	1228	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
14	a	1135	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
14	b	1233	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
14	G	1116	CLA	CMD-C2D-C3D	-2.69	121.53	127.69
14	H	1216	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
14	B	1211	CLA	C4D-C3D-CAD	2.69	111.03	108.11
18	b	4010	BCR	C36-C18-C17	-2.69	118.46	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1217	CLA	C3C-C4C-NC	2.69	113.87	110.43
14	H	1228	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
14	A	1127	CLA	CAC-C3C-C4C	2.68	128.28	124.79
14	A	1140	CLA	CMC-C2C-C1C	2.68	129.23	125.03
14	G	1140	CLA	CMC-C2C-C1C	2.68	129.23	125.03
14	B	1206	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
14	B	1226	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
14	A	1136	CLA	C3C-C4C-NC	2.68	113.87	110.43
14	A	1105	CLA	C3D-C4D-ND	2.68	114.35	109.99
14	b	1022	CLA	C4D-C3D-CAD	2.68	111.02	108.11
18	A	4011	BCR	C1-C6-C5	-2.68	118.97	122.64
14	b	1222	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	B	1022	CLA	C4D-C3D-CAD	2.68	111.02	108.11
14	b	1228	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
14	a	1116	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
14	B	1222	CLA	C3D-C4D-ND	2.68	114.34	109.99
18	B	4016	BCR	C34-C9-C8	2.68	122.18	118.09
14	A	1116	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
14	H	1210	CLA	CAA-CBA-CGA	-2.68	105.60	113.21
14	G	1122	CLA	C4D-C3D-CAD	2.68	111.02	108.11
14	B	1221	CLA	C3C-C4C-NC	2.68	113.86	110.43
15	A	1121	F6C	C3C-C4C-NC	2.68	113.26	110.32
14	H	1234	CLA	C4-C3-C5	2.68	119.88	115.23
14	l	1503	CLA	C3D-C4D-ND	2.68	114.34	109.99
15	b	1230	F6C	CMA-C3A-C4A	-2.68	120.01	124.73
14	B	1207	CLA	CMB-C2B-C1B	2.68	129.50	125.42
14	A	1137	CLA	C3C-C4C-NC	2.68	113.86	110.43
14	b	1213	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	H	1021	CLA	C4D-C3D-CAD	2.68	111.01	108.11
14	H	1207	CLA	CMB-C2B-C1B	2.68	129.50	125.42
14	H	1211	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	a	1129	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	b	1211	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	A	1135	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	H	1233	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	b	1235	CLA	C4-C3-C5	2.67	119.87	115.23
14	a	1114	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
14	G	1101	CLA	CMB-C2B-C1B	2.67	129.49	125.42
15	G	1121	F6C	C3C-C4C-NC	2.67	113.25	110.32
18	V	4021	BCR	C39-C30-C25	-2.67	106.05	110.24
14	G	1139	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	a	1140	CLA	CMC-C2C-C1C	2.67	129.21	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1101	CLA	CMB-C2B-C1B	2.67	129.49	125.42
14	a	1136	CLA	CMC-C2C-C1C	2.67	129.21	125.03
14	H	1226	CLA	CMC-C2C-C3C	2.67	133.37	126.15
14	H	1217	CLA	CMC-C2C-C1C	2.67	129.21	125.03
18	H	4013	BCR	C2-C1-C6	2.67	114.32	110.44
14	B	1207	CLA	CAC-C3C-C4C	2.67	128.26	124.79
14	B	1234	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	a	1107	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	a	1118	CLA	C4D-C3D-CAD	2.67	111.01	108.11
14	G	1013	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
14	H	1235	CLA	CMC-C2C-C1C	2.67	129.21	125.03
14	B	1235	CLA	C4-C3-C5	2.67	119.86	115.23
14	b	1207	CLA	CMB-C2B-C1B	2.67	129.48	125.42
18	b	4010	BCR	C34-C9-C8	2.67	122.17	118.09
14	A	1129	CLA	C3D-C4D-ND	2.67	114.33	109.99
14	B	1213	CLA	O1D-CGD-CBD	-2.67	119.25	124.52
14	a	1136	CLA	C3C-C4C-NC	2.67	113.85	110.43
15	a	1121	F6C	C3C-C4C-NC	2.67	113.24	110.32
14	H	1213	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
14	a	1116	CLA	CMD-C2D-C3D	-2.67	121.57	127.69
14	b	1021	CLA	C4D-C3D-CAD	2.67	111.00	108.11
14	G	1138	CLA	CMC-C2C-C1C	2.67	129.20	125.03
14	b	1235	CLA	CMC-C2C-C1C	2.67	129.20	125.03
14	B	1204	CLA	C4D-C3D-CAD	2.67	111.00	108.11
14	H	1234	CLA	C4D-C3D-CAD	2.67	111.00	108.11
14	B	1214	CLA	CAA-C2A-C3A	-2.67	105.80	113.00
18	l	4019	BCR	C7-C8-C9	-2.66	122.29	126.23
13	a	1011	CL0	C4D-ND-C1D	-2.66	103.20	105.22
14	b	1226	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
14	B	1233	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	b	1203	CLA	C4D-C3D-CAD	2.66	111.00	108.11
14	B	1217	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	G	1115	CLA	C3D-C4D-ND	2.66	114.31	109.99
14	G	1129	CLA	C3D-C4D-ND	2.66	114.31	109.99
14	H	1213	CLA	C3D-C4D-ND	2.66	114.31	109.99
13	G	1011	CL0	C4D-ND-C1D	-2.66	103.20	105.22
14	B	1234	CLA	CGD-CBD-CAD	-2.66	102.23	110.85
18	H	4010	BCR	C34-C9-C8	2.66	122.15	118.09
14	a	1127	CLA	CAC-C3C-C4C	2.66	128.25	124.79
14	b	1239	CLA	C2B-C1B-NB	2.66	113.08	110.33
18	l	4019	BCR	C34-C9-C8	2.66	122.15	118.09
14	G	1107	CLA	C3C-C4C-NC	2.66	113.84	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1226	CLA	CMC-C2C-C3C	2.66	133.34	126.15
14	H	1214	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
14	H	1234	CLA	CGD-CBD-CAD	-2.66	102.24	110.85
14	G	1111	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	G	1136	CLA	C3C-C4C-NC	2.66	113.84	110.43
14	b	1214	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
14	B	1211	CLA	C3D-C4D-ND	2.66	114.31	109.99
14	U	1502	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
14	G	1119	CLA	C1-C2-C3	-2.66	121.84	126.20
18	U	4019	BCR	C1-C6-C5	-2.66	119.00	122.64
14	H	1204	CLA	C4D-C3D-CAD	2.66	110.99	108.11
14	a	1122	CLA	C4D-C3D-CAD	2.66	110.99	108.11
14	B	1234	CLA	C4-C3-C5	2.66	119.84	115.23
14	A	1114	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	B	1217	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	b	1023	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	B	1213	CLA	C3D-C4D-ND	2.65	114.30	109.99
18	B	4004	BCR	C15-C14-C13	-2.65	123.56	127.28
14	H	1239	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
18	H	4010	BCR	C36-C18-C17	-2.65	118.52	122.82
14	b	1234	CLA	CGD-CBD-CAD	-2.65	102.26	110.85
14	G	1127	CLA	CAC-C3C-C4C	2.65	128.24	124.79
14	B	1231	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
14	G	1112	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
18	H	4016	BCR	C34-C9-C8	2.65	122.14	118.09
14	B	1023	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	H	1210	CLA	C3D-C4D-ND	2.65	114.30	109.99
14	b	1239	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
18	U	4019	BCR	C34-C9-C8	2.65	122.14	118.09
14	a	1106	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	b	1213	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
14	A	1115	CLA	C3D-C4D-ND	2.65	114.29	109.99
14	a	1105	CLA	CAC-C3C-C4C	2.65	128.24	124.79
14	B	1238	CLA	CHD-C1D-ND	-2.65	121.07	124.80
14	G	1136	CLA	CMC-C2C-C1C	2.65	129.17	125.03
18	B	4010	BCR	C36-C18-C17	-2.65	118.52	122.82
18	b	4014	BCR	C37-C22-C21	-2.65	118.52	122.82
18	A	4007	BCR	C7-C8-C9	-2.65	122.32	126.23
18	b	4004	BCR	C15-C14-C13	-2.65	123.56	127.28
14	b	1238	CLA	CMA-C3A-C4A	2.65	118.89	111.77
14	G	1137	CLA	C3C-C4C-NC	2.65	113.82	110.43
14	b	1217	CLA	C3C-C4C-NC	2.65	113.82	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1123	CLA	CMC-C2C-C1C	2.65	129.17	125.03
14	A	1139	CLA	C4D-C3D-CAD	2.65	110.98	108.11
18	H	4004	BCR	C27-C26-C25	-2.65	119.13	122.70
14	A	1138	CLA	CMC-C2C-C1C	2.65	129.17	125.03
14	a	1111	CLA	CMC-C2C-C1C	2.65	129.17	125.03
14	B	1224	CLA	C6-C7-C8	-2.65	107.17	115.97
14	b	1023	CLA	C4-C3-C5	2.65	119.82	115.23
14	B	1023	CLA	CMB-C2B-C1B	2.65	129.45	125.42
18	L	4019	BCR	C34-C9-C8	2.65	122.13	118.09
18	H	4014	BCR	C37-C22-C21	-2.65	118.53	122.82
18	B	4010	BCR	C34-C9-C8	2.64	122.13	118.09
14	a	1138	CLA	CMC-C2C-C1C	2.64	129.17	125.03
18	b	4016	BCR	C34-C9-C8	2.64	122.13	118.09
14	B	1206	CLA	C3C-C4C-NC	2.64	113.82	110.43
18	H	4004	BCR	C36-C18-C17	-2.64	118.53	122.82
14	b	1217	CLA	CMC-C2C-C1C	2.64	129.16	125.03
14	H	1231	CLA	CAC-C3C-C4C	2.64	128.23	124.79
14	b	1226	CLA	CMC-C2C-C3C	2.64	133.30	126.15
14	G	1106	CLA	C3C-C4C-NC	2.64	113.82	110.43
14	A	1119	CLA	C1-C2-C3	-2.64	121.87	126.20
14	B	1023	CLA	C4-C3-C5	2.64	119.81	115.23
14	a	1119	CLA	C1-C2-C3	-2.64	121.87	126.20
14	H	1206	CLA	C3C-C4C-NC	2.64	113.81	110.43
14	H	1023	CLA	CMB-C2B-C1B	2.64	129.44	125.42
14	a	1101	CLA	CMB-C2B-C1B	2.64	129.44	125.42
14	A	1116	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
18	H	4004	BCR	C15-C14-C13	-2.64	123.58	127.28
15	H	1230	F6C	CMA-C3A-C4A	-2.64	120.08	124.73
14	G	1114	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
18	m	4021	BCR	C39-C30-C25	-2.64	106.11	110.24
18	H	4006	BCR	C38-C26-C25	-2.64	121.61	124.48
14	a	1112	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
14	B	1235	CLA	CMC-C2C-C1C	2.64	129.16	125.03
14	B	1220	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
14	H	1226	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
14	H	1023	CLA	C4-C3-C5	2.64	119.81	115.23
14	G	1119	CLA	CMB-C2B-C3B	2.64	132.75	126.55
14	H	1224	CLA	C6-C7-C8	-2.64	107.20	115.97
14	G	1105	CLA	CAC-C3C-C4C	2.64	128.22	124.79
14	G	1107	CLA	C4D-C3D-CAD	2.64	110.97	108.11
18	B	4006	BCR	C38-C26-C25	-2.64	121.61	124.48
14	a	1012	CLA	C6-C5-C3	-2.64	107.05	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1139	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	b	1221	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	b	1231	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
18	L	4022	BCR	C36-C18-C17	-2.63	118.55	122.82
18	b	4004	BCR	C36-C18-C17	-2.63	118.55	122.82
14	B	1221	CLA	C4D-C3D-CAD	2.63	110.97	108.11
18	H	4016	BCR	C33-C5-C6	-2.63	121.61	124.48
15	B	1230	F6C	O2D-CGD-O1D	-2.63	118.72	123.85
18	l	4022	BCR	C15-C14-C13	-2.63	123.58	127.28
14	L	1502	CLA	C3D-C4D-ND	2.63	114.27	109.99
14	U	1502	CLA	C3D-C4D-ND	2.63	114.27	109.99
14	H	1231	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	G	1123	CLA	CMC-C2C-C1C	2.63	129.15	125.03
18	B	4004	BCR	C27-C26-C25	-2.63	119.15	122.70
14	a	1107	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	a	1115	CLA	C3D-C4D-ND	2.63	114.27	109.99
14	H	1220	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
14	B	1238	CLA	CMA-C3A-C4A	2.63	118.85	111.77
14	A	1107	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	A	1119	CLA	CMB-C2B-C3B	2.63	132.74	126.55
14	A	1112	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
14	G	1105	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
14	L	1502	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
14	b	1206	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	G	1116	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
14	b	1231	CLA	CAC-C3C-C4C	2.63	128.21	124.79
18	b	4004	BCR	C27-C26-C25	-2.63	119.15	122.70
14	a	1113	CLA	CMA-C3A-C4A	2.63	118.84	111.77
14	l	1502	CLA	C3D-C4D-ND	2.63	114.26	109.99
18	B	4014	BCR	C37-C22-C21	-2.63	118.56	122.82
14	H	1238	CLA	CMA-C3A-C4A	2.63	118.84	111.77
14	a	1132	CLA	O1D-CGD-CBD	-2.63	119.33	124.52
14	b	1231	CLA	CMD-C2D-C3D	-2.63	121.66	127.69
18	l	4022	BCR	C36-C18-C17	-2.63	118.56	122.82
18	M	4021	BCR	C39-C30-C25	-2.63	106.12	110.24
18	a	4007	BCR	C7-C8-C9	-2.63	122.35	126.23
14	B	1226	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
14	A	1118	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	G	1113	CLA	CMA-C3A-C4A	2.63	118.83	111.77
14	a	1117	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
14	b	1238	CLA	CHD-C1D-ND	-2.63	121.11	124.80
14	b	1226	CLA	CHC-C1C-C2C	-2.63	119.48	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1236	CLA	O1D-CGD-CBD	-2.63	119.34	124.52
14	B	1218	CLA	CMC-C2C-C1C	2.62	129.14	125.03
15	B	1237	F6C	C3D-C4D-ND	2.62	114.25	109.93
14	A	1106	CLA	C3C-C4C-NC	2.62	113.79	110.43
14	B	1239	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	A	1113	CLA	CMA-C3A-C4A	2.62	118.82	111.77
14	B	1231	CLA	CAC-C3C-C4C	2.62	128.20	124.79
14	l	1502	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
14	A	1012	CLA	C6-C5-C3	-2.62	107.08	113.47
14	b	1224	CLA	C6-C7-C8	-2.62	107.25	115.97
14	A	1111	CLA	CMC-C2C-C1C	2.62	129.13	125.03
14	G	1118	CLA	C4D-C3D-CAD	2.62	110.95	108.11
14	H	1239	CLA	C2B-C1B-NB	2.62	113.05	110.33
15	G	1121	F6C	OMB-CMB-C2B	-2.62	119.70	125.62
14	G	1110	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
14	H	1238	CLA	CHD-C1D-ND	-2.62	121.11	124.80
14	a	1123	CLA	CMC-C2C-C1C	2.62	129.13	125.03
14	A	1115	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
13	G	1011	CL0	O1D-CGD-CBD	-2.62	120.75	124.72
14	H	1218	CLA	CMC-C2C-C1C	2.62	129.13	125.03
14	G	1108	CLA	CMB-C2B-C1B	2.62	129.41	125.42
14	a	1119	CLA	CMB-C2B-C3B	2.62	132.71	126.55
14	b	1223	CLA	C1-C2-C3	-2.62	121.90	126.20
14	B	1212	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
14	G	1118	CLA	CMB-C2B-C1B	2.62	129.41	125.42
14	b	1023	CLA	CMB-C2B-C1B	2.62	129.41	125.42
14	H	1205	CLA	C3C-C4C-NC	2.62	113.79	110.43
18	L	4022	BCR	C15-C14-C13	-2.62	123.60	127.28
18	B	4004	BCR	C36-C18-C17	-2.62	118.57	122.82
14	A	1110	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
18	G	4007	BCR	C7-C8-C9	-2.62	122.36	126.23
14	b	1212	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
14	G	1115	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
14	G	1101	CLA	CMA-C3A-C4A	2.62	118.81	111.77
14	G	1117	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
14	G	1124	CLA	C4D-C3D-CAD	2.62	110.95	108.11
14	a	1106	CLA	C4D-C3D-CAD	2.62	110.95	108.11
14	a	1118	CLA	C3D-C4D-ND	2.62	114.24	109.99
18	b	4013	BCR	C34-C9-C10	-2.62	118.58	122.82
14	b	1204	CLA	C4D-C3D-CAD	2.62	110.95	108.11
14	A	1117	CLA	CHC-C1C-C2C	-2.62	119.52	126.95
15	a	1121	F6C	OMB-CMB-C2B	-2.62	119.72	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1237	F6C	C3D-C4D-ND	2.62	114.24	109.93
14	H	1219	CLA	C3C-C4C-NC	2.62	113.78	110.43
14	a	1115	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
14	B	1021	CLA	C4D-C3D-CAD	2.61	110.95	108.11
13	A	1011	CL0	O1D-CGD-CBD	-2.61	120.76	124.72
14	H	1023	CLA	C3C-C4C-NC	2.61	113.78	110.43
14	A	1105	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
14	A	1132	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
14	H	1212	CLA	O1D-CGD-CBD	-2.61	119.36	124.52
14	A	1105	CLA	CAC-C3C-C4C	2.61	128.19	124.79
14	G	1107	CLA	CAC-C3C-C4C	2.61	128.19	124.79
14	A	1101	CLA	CMA-C3A-C4A	2.61	118.79	111.77
14	a	1105	CLA	C4D-C3D-CAD	2.61	110.94	108.11
14	a	1108	CLA	CMB-C2B-C1B	2.61	129.40	125.42
14	G	1117	CLA	CMA-C3A-C4A	2.61	118.79	111.77
14	a	1117	CLA	CMA-C3A-C4A	2.61	118.79	111.77
14	A	1106	CLA	C4D-C3D-CAD	2.61	110.94	108.11
14	a	1105	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
14	B	1216	CLA	C4-C3-C5	2.61	119.75	115.23
14	B	1228	CLA	C3D-C4D-ND	2.61	114.22	109.99
14	b	1208	CLA	C3D-C4D-ND	2.61	114.22	109.99
18	H	4013	BCR	C34-C9-C10	-2.61	118.59	122.82
14	a	1127	CLA	CMB-C2B-C3B	2.61	132.68	126.55
14	B	1231	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
14	H	1231	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
14	G	1127	CLA	CMB-C2B-C3B	2.61	132.68	126.55
14	A	1124	CLA	C4D-C3D-CAD	2.61	110.94	108.11
14	B	1219	CLA	C3C-C4C-NC	2.61	113.77	110.43
14	G	1133	CLA	CMC-C2C-C1C	2.61	129.11	125.03
15	B	1230	F6C	CMA-C3A-C4A	-2.61	120.14	124.73
14	a	1110	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
14	G	1012	CLA	C6-C5-C3	-2.61	107.12	113.47
14	a	1122	CLA	C3C-C4C-NC	2.60	113.77	110.43
14	b	1220	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
14	a	1101	CLA	CMA-C3A-C4A	2.60	118.77	111.77
15	H	1237	F6C	C3D-C4D-ND	2.60	114.22	109.93
18	A	4008	BCR	C35-C13-C12	2.60	122.07	118.09
14	B	1210	CLA	C3D-C4D-ND	2.60	114.22	109.99
14	B	1236	CLA	O1D-CGD-CBD	-2.60	119.38	124.52
14	G	1106	CLA	C4D-C3D-CAD	2.60	110.93	108.11
18	A	4007	BCR	C1-C6-C5	-2.60	119.08	122.64
18	G	4007	BCR	C1-C6-C5	-2.60	119.08	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	1011	CL0	O1D-CGD-CBD	-2.60	120.78	124.72
14	A	1118	CLA	CMB-C2B-C1B	2.60	129.38	125.42
14	a	1118	CLA	CMB-C2B-C1B	2.60	129.38	125.42
15	b	1237	F6C	CHD-C1D-ND	-2.60	120.39	124.31
14	A	1110	CLA	C4D-C3D-CAD	2.60	110.93	108.11
14	G	1132	CLA	O1D-CGD-CBD	-2.60	119.39	124.52
14	b	1222	CLA	C1-C2-C3	-2.60	121.93	126.20
14	H	1227	CLA	C3D-C4D-ND	2.60	114.22	109.99
15	A	1121	F6C	OMB-CMB-C2B	-2.60	119.75	125.62
14	G	1110	CLA	CMC-C2C-C1C	2.60	129.10	125.03
14	G	1110	CLA	C4D-C3D-CAD	2.60	110.93	108.11
14	A	1128	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
14	G	1128	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
14	G	1122	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	a	1110	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
18	I	4020	BCR	C33-C5-C6	-2.60	121.65	124.48
14	b	1205	CLA	C3C-C4C-NC	2.60	113.76	110.43
18	U	4022	BCR	C36-C18-C17	-2.60	118.61	122.82
18	U	4022	BCR	C15-C14-C13	-2.60	123.63	127.28
14	A	1110	CLA	CAA-C2A-C3A	-2.60	105.98	113.00
14	b	1213	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
14	A	1133	CLA	CMC-C2C-C1C	2.60	129.09	125.03
14	a	1133	CLA	CMC-C2C-C1C	2.60	129.09	125.03
14	A	1122	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	B	1205	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	H	1201	CLA	C3C-C4C-NC	2.60	113.76	110.43
14	B	1227	CLA	CMA-C3A-C4A	2.60	118.75	111.77
14	A	1110	CLA	CMC-C2C-C1C	2.60	129.09	125.03
14	A	1108	CLA	CMB-C2B-C1B	2.60	129.37	125.42
14	a	1128	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
14	B	1227	CLA	C3D-C4D-ND	2.60	114.21	109.99
14	b	1227	CLA	C3D-C4D-ND	2.60	114.20	109.99
14	a	1110	CLA	CMC-C2C-C1C	2.59	129.09	125.03
18	A	4003	BCR	C39-C30-C25	-2.59	106.17	110.24
18	G	4001	BCR	C33-C5-C6	-2.59	121.65	124.48
14	B	1239	CLA	C2B-C1B-NB	2.59	113.02	110.33
14	G	1118	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	b	1021	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	B	1223	CLA	C1-C2-C3	-2.59	121.95	126.20
18	B	4016	BCR	C33-C5-C6	-2.59	121.66	124.48
18	b	4016	BCR	C33-C5-C6	-2.59	121.66	124.48
18	A	4001	BCR	C33-C5-C6	-2.59	121.66	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1222	CLA	C1-C2-C3	-2.59	121.95	126.20
14	b	1227	CLA	CMA-C3A-C4A	2.59	118.74	111.77
18	G	4003	BCR	C39-C30-C25	-2.59	106.18	110.24
14	a	1133	CLA	CMB-C2B-C1B	2.59	129.36	125.42
14	B	1208	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	B	1209	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	H	1223	CLA	C1-C2-C3	-2.59	121.95	126.20
14	H	1217	CLA	CMA-C3A-C4A	2.59	118.73	111.77
14	H	1213	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
14	H	1227	CLA	CMA-C3A-C4A	2.59	118.73	111.77
14	H	1221	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	H	1208	CLA	C3D-C4D-ND	2.59	114.19	109.99
14	G	1110	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
14	b	1218	CLA	CMC-C2C-C1C	2.59	129.08	125.03
14	b	1201	CLA	C3C-C4C-NC	2.59	113.75	110.43
14	a	1119	CLA	C3D-C4D-ND	2.59	114.19	109.99
14	G	1105	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	B	1229	CLA	CAA-C2A-C1A	-2.59	103.49	111.97
14	G	1135	CLA	C3D-C4D-ND	2.59	114.19	109.99
18	a	4003	BCR	C39-C30-C25	-2.59	106.19	110.24
18	l	4022	BCR	C19-C18-C17	2.59	123.08	119.01
18	a	4007	BCR	C1-C6-C5	-2.59	119.10	122.64
14	H	1021	CLA	C3D-C4D-ND	2.59	114.19	109.99
18	a	4008	BCR	C35-C13-C12	2.59	122.04	118.09
14	A	1117	CLA	CMA-C3A-C4A	2.58	118.72	111.77
14	B	1217	CLA	CMA-C3A-C4A	2.58	118.72	111.77
14	H	1216	CLA	C4-C3-C5	2.58	119.71	115.23
15	G	1120	F6C	C3D-C4D-ND	2.58	114.19	109.93
14	A	1119	CLA	C3D-C4D-ND	2.58	114.19	109.99
18	B	4013	BCR	C34-C9-C10	-2.58	118.63	122.82
14	H	1236	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
14	a	1124	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	H	1228	CLA	C3D-C4D-ND	2.58	114.19	109.99
14	a	1107	CLA	CAC-C3C-C4C	2.58	128.15	124.79
14	B	1228	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	a	1114	CLA	C4D-C3D-CAD	2.58	110.91	108.11
18	a	4001	BCR	C33-C5-C6	-2.58	121.67	124.48
14	G	1127	CLA	C6-C5-C3	-2.58	107.18	113.47
15	H	1237	F6C	CHD-C1D-ND	-2.58	120.42	124.31
18	R	4020	BCR	C33-C5-C6	-2.58	121.67	124.48
14	B	1201	CLA	C3C-C4C-NC	2.58	113.74	110.43
14	a	1135	CLA	CMD-C2D-C3D	-2.58	121.77	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1107	CLA	CAC-C3C-C4C	2.58	128.15	124.79
18	i	4018	BCR	C1-C6-C5	-2.58	119.11	122.64
15	A	1121	F6C	CAC-C3C-C4C	2.58	128.46	124.91
14	H	1222	CLA	C1-C2-C3	-2.58	121.97	126.20
14	A	1105	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	b	1210	CLA	C3D-C4D-ND	2.58	114.18	109.99
14	A	1133	CLA	CMB-C2B-C1B	2.58	129.34	125.42
18	G	4002	BCR	C3-C4-C5	-2.58	109.46	114.06
14	a	1127	CLA	C6-C5-C3	-2.58	107.19	113.47
14	b	1203	CLA	CMC-C2C-C1C	2.58	129.06	125.03
14	b	1223	CLA	C4D-C3D-CAD	2.58	110.91	108.11
18	H	4013	BCR	C33-C5-C6	-2.58	121.67	124.48
18	a	4002	BCR	C3-C4-C5	-2.58	109.46	114.06
14	H	1229	CLA	CAA-C2A-C1A	-2.58	103.53	111.97
14	b	1204	CLA	CMC-C2C-C1C	2.58	129.06	125.03
15	a	1120	F6C	C3D-C4D-ND	2.58	114.17	109.93
18	B	4010	BCR	C40-C30-C25	2.58	114.28	110.24
14	B	1213	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
14	A	1127	CLA	CMB-C2B-C3B	2.58	132.61	126.55
18	U	4022	BCR	C37-C22-C21	-2.58	118.64	122.82
14	A	1108	CLA	C3D-C4D-ND	2.57	114.17	109.99
14	b	1216	CLA	C4-C3-C5	2.57	119.70	115.23
14	b	1217	CLA	CMA-C3A-C4A	2.57	118.69	111.77
14	G	1105	CLA	CMC-C2C-C1C	2.57	129.06	125.03
14	a	1132	CLA	C3C-C4C-NC	2.57	113.73	110.43
18	G	4008	BCR	C35-C13-C12	2.57	122.02	118.09
14	B	1203	CLA	CMC-C2C-C1C	2.57	129.05	125.03
14	H	1203	CLA	CMC-C2C-C1C	2.57	129.05	125.03
14	H	1228	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	B	1216	CLA	C1-C2-C3	-2.57	121.98	126.20
14	H	1202	CLA	CMB-C2B-C1B	2.57	129.33	125.42
18	b	4010	BCR	C40-C30-C25	2.57	114.27	110.24
14	A	1127	CLA	C6-C5-C3	-2.57	107.21	113.47
15	b	1237	F6C	C2B-C3B-C4B	-2.57	105.14	106.46
18	L	4022	BCR	C37-C22-C21	-2.57	118.65	122.82
14	b	1229	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
14	b	1215	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
15	b	1230	F6C	O2D-CGD-O1D	-2.57	118.85	123.85
18	B	4013	BCR	C34-C9-C8	2.57	122.01	118.09
14	H	1209	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	b	1235	CLA	CBA-CAA-C2A	2.57	121.43	113.79
14	B	1215	CLA	O2D-CGD-O1D	-2.57	118.85	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1120	F6C	C3D-C4D-ND	2.57	114.16	109.93
18	i	4020	BCR	C33-C5-C6	-2.57	121.68	124.48
14	a	1105	CLA	CMC-C2C-C1C	2.57	129.04	125.03
14	G	1135	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
18	l	4022	BCR	C29-C30-C25	2.57	114.17	110.44
14	A	1118	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	H	1235	CLA	CBA-CAA-C2A	2.57	121.43	113.79
15	B	1237	F6C	CMC-C2C-C1C	2.57	129.33	125.42
14	a	1118	CLA	C1-O2A-CGA	2.57	122.86	116.65
14	b	1228	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
14	b	1209	CLA	C3D-C4D-ND	2.56	114.16	109.99
18	U	4022	BCR	C19-C18-C17	2.56	123.04	119.01
14	B	1216	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	G	1114	CLA	C4D-C3D-CAD	2.56	110.89	108.11
15	a	1121	F6C	CAC-C3C-C4C	2.56	128.44	124.91
14	A	1124	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
14	A	1118	CLA	C1-O2A-CGA	2.56	122.86	116.65
14	a	1117	CLA	CAA-C2A-C3A	-2.56	106.07	113.00
18	L	4022	BCR	C29-C30-C25	2.56	114.16	110.44
14	a	1130	CLA	CMB-C2B-C3B	2.56	132.58	126.55
14	b	1219	CLA	C3C-C4C-NC	2.56	113.71	110.43
14	A	1139	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
14	A	1112	CLA	C4D-C3D-CAD	2.56	110.89	108.11
18	l	4022	BCR	C37-C22-C21	-2.56	118.67	122.82
18	L	4022	BCR	C19-C18-C17	2.56	123.04	119.01
14	H	1215	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
14	A	1122	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	b	1203	CLA	OBD-CAD-C3D	-2.56	122.43	128.42
14	a	1108	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	b	1228	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	B	1235	CLA	CBA-CAA-C2A	2.56	121.41	113.79
14	G	1118	CLA	C1-O2A-CGA	2.56	122.84	116.65
14	A	1132	CLA	C3C-C4C-NC	2.56	113.71	110.43
15	B	1237	F6C	CHD-C1D-ND	-2.56	120.46	124.31
18	B	4013	BCR	C33-C5-C6	-2.56	121.69	124.48
18	B	4012	BCR	C3-C4-C5	-2.56	109.50	114.06
14	G	1117	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
14	A	1117	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
14	A	1013	CLA	C4-C3-C5	2.56	119.67	115.23
14	G	1119	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	A	1135	CLA	CMD-C2D-C3D	-2.56	121.83	127.69
18	a	4001	BCR	C29-C30-C25	2.56	114.15	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1133	CLA	CMB-C2B-C1B	2.56	129.31	125.42
18	I	4018	BCR	C1-C6-C5	-2.56	119.14	122.64
14	A	1135	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	a	1139	CLA	O1D-CGD-CBD	-2.56	119.48	124.52
18	A	4011	BCR	C19-C18-C17	2.55	123.03	119.01
14	H	1203	CLA	OBD-CAD-C3D	-2.55	122.45	128.42
15	G	1121	F6C	CAC-C3C-C4C	2.55	128.43	124.91
18	A	4002	BCR	C3-C4-C5	-2.55	109.50	114.06
14	a	1123	CLA	C4-C3-C5	2.55	119.66	115.23
14	H	1216	CLA	C1-C2-C3	-2.55	122.02	126.20
14	B	1223	CLA	C4D-C3D-CAD	2.55	110.88	108.11
14	b	1202	CLA	CMB-C2B-C1B	2.55	129.30	125.42
14	H	1205	CLA	C3D-C4D-ND	2.55	114.13	109.99
18	U	4022	BCR	C29-C30-C25	2.55	114.14	110.44
18	a	4007	BCR	C33-C5-C4	2.55	119.03	113.60
18	H	4012	BCR	C3-C4-C5	-2.55	109.51	114.06
14	a	1138	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
14	G	1132	CLA	C3C-C4C-NC	2.55	113.70	110.43
14	a	1101	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	B	1205	CLA	CMC-C2C-C1C	2.55	129.02	125.03
14	H	1219	CLA	CMC-C2C-C1C	2.55	129.02	125.03
14	b	1216	CLA	C1-C2-C3	-2.55	122.02	126.20
14	A	1117	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
14	a	1135	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	b	1023	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
14	G	1117	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
14	A	1130	CLA	CMB-C2B-C3B	2.55	132.54	126.55
18	H	4010	BCR	C40-C30-C25	2.55	114.24	110.24
14	a	1102	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	A	1138	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
14	a	1117	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
14	B	1021	CLA	C3D-C4D-ND	2.55	114.13	109.99
15	A	1120	F6C	CHA-C4D-ND	2.55	135.49	133.05
14	B	1203	CLA	C3C-C4C-NC	2.55	113.69	110.43
14	H	1204	CLA	CMC-C2C-C1C	2.55	129.01	125.03
14	B	1219	CLA	C3D-C4D-ND	2.55	114.12	109.99
14	b	1236	CLA	CMC-C2C-C1C	2.54	129.01	125.03
14	G	1124	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	a	1124	CLA	CMD-C2D-C3D	-2.54	121.85	127.69
15	a	1120	F6C	CHA-C4D-ND	2.54	135.48	133.05
14	H	1023	CLA	C1C-C2C-C3C	-2.54	104.30	106.98
14	A	1123	CLA	C4-C3-C5	2.54	119.64	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1104	CLA	C4D-C3D-CAD	2.54	110.87	108.11
14	a	1122	CLA	CED-O2D-CGD	2.54	121.69	115.92
14	B	1226	CLA	C1-O2A-CGA	2.54	122.81	116.65
14	A	1114	CLA	C4D-C3D-CAD	2.54	110.87	108.11
18	B	4013	BCR	C37-C22-C21	-2.54	118.70	122.82
14	H	1216	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	G	1124	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
14	G	1138	CLA	O1D-CGD-CBD	-2.54	119.50	124.52
18	b	4013	BCR	C34-C9-C8	2.54	121.97	118.09
14	H	1203	CLA	C3C-C4C-NC	2.54	113.69	110.43
14	B	1202	CLA	CMB-C2B-C1B	2.54	129.29	125.42
14	a	1104	CLA	C4D-C3D-CAD	2.54	110.87	108.11
14	B	1236	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	H	1236	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	H	1213	CLA	C4-C3-C5	2.54	119.63	115.23
14	G	1122	CLA	CED-O2D-CGD	2.54	121.67	115.92
14	a	1124	CLA	C3D-C4D-ND	2.54	114.11	109.99
18	A	4002	BCR	C38-C26-C27	2.54	119.01	113.60
14	H	1023	CLA	CHC-C1C-C2C	-2.54	119.74	126.95
14	G	1108	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	b	1219	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	b	1216	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	W	1701	CLA	C4D-C3D-CAD	2.54	110.86	108.11
14	H	1226	CLA	C1-O2A-CGA	2.53	122.79	116.65
14	b	1213	CLA	C4-C3-C5	2.53	119.63	115.23
14	A	1102	CLA	C3D-C4D-ND	2.53	114.11	109.99
14	H	1229	CLA	CMC-C2C-C1C	2.53	129.00	125.03
18	a	4011	BCR	C19-C18-C17	2.53	123.00	119.01
18	A	4007	BCR	C33-C5-C4	2.53	119.00	113.60
18	R	4018	BCR	C1-C6-C5	-2.53	119.17	122.64
14	b	1224	CLA	CHD-C4C-C3C	-2.53	121.08	124.77
14	A	1124	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	G	1112	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	H	1223	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	x	1701	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	A	1105	CLA	CMC-C2C-C1C	2.53	128.99	125.03
18	b	4006	BCR	C15-C14-C13	-2.53	123.73	127.28
14	A	1138	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
14	G	1013	CLA	C4-C3-C5	2.53	119.62	115.23
14	G	1125	CLA	CMB-C2B-C3B	2.53	132.51	126.55
14	B	1204	CLA	CMC-C2C-C1C	2.53	128.99	125.03
14	b	1205	CLA	C3D-C4D-ND	2.53	114.10	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1023	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
14	G	1130	CLA	CMB-C2B-C3B	2.53	132.50	126.55
14	b	1211	CLA	C4-C3-C5	2.53	119.62	115.23
14	B	1207	CLA	C4B-CHC-C1C	2.53	132.20	126.25
14	B	1219	CLA	CMC-C2C-C1C	2.53	128.99	125.03
14	b	1226	CLA	C1-O2A-CGA	2.53	122.77	116.65
14	A	1139	CLA	C3C-C4C-NC	2.53	113.67	110.43
14	G	1116	CLA	CBA-CAA-C2A	2.53	121.32	113.79
14	a	1124	CLA	CAA-C2A-C1A	-2.53	103.69	111.97
14	A	1122	CLA	CED-O2D-CGD	2.53	121.65	115.92
14	b	1023	CLA	C3D-C4D-ND	2.53	114.09	109.99
18	H	4013	BCR	C37-C22-C21	-2.53	118.72	122.82
18	G	4001	BCR	C29-C30-C25	2.53	114.11	110.44
14	G	1123	CLA	C4-C3-C5	2.53	119.61	115.23
14	A	1139	CLA	C3D-C4D-ND	2.53	114.09	109.99
14	G	1102	CLA	C3D-C4D-ND	2.53	114.09	109.99
14	A	1124	CLA	CAA-C2A-C1A	-2.53	103.70	111.97
14	B	1213	CLA	C4-C3-C5	2.53	119.61	115.23
14	G	1122	CLA	C3D-C4D-ND	2.53	114.09	109.99
14	A	1012	CLA	C3C-C4C-NC	2.53	113.67	110.43
18	b	4013	BCR	C37-C22-C21	-2.53	118.72	122.82
14	U	1503	CLA	C4-C3-C5	2.53	119.61	115.23
14	H	1224	CLA	CHD-C4C-C3C	-2.52	121.09	124.77
14	G	1101	CLA	C3D-C4D-ND	2.52	114.09	109.99
18	H	4013	BCR	C34-C9-C8	2.52	121.94	118.09
14	B	1222	CLA	CMA-C3A-C4A	2.52	118.56	111.77
14	G	1139	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
18	G	4011	BCR	C4-C5-C6	-2.52	119.29	122.70
14	A	1012	CLA	CHA-C1A-NA	-2.52	120.67	126.39
14	G	1104	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	H	1207	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	B	1228	CLA	C4D-C3D-CAD	2.52	110.85	108.11
14	a	1112	CLA	C4D-C3D-CAD	2.52	110.85	108.11
14	G	1138	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
14	H	1227	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
14	H	1211	CLA	C4-C3-C5	2.52	119.61	115.23
18	G	4002	BCR	C38-C26-C27	2.52	118.97	113.60
18	G	4007	BCR	C33-C5-C4	2.52	118.97	113.60
14	l	1503	CLA	C4-C3-C5	2.52	119.61	115.23
14	a	1122	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	B	1023	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
14	B	1203	CLA	OBD-CAD-C3D	-2.52	122.52	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1104	CLA	C4D-C3D-CAD	2.52	110.84	108.11
14	B	1233	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	a	1139	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	b	1207	CLA	C4B-CHC-C1C	2.52	132.18	126.25
14	a	1106	CLA	CBA-CAA-C2A	2.52	121.30	113.79
14	a	1110	CLA	C4D-C3D-CAD	2.52	110.84	108.11
14	G	1124	CLA	CAA-C2A-C1A	-2.52	103.71	111.97
18	I	4020	BCR	C23-C22-C21	-2.52	115.04	119.01
14	G	1012	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	B	1205	CLA	C3D-C4D-ND	2.52	114.08	109.99
18	a	4002	BCR	C38-C26-C27	2.52	118.97	113.60
14	b	1222	CLA	CMA-C3A-C4A	2.52	118.55	111.77
14	B	1227	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
18	H	4006	BCR	C15-C14-C13	-2.52	123.74	127.28
14	b	1227	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
14	A	1111	CLA	C4D-C3D-CAD	2.52	110.84	108.11
18	b	4012	BCR	C3-C4-C5	-2.52	109.56	114.06
14	a	1108	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	a	1013	CLA	C4-C3-C5	2.52	119.60	115.23
14	b	1205	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
18	b	4013	BCR	C33-C5-C6	-2.52	121.74	124.48
14	A	1116	CLA	CBA-CAA-C2A	2.52	121.28	113.79
21	a	6001	LMT	C1'-O5'-C5'	2.52	118.64	113.72
14	a	1013	CLA	C1-O2A-CGA	2.52	122.74	116.65
18	B	4006	BCR	C15-C14-C13	-2.52	123.75	127.28
21	A	6001	LMT	C1'-O5'-C5'	2.52	118.64	113.72
14	a	1116	CLA	CBA-CAA-C2A	2.52	121.28	113.79
14	G	1139	CLA	C3D-C4D-ND	2.52	114.08	109.99
14	a	1135	CLA	C3C-C4C-NC	2.52	113.65	110.43
14	B	1238	CLA	C1-C2-C3	-2.52	122.08	126.20
14	G	1108	CLA	C3C-C4C-NC	2.52	113.65	110.43
14	b	1203	CLA	C3C-C4C-NC	2.52	113.65	110.43
14	a	1138	CLA	CMD-C2D-C3D	-2.51	121.92	127.69
15	b	1237	F6C	CMC-C2C-C1C	2.51	129.25	125.42
14	L	1503	CLA	C4-C3-C5	2.51	119.59	115.23
14	H	1207	CLA	C4B-CHC-C1C	2.51	132.16	126.25
15	G	1120	F6C	CHA-C4D-ND	2.51	135.46	133.05
15	H	1237	F6C	CMC-C2C-C1C	2.51	129.25	125.42
14	b	1233	CLA	C3D-C4D-ND	2.51	114.07	109.99
15	H	1237	F6C	C2B-C3B-C4B	-2.51	105.17	106.46
14	H	1205	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
14	a	1125	CLA	CMB-C2B-C3B	2.51	132.46	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	4020	BCR	C23-C22-C21	-2.51	115.06	119.01
14	H	1208	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	a	1101	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	a	1104	CLA	C3D-C4D-ND	2.51	114.07	109.99
14	b	1208	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	b	1229	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	A	1106	CLA	CBA-CAA-C2A	2.51	121.27	113.79
18	i	4020	BCR	C23-C22-C21	-2.51	115.06	119.01
14	B	1219	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
14	H	1219	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
14	U	1501	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	l	1501	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	B	1023	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
14	G	1111	CLA	C4D-C3D-CAD	2.51	110.83	108.11
18	G	4002	BCR	C37-C22-C21	-2.51	118.75	122.82
14	b	1219	CLA	O1D-CGD-CBD	-2.51	119.57	124.52
14	A	1109	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
14	X	1701	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	G	1135	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	a	1012	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	a	1105	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
15	H	1237	F6C	CHA-C1A-C2A	-2.51	123.67	130.41
14	H	1023	CLA	C3D-C4D-ND	2.51	114.06	109.99
18	I	4020	BCR	C23-C24-C25	-2.51	120.30	127.00
14	A	1125	CLA	CMB-C2B-C3B	2.51	132.45	126.55
18	b	4014	BCR	C33-C5-C4	2.51	118.94	113.60
14	b	1231	CLA	C4-C3-C5	2.51	119.58	115.23
14	G	1139	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	B	1227	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
14	B	1208	CLA	CMC-C2C-C1C	2.51	128.95	125.03
14	a	1133	CLA	C6-C5-C3	-2.51	107.36	113.47
14	B	1222	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	G	1012	CLA	CHA-C1A-NA	-2.51	120.72	126.39
15	b	1237	F6C	CHA-C1A-C2A	-2.51	123.67	130.41
14	H	1222	CLA	CMA-C3A-C4A	2.51	118.51	111.77
14	A	1101	CLA	C3D-C4D-ND	2.51	114.06	109.99
18	G	4011	BCR	C19-C18-C17	2.50	122.95	119.01
14	a	1012	CLA	CHA-C1A-NA	-2.50	120.72	126.39
14	G	1133	CLA	C6-C5-C3	-2.50	107.37	113.47
18	R	4020	BCR	C23-C24-C25	-2.50	120.31	127.00
14	B	1224	CLA	CHD-C4C-C3C	-2.50	121.12	124.77
14	k	1401	CLA	C3C-C4C-NC	2.50	113.64	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1105	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
14	G	1105	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
14	B	1203	CLA	C4-C3-C2	-2.50	117.20	123.63
21	G	6001	LMT	C1'-O5'-C5'	2.50	118.61	113.72
14	A	1133	CLA	C6-C5-C3	-2.50	107.37	113.47
14	B	1209	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	G	1126	CLA	C3D-C4D-ND	2.50	114.05	109.99
18	a	4011	BCR	C4-C5-C6	-2.50	119.32	122.70
14	a	1122	CLA	CAA-CBA-CGA	-2.50	106.11	113.21
14	H	1238	CLA	C1-C2-C3	-2.50	122.10	126.20
14	G	1122	CLA	CAA-CBA-CGA	-2.50	106.11	113.21
18	a	4002	BCR	C37-C22-C21	-2.50	118.77	122.82
14	a	1117	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	a	1117	CLA	C1-C2-C3	-2.50	122.10	126.20
14	H	1203	CLA	C4-C3-C2	-2.50	117.21	123.63
14	A	1108	CLA	C3C-C4C-NC	2.50	113.63	110.43
14	a	1139	CLA	C3C-C4C-NC	2.50	113.63	110.43
14	B	1229	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	b	1216	CLA	CHC-C1C-C2C	-2.50	119.85	126.95
15	B	1237	F6C	CHA-C1A-C2A	-2.50	123.70	130.41
14	b	1209	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	a	1110	CLA	CMB-C2B-C1B	2.50	129.22	125.42
18	A	4001	BCR	C29-C30-C25	2.50	114.06	110.44
14	B	1213	CLA	CAC-C3C-C4C	2.50	128.04	124.79
18	B	4014	BCR	C33-C5-C4	2.50	118.92	113.60
18	A	4002	BCR	C37-C22-C21	-2.50	118.77	122.82
14	b	1227	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
18	i	4020	BCR	C23-C24-C25	-2.50	120.33	127.00
14	b	1231	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	A	1122	CLA	CAA-CBA-CGA	-2.49	106.12	113.21
14	G	1138	CLA	CBA-CAA-C2A	2.49	121.22	113.79
14	A	1110	CLA	CMB-C2B-C1B	2.49	129.22	125.42
18	b	4006	BCR	C36-C18-C17	-2.49	118.78	122.82
14	G	1106	CLA	CBA-CAA-C2A	2.49	121.21	113.79
14	b	1205	CLA	CMC-C2C-C1C	2.49	128.93	125.03
14	L	1501	CLA	CMC-C2C-C1C	2.49	128.93	125.03
14	B	1023	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	G	1117	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	H	1221	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	H	1211	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
14	H	1228	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	H	1233	CLA	C3D-C4D-ND	2.49	114.04	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	1401	CLA	C3C-C4C-NC	2.49	113.62	110.43
14	a	1116	CLA	C4-C3-C5	2.49	119.55	115.23
14	B	1211	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
14	a	1125	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	A	1013	CLA	C1-O2A-CGA	2.49	122.68	116.65
15	B	1230	F6C	CHB-C4A-C3A	-2.49	120.31	125.49
14	B	1210	CLA	CMA-C3A-C4A	2.49	118.47	111.77
14	G	1013	CLA	C1-O2A-CGA	2.49	122.68	116.65
14	H	1209	CLA	CMC-C2C-C1C	2.49	128.93	125.03
14	a	1108	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	G	1101	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	T	1401	CLA	C3C-C4C-NC	2.49	113.62	110.43
14	G	1109	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
14	b	1211	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
14	H	1223	CLA	CHD-C1D-ND	-2.49	121.30	124.80
14	H	1231	CLA	C4-C3-C5	2.49	119.55	115.23
14	a	1138	CLA	CBA-CAA-C2A	2.49	121.20	113.79
14	B	1212	CLA	CMA-C3A-C4A	2.49	118.46	111.77
18	A	4011	BCR	C4-C5-C6	-2.49	119.34	122.70
14	G	1123	CLA	C1-O2A-CGA	2.49	122.67	116.65
14	H	1219	CLA	C3D-C4D-ND	2.49	114.03	109.99
14	B	1205	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
14	b	1203	CLA	C4-C3-C2	-2.49	117.24	123.63
15	A	1121	F6C	O2D-CGD-O1D	-2.49	119.01	123.85
14	B	1201	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
14	a	1116	CLA	C1-O2A-CGA	2.49	122.67	116.65
14	G	1107	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
14	A	1138	CLA	CBA-CAA-C2A	2.49	121.19	113.79
14	A	1135	CLA	C3C-C4C-NC	2.49	113.61	110.43
14	B	1231	CLA	C3D-C4D-ND	2.49	114.03	109.99
14	a	1109	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
14	A	1107	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
14	b	1238	CLA	C1-C2-C3	-2.48	122.13	126.20
14	G	1117	CLA	C1-C2-C3	-2.48	122.13	126.20
14	A	1108	CLA	C4D-C3D-CAD	2.48	110.80	108.11
14	H	1218	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	G	1131	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
14	B	1207	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	a	1126	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	a	1114	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
14	G	1114	CLA	CMD-C2D-C3D	-2.48	121.99	127.69
14	B	1231	CLA	C4-C3-C5	2.48	119.54	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4011	BCR	C28-C27-C26	-2.48	109.63	114.06
14	B	1211	CLA	C4-C3-C5	2.48	119.54	115.23
14	b	1218	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	A	1113	CLA	C4D-C3D-CAD	2.48	110.80	108.11
14	L	1502	CLA	C1-O2A-CGA	2.48	122.66	116.65
14	A	1117	CLA	C1-C2-C3	-2.48	122.13	126.20
14	B	1212	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	a	1123	CLA	OBD-CAD-C3D	-2.48	122.62	128.42
18	B	4006	BCR	C36-C18-C17	-2.48	118.80	122.82
15	b	1230	F6C	CHB-C4A-C3A	-2.48	120.33	125.49
18	A	4002	BCR	C30-C25-C24	2.48	122.38	115.65
14	b	1201	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
14	B	1021	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
14	A	1116	CLA	C1-O2A-CGA	2.48	122.66	116.65
14	a	1113	CLA	C4D-C3D-CAD	2.48	110.80	108.11
14	b	1021	CLA	CBC-CAC-C3C	-2.48	105.70	112.42
18	H	4014	BCR	C33-C5-C4	2.48	118.88	113.60
14	a	1138	CLA	CED-O2D-CGD	2.48	121.54	115.92
14	a	1108	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	b	1238	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	a	1107	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
14	A	1117	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	B	1218	CLA	C3C-C4C-NC	2.48	113.61	110.43
14	b	1209	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	A	1123	CLA	C1-O2A-CGA	2.48	122.65	116.65
14	A	1104	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	H	1201	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	b	1219	CLA	C3D-C4D-ND	2.48	114.01	109.99
14	B	1226	CLA	CAA-CBA-CGA	-2.48	106.17	113.21
14	G	1110	CLA	CMB-C2B-C1B	2.48	129.19	125.42
14	H	1205	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	a	1131	CLA	CAA-C2A-C3A	-2.48	106.31	113.00
14	b	1213	CLA	CAC-C3C-C4C	2.48	128.01	124.79
14	H	1231	CLA	C3D-C4D-ND	2.48	114.01	109.99
14	H	1201	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
14	b	1212	CLA	CMA-C3A-C4A	2.48	118.43	111.77
14	B	1238	CLA	CMD-C2D-C3D	-2.48	122.01	127.69
14	A	1126	CLA	C3D-C4D-ND	2.48	114.01	109.99
14	H	1208	CLA	C4-C3-C5	2.48	119.53	115.23
14	A	1127	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
14	A	1116	CLA	C4-C3-C5	2.47	119.52	115.23
14	a	1111	CLA	C4D-C3D-CAD	2.47	110.79	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1227	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
15	G	1121	F6C	O2D-CGD-O1D	-2.47	119.03	123.85
18	G	4011	BCR	C28-C27-C26	-2.47	109.64	114.06
14	H	1235	CLA	C4-C3-C2	-2.47	117.27	123.63
14	H	1212	CLA	CMA-C3A-C4A	2.47	118.42	111.77
14	H	1213	CLA	CAC-C3C-C4C	2.47	128.01	124.79
15	A	1120	F6C	CMC-C2C-C1C	2.47	129.19	125.42
14	b	1223	CLA	CHD-C1D-ND	-2.47	121.32	124.80
14	b	1212	CLA	CMC-C2C-C1C	2.47	128.90	125.03
14	G	1127	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
14	B	1209	CLA	CMA-C3A-C4A	2.47	118.42	111.77
14	H	1209	CLA	CMA-C3A-C4A	2.47	118.42	111.77
14	b	1210	CLA	CMA-C3A-C4A	2.47	118.42	111.77
14	G	1115	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	G	1133	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	H	1218	CLA	C3D-C4D-ND	2.47	114.01	109.99
14	H	1220	CLA	C3D-C4D-ND	2.47	114.01	109.99
14	b	1207	CLA	C3D-C4D-ND	2.47	114.01	109.99
14	G	1114	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
14	a	1128	CLA	CHB-C1B-C2B	-2.47	120.25	127.43
14	A	1111	CLA	C3C-C4C-NC	2.47	113.60	110.43
18	H	4006	BCR	C36-C18-C17	-2.47	118.81	122.82
14	a	1133	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	H	1226	CLA	CAA-CBA-CGA	-2.47	106.19	113.21
15	a	1121	F6C	O2D-CGD-O1D	-2.47	119.04	123.85
14	B	1221	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	H	1021	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
14	b	1209	CLA	CMA-C3A-C4A	2.47	118.41	111.77
14	U	1502	CLA	C1-O2A-CGA	2.47	122.63	116.65
14	H	1210	CLA	CMA-C3A-C4A	2.47	118.41	111.77
14	b	1218	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	G	1116	CLA	C4-C3-C5	2.47	119.52	115.23
14	H	1209	CLA	CMB-C2B-C1B	2.47	129.18	125.42
14	l	1502	CLA	C1-O2A-CGA	2.47	122.63	116.65
15	H	1230	F6C	CHB-C4A-C3A	-2.47	120.35	125.49
14	a	1112	CLA	CAC-C3C-C4C	2.47	128.00	124.79
14	A	1114	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	G	1123	CLA	OBD-CAD-C3D	-2.47	122.65	128.42
14	T	1401	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	b	1238	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	a	1123	CLA	C1-O2A-CGA	2.47	122.62	116.65
14	A	1114	CLA	CHC-C1C-C2C	-2.47	119.94	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1128	CLA	CHB-C1B-C2B	-2.47	120.26	127.43
14	A	1131	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
14	k	1401	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	A	1133	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
18	G	4002	BCR	C30-C25-C24	2.47	122.34	115.65
14	B	1225	CLA	C4D-C3D-CAD	2.47	110.78	108.11
18	U	4019	BCR	C15-C14-C13	-2.47	123.82	127.28
14	G	1138	CLA	CED-O2D-CGD	2.47	121.51	115.92
14	H	1212	CLA	CMC-C2C-C1C	2.47	128.89	125.03
14	A	1123	CLA	OBD-CAD-C3D	-2.47	122.65	128.42
14	H	1222	CLA	C3C-C4C-NC	2.47	113.59	110.43
14	b	1202	CLA	C3C-C4C-NC	2.47	113.59	110.43
14	G	1116	CLA	C1-O2A-CGA	2.47	122.62	116.65
14	H	1238	CLA	CMC-C2C-C1C	2.46	128.89	125.03
15	b	1230	F6C	CMC-C2C-C1C	2.46	129.17	125.42
15	a	1121	F6C	C3D-C4D-ND	2.46	113.99	109.93
14	B	1215	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
14	b	1238	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
14	b	1221	CLA	C3D-C4D-ND	2.46	113.99	109.99
14	H	1209	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	H	1210	CLA	C4C-C3C-C2C	-2.46	103.31	106.89
14	A	1108	CLA	CMC-C2C-C1C	2.46	128.88	125.03
14	G	1111	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	A	1107	CLA	C3D-C4D-ND	2.46	113.99	109.99
14	G	1128	CLA	CHB-C1B-C2B	-2.46	120.28	127.43
14	B	1223	CLA	CHD-C1D-ND	-2.46	121.34	124.80
14	b	1226	CLA	CAA-CBA-CGA	-2.46	106.22	113.21
14	G	1108	CLA	CMC-C2C-C1C	2.46	128.88	125.03
18	G	4007	BCR	C23-C24-C25	-2.46	120.42	127.00
14	H	1231	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	G	1133	CLA	C4-C3-C5	2.46	119.50	115.23
14	b	1215	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
14	A	1101	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	H	1216	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
15	A	1121	F6C	C3D-C4D-ND	2.46	113.98	109.93
14	B	1209	CLA	CMC-C2C-C1C	2.46	128.88	125.03
18	a	4011	BCR	C28-C27-C26	-2.46	109.67	114.06
14	b	1222	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	b	1021	CLA	CHD-C1D-ND	-2.46	121.34	124.80
14	a	1138	CLA	C3D-C4D-ND	2.46	113.99	109.99
14	B	1234	CLA	C3D-C4D-ND	2.46	113.98	109.99
14	b	1210	CLA	C1-O2A-CGA	2.46	122.60	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1238	CLA	CMC-C2C-C1C	2.46	128.88	125.03
15	G	1121	F6C	C3D-C4D-ND	2.46	113.98	109.93
14	K	1401	CLA	C3D-C4D-ND	2.46	113.98	109.99
14	A	1138	CLA	CED-O2D-CGD	2.46	121.49	115.92
14	l	1501	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	L	1502	CLA	CMC-C2C-C1C	2.46	128.87	125.03
14	B	1238	CLA	C3D-C4D-ND	2.46	113.98	109.99
14	G	1124	CLA	C1-O2A-CGA	2.46	122.60	116.65
14	H	1232	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
14	H	1214	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	b	1201	CLA	CHB-C4A-NA	2.46	127.94	124.40
18	A	4007	BCR	C23-C24-C25	-2.46	120.44	127.00
14	B	1218	CLA	C3D-C4D-ND	2.46	113.98	109.99
14	b	1234	CLA	C3D-C4D-ND	2.46	113.98	109.99
14	B	1232	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
14	a	1114	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
18	A	4008	BCR	C19-C18-C17	2.45	122.87	119.01
14	H	1202	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	b	1233	CLA	C3C-C4C-NC	2.45	113.57	110.43
18	B	4005	BCR	C34-C9-C8	2.45	121.84	118.09
14	B	1210	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
14	a	1137	CLA	CMC-C2C-C1C	2.45	128.87	125.03
14	G	1112	CLA	CAC-C3C-C4C	2.45	127.98	124.79
14	B	1210	CLA	C1-O2A-CGA	2.45	122.59	116.65
14	b	1228	CLA	C4D-C3D-CAD	2.45	110.77	108.11
14	b	1232	CLA	CMD-C2D-C3D	-2.45	122.06	127.69
14	H	1215	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
14	B	1231	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	b	1235	CLA	C4-C3-C2	-2.45	117.33	123.63
14	x	1701	CLA	CMB-C2B-C1B	2.45	129.15	125.42
14	B	1223	CLA	CMB-C2B-C3B	2.45	132.32	126.55
14	A	1140	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	H	1223	CLA	CMC-C2C-C1C	2.45	128.86	125.03
14	A	1124	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	b	1231	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	B	1235	CLA	C4-C3-C2	-2.45	117.34	123.63
14	B	1209	CLA	CMB-C2B-C1B	2.45	129.15	125.42
14	b	1208	CLA	C4-C3-C5	2.45	119.48	115.23
18	G	4008	BCR	C19-C18-C17	2.45	122.86	119.01
14	A	1112	CLA	CAC-C3C-C4C	2.45	127.97	124.79
14	a	1107	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	a	1127	CLA	O2D-CGD-O1D	-2.45	119.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1133	CLA	C4-C3-C5	2.45	119.48	115.23
14	B	1216	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
14	B	1229	CLA	CMD-C2D-C3D	-2.45	122.08	127.69
18	a	4002	BCR	C30-C25-C24	2.45	122.29	115.65
18	b	4009	BCR	C37-C22-C21	-2.45	118.85	122.82
14	A	1128	CLA	C3C-C4C-NC	2.45	113.56	110.43
14	b	1220	CLA	C3D-C4D-ND	2.45	113.96	109.99
14	U	1502	CLA	CMC-C2C-C1C	2.45	128.86	125.03
14	B	1203	CLA	CMB-C2B-C1B	2.45	129.14	125.42
15	G	1120	F6C	CMC-C2C-C1C	2.45	129.14	125.42
14	a	1140	CLA	C3D-C4D-ND	2.45	113.96	109.99
14	b	1239	CLA	CHC-C1C-C2C	-2.45	120.00	126.95
14	H	1216	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	G	1140	CLA	C3D-C4D-ND	2.44	113.96	109.99
14	B	1202	CLA	C3C-C4C-NC	2.44	113.56	110.43
14	B	1208	CLA	C4-C3-C5	2.44	119.47	115.23
14	G	1138	CLA	C3D-C4D-ND	2.44	113.96	109.99
14	b	1226	CLA	C1D-ND-C4D	-2.44	104.60	106.31
18	a	4007	BCR	C23-C24-C25	-2.44	120.47	127.00
14	a	1012	CLA	CMC-C2C-C1C	2.44	128.85	125.03
14	H	1203	CLA	CMB-C2B-C1B	2.44	129.14	125.42
18	H	4005	BCR	C34-C9-C8	2.44	121.82	118.09
18	b	4005	BCR	C34-C9-C8	2.44	121.82	118.09
14	a	1133	CLA	C4-C3-C5	2.44	119.47	115.23
14	H	1239	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
14	b	1210	CLA	C4C-C3C-C2C	-2.44	103.34	106.89
14	A	1119	CLA	C1-O2A-CGA	2.44	122.56	116.65
14	B	1223	CLA	CMC-C2C-C1C	2.44	128.85	125.03
14	H	1238	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
18	l	4019	BCR	C15-C14-C13	-2.44	123.85	127.28
15	a	1120	F6C	CMC-C2C-C1C	2.44	129.14	125.42
14	A	1115	CLA	C3C-C4C-NC	2.44	113.56	110.43
18	H	4005	BCR	C15-C14-C13	-2.44	123.86	127.28
18	G	4003	BCR	C4-C5-C6	-2.44	119.41	122.70
14	A	1115	CLA	C4D-C3D-CAD	2.44	110.76	108.11
14	b	1216	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	H	1234	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	H	1233	CLA	C3C-C4C-NC	2.44	113.56	110.43
14	H	1229	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
14	H	1225	CLA	C4C-C3C-C2C	-2.44	103.34	106.89
14	H	1210	CLA	C1-O2A-CGA	2.44	122.55	116.65
14	B	1233	CLA	C3C-C4C-NC	2.44	113.55	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	4019	BCR	C15-C14-C13	-2.44	123.86	127.28
14	H	1238	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	b	1229	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
18	R	4020	BCR	C37-C22-C23	2.44	121.81	118.09
14	B	1220	CLA	C3D-C4D-ND	2.44	113.95	109.99
18	a	4003	BCR	C4-C5-C6	-2.44	119.41	122.70
14	H	1021	CLA	CHD-C1D-ND	-2.44	121.37	124.80
14	b	1223	CLA	CMC-C2C-C1C	2.44	128.84	125.03
18	i	4020	BCR	C37-C22-C23	2.44	121.81	118.09
14	b	1209	CLA	CMB-C2B-C1B	2.44	129.13	125.42
14	G	1108	CLA	C4D-C3D-CAD	2.43	110.75	108.11
14	H	1219	CLA	CAC-C3C-C4C	2.43	127.96	124.79
14	A	1125	CLA	C4D-C3D-CAD	2.43	110.75	108.11
14	A	1118	CLA	CMA-C3A-C4A	2.43	118.31	111.77
14	a	1118	CLA	CMA-C3A-C4A	2.43	118.31	111.77
14	G	1115	CLA	C3C-C4C-NC	2.43	113.55	110.43
14	A	1138	CLA	C3D-C4D-ND	2.43	113.94	109.99
14	G	1125	CLA	C4D-C3D-CAD	2.43	110.75	108.11
14	U	1501	CLA	C4D-C3D-CAD	2.43	110.75	108.11
14	G	1130	CLA	C3C-C4C-NC	2.43	113.55	110.43
14	H	1021	CLA	C1-C2-C3	-2.43	122.21	126.20
14	H	1239	CLA	C3D-C4D-ND	2.43	113.94	109.99
14	b	1021	CLA	C1-C2-C3	-2.43	122.21	126.20
14	A	1130	CLA	C3C-C4C-NC	2.43	113.55	110.43
18	I	4020	BCR	C37-C22-C23	2.43	121.80	118.09
14	l	1502	CLA	CMC-C2C-C1C	2.43	128.83	125.03
14	G	1125	CLA	CMC-C2C-C3C	2.43	132.72	126.15
14	G	1107	CLA	C3D-C4D-ND	2.43	113.94	109.99
14	H	1225	CLA	C4D-C3D-CAD	2.43	110.75	108.11
14	A	1125	CLA	CMC-C2C-C3C	2.43	132.72	126.15
14	A	1124	CLA	C1-O2A-CGA	2.43	122.53	116.65
14	G	1137	CLA	CMC-C2C-C1C	2.43	128.83	125.03
14	a	1111	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	b	1203	CLA	CMB-C2B-C1B	2.43	129.12	125.42
14	a	1119	CLA	C1-O2A-CGA	2.43	122.53	116.65
18	a	4007	BCR	C38-C26-C27	2.43	118.78	113.60
14	G	1128	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	B	1214	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	a	1124	CLA	C1-O2A-CGA	2.43	122.53	116.65
14	B	1239	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
18	M	4021	BCR	C37-C22-C21	-2.43	118.88	122.82
14	G	1119	CLA	C1-O2A-CGA	2.43	122.53	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1211	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
14	A	1137	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
14	a	1125	CLA	CMC-C2C-C3C	2.43	132.71	126.15
14	H	1220	CLA	CED-O2D-CGD	2.43	121.42	115.92
14	H	1238	CLA	CHB-C1B-C2B	-2.43	120.39	127.43
18	H	4009	BCR	C37-C22-C21	-2.43	118.89	122.82
14	T	1401	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
14	k	1401	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
14	A	1125	CLA	CHD-C1D-ND	-2.42	121.39	124.80
14	b	1223	CLA	CMB-C2B-C3B	2.42	132.25	126.55
18	b	4010	BCR	C34-C9-C10	-2.42	118.89	122.82
14	H	1213	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
18	a	4008	BCR	C19-C18-C17	2.42	122.82	119.01
14	B	1238	CLA	CHB-C1B-C2B	-2.42	120.40	127.43
18	B	4009	BCR	C37-C22-C21	-2.42	118.89	122.82
14	b	1218	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
14	G	1137	CLA	C3D-C4D-ND	2.42	113.92	109.99
14	X	1701	CLA	CMB-C2B-C1B	2.42	129.10	125.42
14	G	1113	CLA	C4D-C3D-CAD	2.42	110.73	108.11
14	a	1115	CLA	C4D-C3D-CAD	2.42	110.73	108.11
14	B	1218	CLA	CAA-C2A-C3A	-2.42	106.46	113.00
14	H	1223	CLA	CMB-C2B-C3B	2.42	132.24	126.55
14	G	1139	CLA	CMA-C3A-C4A	2.42	118.28	111.77
14	b	1214	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	G	1137	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
14	B	1208	CLA	C4D-C3D-CAD	2.42	110.73	108.11
14	B	1021	CLA	CHD-C1D-ND	-2.42	121.40	124.80
14	G	1124	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	a	1130	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	H	1233	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
14	G	1130	CLA	C1-O2A-CGA	2.42	122.50	116.65
14	a	1102	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	G	1125	CLA	CHD-C1D-ND	-2.42	121.40	124.80
14	B	1220	CLA	CED-O2D-CGD	2.42	121.40	115.92
18	A	4003	BCR	C4-C5-C6	-2.42	119.44	122.70
14	b	1225	CLA	C4D-C3D-CAD	2.42	110.73	108.11
14	b	1238	CLA	CHB-C1B-C2B	-2.42	120.41	127.43
14	b	1213	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
14	G	1118	CLA	CMA-C3A-C4A	2.42	118.27	111.77
14	a	1125	CLA	CHD-C1D-ND	-2.42	121.40	124.80
14	H	1201	CLA	C1-O2A-CGA	2.42	122.50	116.65
14	A	1116	CLA	C3D-C4D-ND	2.42	113.91	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	1401	CLA	CMD-C2D-C3D	-2.42	122.15	127.69
14	A	1012	CLA	CMC-C2C-C1C	2.42	128.81	125.03
14	A	1137	CLA	CMC-C2C-C1C	2.42	128.81	125.03
14	G	1012	CLA	CMC-C2C-C1C	2.42	128.81	125.03
14	H	1235	CLA	O1D-CGD-CBD	-2.41	119.75	124.52
14	U	1501	CLA	O1D-CGD-CBD	-2.41	119.75	124.52
14	B	1239	CLA	C3D-C4D-ND	2.41	113.91	109.99
14	H	1239	CLA	C1-O2A-CGA	2.41	122.50	116.65
14	B	1021	CLA	C1-C2-C3	-2.41	122.24	126.20
14	B	1201	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	G	1127	CLA	C3D-C4D-ND	2.41	113.91	109.99
14	b	1239	CLA	C1-O2A-CGA	2.41	122.49	116.65
14	L	1501	CLA	CMB-C2B-C3B	2.41	132.22	126.55
14	a	1130	CLA	C1-O2A-CGA	2.41	122.49	116.65
14	B	1225	CLA	C4C-C3C-C2C	-2.41	103.38	106.89
14	b	1213	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	b	1214	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	b	1225	CLA	C4C-C3C-C2C	-2.41	103.38	106.89
14	b	1235	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
14	b	1021	CLA	CHD-C4C-C3C	-2.41	121.26	124.77
14	H	1229	CLA	C4D-C3D-CAD	2.41	110.72	108.11
14	W	1701	CLA	CMB-C2B-C1B	2.41	129.09	125.42
14	a	1127	CLA	CMC-C2C-C1C	2.41	128.80	125.03
14	A	1127	CLA	C3D-C4D-ND	2.41	113.90	109.99
18	m	4021	BCR	C37-C22-C21	-2.41	118.91	122.82
18	a	4011	BCR	C1-C6-C7	2.41	122.19	115.65
14	B	1239	CLA	C1-O2A-CGA	2.41	122.48	116.65
14	A	1127	CLA	CMC-C2C-C1C	2.41	128.80	125.03
14	B	1233	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
14	G	1012	CLA	C1-C2-C3	-2.41	122.25	126.20
18	B	4006	BCR	C35-C13-C12	2.41	121.77	118.09
18	B	4014	BCR	C29-C28-C27	-2.41	105.98	111.28
14	B	1223	CLA	C4-C3-C5	2.41	119.41	115.23
18	b	4005	BCR	C15-C14-C13	-2.41	123.90	127.28
18	G	4011	BCR	C1-C6-C7	2.41	122.18	115.65
14	G	1122	CLA	CMB-C2B-C1B	2.41	129.09	125.42
14	A	1112	CLA	C3C-C4C-NC	2.41	113.51	110.43
14	H	1216	CLA	C1-O2A-CGA	2.41	122.48	116.65
14	B	1213	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
14	L	1501	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
14	H	1218	CLA	CAA-C2A-C3A	-2.41	106.50	113.00
18	H	4010	BCR	C34-C9-C10	-2.41	118.92	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	4019	BCR	C32-C1-C6	-2.41	106.47	110.24
18	l	4022	BCR	C1-C6-C5	-2.41	119.35	122.64
14	x	1701	CLA	O2D-CGD-O1D	-2.41	119.17	123.85
14	a	1139	CLA	CMA-C3A-C4A	2.41	118.24	111.77
15	a	1121	F6C	CHA-C1A-C2A	-2.41	123.94	130.41
14	G	1127	CLA	CMC-C2C-C1C	2.41	128.79	125.03
18	b	4013	BCR	C31-C1-C6	-2.41	106.47	110.24
14	b	1219	CLA	CAC-C3C-C4C	2.41	127.92	124.79
14	a	1137	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
14	B	1211	CLA	CAA-C2A-C3A	-2.40	106.50	113.00
15	A	1121	F6C	CHA-C1A-C2A	-2.40	123.94	130.41
18	U	4022	BCR	C1-C6-C5	-2.40	119.35	122.64
14	b	1220	CLA	CED-O2D-CGD	2.40	121.37	115.92
18	V	4021	BCR	C37-C22-C21	-2.40	118.92	122.82
14	B	1022	CLA	C4-C3-C5	2.40	119.40	115.23
14	B	1216	CLA	C1-O2A-CGA	2.40	122.47	116.65
14	a	1138	CLA	C4D-C3D-CAD	2.40	110.72	108.11
14	H	1012	CLA	C4-C3-C5	2.40	119.40	115.23
14	H	1226	CLA	CAC-C3C-C4C	2.40	127.92	124.79
14	a	1012	CLA	C1-C2-C3	-2.40	122.26	126.20
14	B	1215	CLA	CMA-C3A-C4A	2.40	118.23	111.77
14	H	1211	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
18	B	4005	BCR	C15-C14-C13	-2.40	123.91	127.28
14	G	1122	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
18	G	4007	BCR	C38-C26-C27	2.40	118.72	113.60
18	B	4012	BCR	C37-C22-C21	-2.40	118.93	122.82
14	U	1501	CLA	CMB-C2B-C3B	2.40	132.20	126.55
14	a	1119	CLA	C3C-C4C-NC	2.40	113.50	110.43
14	B	1219	CLA	CAC-C3C-C4C	2.40	127.91	124.79
14	G	1116	CLA	CAC-C3C-C4C	2.40	127.91	124.79
18	H	4014	BCR	C29-C28-C27	-2.40	106.00	111.28
14	B	1210	CLA	C4-C3-C2	-2.40	117.47	123.63
14	W	1701	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	b	1219	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	a	1128	CLA	C3C-C4C-NC	2.40	113.50	110.43
18	B	4010	BCR	C34-C9-C10	-2.40	118.93	122.82
18	A	4007	BCR	C38-C26-C27	2.40	118.71	113.60
14	l	1501	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
14	B	1210	CLA	C3C-C4C-NC	2.40	113.50	110.43
14	A	1139	CLA	CMA-C3A-C4A	2.40	118.22	111.77
14	A	1133	CLA	C1-O2A-CGA	2.40	122.45	116.65
14	B	1216	CLA	CAC-C3C-C4C	2.40	127.91	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1130	CLA	C1-O2A-CGA	2.40	122.45	116.65
14	b	1022	CLA	C1-O2A-CGA	2.40	122.45	116.65
14	b	1022	CLA	C4-C3-C5	2.40	119.39	115.23
15	G	1121	F6C	CHA-C1A-C2A	-2.40	123.97	130.41
14	A	1102	CLA	CMC-C2C-C1C	2.40	128.78	125.03
14	G	1119	CLA	C3C-C4C-NC	2.40	113.50	110.43
14	B	1216	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	1012	CLA	C4-C3-C5	2.40	119.39	115.23
14	b	1201	CLA	CAA-C2A-C3A	-2.40	106.53	113.00
14	b	1215	CLA	CMA-C3A-C4A	2.40	118.21	111.77
14	b	1224	CLA	C3D-C4D-ND	2.40	113.88	109.99
18	b	4014	BCR	C29-C28-C27	-2.40	106.01	111.28
14	b	1208	CLA	C4D-C3D-CAD	2.39	110.71	108.11
18	b	4006	BCR	C35-C13-C12	2.39	121.75	118.09
14	b	1239	CLA	C3D-C4D-ND	2.39	113.88	109.99
14	A	1119	CLA	C4D-C3D-CAD	2.39	110.71	108.11
14	H	1012	CLA	C1-O2A-CGA	2.39	122.44	116.65
14	a	1137	CLA	C3D-C4D-ND	2.39	113.88	109.99
14	G	1012	CLA	C4-C3-C5	2.39	119.38	115.23
14	B	1201	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
14	b	1201	CLA	C1-O2A-CGA	2.39	122.44	116.65
14	a	1102	CLA	CMC-C2C-C1C	2.39	128.77	125.03
14	B	1021	CLA	CHD-C4C-C3C	-2.39	121.28	124.77
14	B	1202	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
14	B	1022	CLA	C1-O2A-CGA	2.39	122.44	116.65
14	H	1208	CLA	C4D-C3D-CAD	2.39	110.70	108.11
14	H	1210	CLA	C4-C3-C2	-2.39	117.49	123.63
14	G	1102	CLA	CMC-C2C-C1C	2.39	128.77	125.03
15	b	1230	F6C	CMA-C3A-C2A	-2.39	119.68	126.15
18	H	4006	BCR	C35-C13-C12	2.39	121.74	118.09
14	A	1116	CLA	CAC-C3C-C4C	2.39	127.90	124.79
14	b	1233	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
15	H	1237	F6C	CAC-C3C-C4C	2.39	128.20	124.91
18	A	4011	BCR	C1-C6-C7	2.39	122.13	115.65
14	a	1133	CLA	C1-O2A-CGA	2.39	122.44	116.65
14	B	1227	CLA	C3C-C4C-NC	2.39	113.49	110.43
18	B	4013	BCR	C31-C1-C6	-2.39	106.50	110.24
14	b	1223	CLA	C4-C3-C5	2.39	119.38	115.23
14	l	1501	CLA	CMB-C2B-C3B	2.39	132.17	126.55
14	b	1210	CLA	C4-C3-C2	-2.39	117.49	123.63
18	b	4006	BCR	C34-C9-C10	-2.39	118.95	122.82
14	b	1227	CLA	C3C-C4C-NC	2.39	113.49	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1235	CLA	CHB-C1B-C2B	-2.39	120.49	127.43
14	a	1122	CLA	C4C-C3C-C2C	-2.39	103.42	106.89
14	H	1224	CLA	C3D-C4D-ND	2.39	113.87	109.99
14	G	1116	CLA	C3D-C4D-ND	2.39	113.87	109.99
14	G	1123	CLA	C1-C2-C3	-2.39	122.28	126.20
14	H	1201	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
14	b	1216	CLA	C1-O2A-CGA	2.39	122.43	116.65
14	a	1115	CLA	C3C-C4C-NC	2.39	113.49	110.43
14	A	1012	CLA	C1-C2-C3	-2.39	122.29	126.20
18	H	4012	BCR	C32-C1-C6	-2.39	106.50	110.24
14	a	1127	CLA	C3D-C4D-ND	2.39	113.87	109.99
15	G	1120	F6C	CMA-C3A-C2A	-2.39	119.69	126.15
14	H	1203	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
14	H	1215	CLA	CMA-C3A-C4A	2.39	118.19	111.77
14	H	1210	CLA	C3C-C4C-NC	2.39	113.49	110.43
14	X	1701	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
21	G	6002	LMT	C1B-O1B-C4'	2.39	123.63	117.98
14	A	1102	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	H	1223	CLA	C4-C3-C5	2.39	119.37	115.23
14	B	1235	CLA	O1D-CGD-CBD	-2.38	119.81	124.52
14	G	1102	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	a	1124	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	A	1137	CLA	C3D-C4D-ND	2.38	113.86	109.99
14	a	1112	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	a	1122	CLA	CMB-C2B-C1B	2.38	129.05	125.42
18	H	4013	BCR	C31-C1-C6	-2.38	106.51	110.24
14	B	1201	CLA	C1-O2A-CGA	2.38	122.42	116.65
14	B	1213	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	b	1229	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	b	1206	CLA	CBA-CAA-C2A	2.38	120.88	113.79
15	B	1237	F6C	C2B-C3B-C4B	-2.38	105.23	106.46
18	L	4022	BCR	C1-C6-C5	-2.38	119.38	122.64
14	b	1235	CLA	CHB-C1B-C2B	-2.38	120.51	127.43
14	B	1206	CLA	CBA-CAA-C2A	2.38	120.88	113.79
14	b	1210	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	b	1201	CLA	C3D-C4D-ND	2.38	113.86	109.99
14	G	1133	CLA	C1-O2A-CGA	2.38	122.41	116.65
14	A	1119	CLA	C3C-C4C-NC	2.38	113.48	110.43
14	B	1214	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	L	1501	CLA	C4D-C3D-CAD	2.38	110.69	108.11
21	G	6002	LMT	C1'-O5'-C5'	-2.38	109.07	113.72
18	M	4021	BCR	C38-C26-C25	-2.38	121.89	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1230	F6C	O1D-CGD-CBD	-2.38	119.82	124.52
14	H	1216	CLA	CAC-C3C-C4C	2.38	127.89	124.79
18	H	4006	BCR	C34-C9-C10	-2.38	118.96	122.82
21	A	6001	LMT	O5'-C5'-C6'	2.38	112.33	106.44
14	A	1129	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
14	G	1102	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	B	1203	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
14	b	1202	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
14	a	1123	CLA	C1-C2-C3	-2.38	122.30	126.20
14	A	1127	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	G	1127	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	a	1119	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	a	1012	CLA	C4-C3-C5	2.38	119.35	115.23
18	B	4006	BCR	C34-C9-C10	-2.38	118.97	122.82
18	L	4022	BCR	C3-C4-C5	-2.38	109.82	114.06
14	B	1228	CLA	CHC-C1C-C2C	-2.38	120.19	126.95
15	A	1120	F6C	CMA-C3A-C2A	-2.38	119.72	126.15
18	b	4012	BCR	C37-C22-C21	-2.38	118.97	122.82
14	H	1205	CLA	OBD-CAD-C3D	-2.37	122.86	128.42
14	H	1021	CLA	CHD-C4C-C3C	-2.37	121.31	124.77
15	B	1230	F6C	CMD-C2D-C3D	-2.37	122.25	127.69
18	B	4017	BCR	C33-C5-C6	-2.37	121.89	124.48
15	a	1120	F6C	CMA-C3A-C2A	-2.37	119.73	126.15
14	A	1122	CLA	C4C-C3C-C2C	-2.37	103.44	106.89
14	B	1224	CLA	C3D-C4D-ND	2.37	113.84	109.99
14	B	1219	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
14	G	1112	CLA	C3C-C4C-NC	2.37	113.47	110.43
14	B	1236	CLA	CMB-C2B-C1B	2.37	129.03	125.42
21	G	6001	LMT	O5'-C5'-C6'	2.37	112.32	106.44
14	H	1228	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
18	B	4012	BCR	C32-C1-C6	-2.37	106.52	110.24
14	a	1102	CLA	C3C-C4C-NC	2.37	113.47	110.43
14	b	1238	CLA	C4C-C3C-C2C	-2.37	103.44	106.89
14	G	1106	CLA	C3D-C4D-ND	2.37	113.84	109.99
18	U	4022	BCR	C35-C13-C12	2.37	121.71	118.09
14	G	1119	CLA	CHB-C1B-C2B	-2.37	120.55	127.43
14	H	1219	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
14	A	1110	CLA	CMA-C3A-C4A	2.37	118.14	111.77
14	A	1124	CLA	CMB-C2B-C3B	2.37	132.12	126.55
14	B	1235	CLA	CHB-C1B-C2B	-2.37	120.55	127.43
14	G	1124	CLA	CMB-C2B-C3B	2.37	132.12	126.55
18	U	4019	BCR	C32-C1-C6	-2.37	106.53	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1201	CLA	C3D-C4D-ND	2.37	113.84	109.99
14	H	1206	CLA	CBA-CAA-C2A	2.37	120.84	113.79
14	a	1116	CLA	CAC-C3C-C4C	2.37	127.87	124.79
14	A	1123	CLA	C1-C2-C3	-2.37	122.32	126.20
14	b	1217	CLA	C3D-C4D-ND	2.37	113.84	109.99
14	H	1227	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	H	1208	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
14	b	1208	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
18	H	4005	BCR	C23-C22-C21	2.37	122.73	119.01
14	b	1207	CLA	CMA-C3A-C4A	2.37	118.14	111.77
14	H	1226	CLA	C1D-ND-C4D	-2.37	104.65	106.31
14	H	1214	CLA	C4D-C3D-CAD	2.37	110.68	108.11
14	a	1116	CLA	C3D-C4D-ND	2.37	113.83	109.99
14	G	1110	CLA	CMA-C3A-C4A	2.37	118.13	111.77
14	a	1110	CLA	CMA-C3A-C4A	2.37	118.13	111.77
18	b	4009	BCR	C8-C7-C6	-2.37	120.68	127.00
21	a	6002	LMT	C1'-O5'-C5'	-2.37	109.10	113.72
18	U	4022	BCR	C3-C4-C5	-2.37	109.84	114.06
14	H	1213	CLA	C4D-C3D-CAD	2.37	110.67	108.11
14	H	1214	CLA	CMB-C2B-C1B	2.36	129.02	125.42
18	B	4009	BCR	C8-C7-C6	-2.36	120.68	127.00
14	b	1228	CLA	CHC-C1C-C2C	-2.36	120.23	126.95
14	A	1115	CLA	CMA-C3A-C4A	2.36	118.13	111.77
14	G	1107	CLA	CBB-CAB-C3B	-2.36	115.71	127.53
18	R	4018	BCR	C38-C26-C27	2.36	118.64	113.60
14	B	1226	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	a	1107	CLA	CBB-CAB-C3B	-2.36	115.72	127.53
14	B	1229	CLA	C4D-C3D-CAD	2.36	110.67	108.11
18	m	4021	BCR	C38-C26-C25	-2.36	121.91	124.48
15	B	1237	F6C	CAC-C3C-C4C	2.36	128.16	124.91
14	A	1138	CLA	C4D-C3D-CAD	2.36	110.67	108.11
14	A	1122	CLA	CMB-C2B-C1B	2.36	129.02	125.42
14	b	1221	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	b	1226	CLA	CAC-C3C-C4C	2.36	127.86	124.79
18	b	4012	BCR	C32-C1-C6	-2.36	106.54	110.24
14	A	1107	CLA	CBB-CAB-C3B	-2.36	115.72	127.53
18	H	4017	BCR	C33-C5-C6	-2.36	121.91	124.48
14	a	1124	CLA	CMB-C2B-C3B	2.36	132.10	126.55
14	b	1205	CLA	OBD-CAD-C3D	-2.36	122.90	128.42
14	b	1214	CLA	CMB-C2B-C1B	2.36	129.01	125.42
18	H	4012	BCR	C37-C22-C21	-2.36	118.99	122.82
14	B	1205	CLA	OBD-CAD-C3D	-2.36	122.90	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1013	CLA	CAA-C2A-C1A	-2.36	104.24	111.97
14	B	1208	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
14	H	1236	CLA	CMB-C2B-C1B	2.36	129.01	125.42
14	A	1119	CLA	CHB-C1B-C2B	-2.36	120.58	127.43
21	A	6002	LMT	C1'-O5'-C5'	-2.36	109.11	113.72
18	B	4005	BCR	C23-C22-C21	2.36	122.72	119.01
14	a	1127	CLA	C4D-C3D-CAD	2.36	110.67	108.11
21	A	6002	LMT	C1B-O1B-C4'	2.36	123.57	117.98
14	A	1013	CLA	CHD-C4C-C3C	-2.36	121.34	124.77
14	H	1202	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
14	a	1119	CLA	CHB-C1B-C2B	-2.36	120.58	127.43
14	H	1225	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	B	1207	CLA	CMA-C3A-C4A	2.36	118.11	111.77
21	a	6001	LMT	O5'-C5'-C6'	2.36	112.28	106.44
14	a	1129	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
18	l	4019	BCR	C32-C1-C6	-2.36	106.55	110.24
14	b	1203	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
14	B	1225	CLA	CAC-C3C-C4C	2.36	127.86	124.79
14	G	1124	CLA	CHB-C1B-C2B	-2.36	120.59	127.43
18	l	4022	BCR	C3-C4-C5	-2.36	109.86	114.06
14	G	1119	CLA	C4D-C3D-CAD	2.36	110.66	108.11
14	A	1106	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	G	1103	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	G	1102	CLA	CHA-C1A-NA	-2.35	121.06	126.39
21	a	6002	LMT	C1B-O1B-C4'	2.35	123.56	117.98
14	a	1132	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	a	1115	CLA	CMA-C3A-C4A	2.35	118.10	111.77
14	a	1013	CLA	CAA-C2A-C1A	-2.35	104.26	111.97
14	G	1132	CLA	C3D-C4D-ND	2.35	113.81	109.99
18	i	4018	BCR	C38-C26-C27	2.35	118.61	113.60
14	A	1108	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	B	1216	CLA	CBB-CAB-C3B	-2.35	115.77	127.53
18	b	4017	BCR	C33-C5-C6	-2.35	121.92	124.48
14	A	1102	CLA	CHA-C1A-NA	-2.35	121.07	126.39
14	B	1236	CLA	C4D-C3D-CAD	2.35	110.66	108.11
14	G	1126	CLA	C4D-C3D-CAD	2.35	110.66	108.11
14	G	1013	CLA	CAA-C2A-C1A	-2.35	104.27	111.97
14	a	1108	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
14	G	1129	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	A	1138	CLA	CMB-C2B-C3B	2.35	132.08	126.55
14	G	1136	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	H	1207	CLA	CMA-C3A-C4A	2.35	118.09	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1238	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
14	H	1201	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	l	1501	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	G	1138	CLA	CMB-C2B-C3B	2.35	132.08	126.55
14	G	1115	CLA	CMA-C3A-C4A	2.35	118.09	111.77
14	A	1112	CLA	C3D-C4D-ND	2.35	113.80	109.99
14	b	1219	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
18	b	4017	BCR	C2-C1-C6	2.35	113.85	110.44
14	b	1216	CLA	CBB-CAB-C3B	-2.35	115.79	127.53
18	H	4009	BCR	C8-C7-C6	-2.35	120.73	127.00
14	G	1138	CLA	C4D-C3D-CAD	2.35	110.66	108.11
14	H	1216	CLA	CBB-CAB-C3B	-2.35	115.80	127.53
14	H	1221	CLA	C1-C2-C3	-2.35	122.35	126.20
15	B	1230	F6C	CMC-C2C-C1C	2.35	128.99	125.42
15	H	1230	F6C	CMC-C2C-C1C	2.35	128.99	125.42
18	H	4017	BCR	C2-C1-C6	2.35	113.85	110.44
14	a	1104	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
14	H	1232	CLA	CMC-C2C-C1C	2.35	128.70	125.03
14	b	1216	CLA	CAC-C3C-C4C	2.35	127.84	124.79
14	b	1236	CLA	CMB-C2B-C1B	2.35	128.99	125.42
14	H	1232	CLA	CAC-C3C-C4C	2.35	127.84	124.79
14	A	1103	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	a	1106	CLA	C3D-C4D-ND	2.34	113.80	109.99
14	X	1701	CLA	CMC-C2C-C1C	2.34	128.70	125.03
14	H	1210	CLA	C4D-C3D-CAD	2.34	110.65	108.11
14	x	1701	CLA	CMC-C2C-C1C	2.34	128.69	125.03
18	I	4018	BCR	C38-C26-C27	2.34	118.59	113.60
14	A	1104	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
14	a	1102	CLA	CHA-C1A-NA	-2.34	121.09	126.39
14	H	1206	CLA	C3D-C4D-ND	2.34	113.79	109.99
14	B	1219	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
14	A	1124	CLA	CHB-C1B-C2B	-2.34	120.63	127.43
14	b	1236	CLA	C4D-C3D-CAD	2.34	110.65	108.11
14	a	1138	CLA	CMB-C2B-C3B	2.34	132.05	126.55
14	G	1013	CLA	CHD-C4C-C3C	-2.34	121.36	124.77
14	a	1131	CLA	C4-C3-C5	2.34	119.29	115.23
14	B	1212	CLA	CAC-C3C-C4C	2.34	127.83	124.79
14	B	1226	CLA	C1D-ND-C4D	-2.34	104.67	106.31
14	b	1225	CLA	CAC-C3C-C4C	2.34	127.83	124.79
14	a	1136	CLA	C3D-C4D-ND	2.34	113.79	109.99
14	G	1103	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	B	1238	CLA	C4C-C3C-C2C	-2.34	103.49	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1103	CLA	C3D-C4D-ND	2.34	113.78	109.99
14	H	1204	CLA	CAC-C3C-C4C	2.34	127.83	124.79
18	a	4001	BCR	C34-C9-C8	2.34	121.66	118.09
14	H	1219	CLA	CAA-C2A-C3A	-2.34	106.69	113.00
14	H	1202	CLA	C3D-C4D-ND	2.34	113.78	109.99
14	a	1124	CLA	CHB-C1B-C2B	-2.34	120.65	127.43
14	G	1108	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
14	a	1013	CLA	CHD-C4C-C3C	-2.33	121.37	124.77
14	H	1228	CLA	OBD-CAD-C3D	-2.33	122.96	128.42
18	b	4005	BCR	C23-C22-C21	2.33	122.68	119.01
18	B	4017	BCR	C2-C1-C6	2.33	113.83	110.44
14	B	1221	CLA	CAC-C3C-C4C	2.33	127.83	124.79
14	a	1108	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
18	V	4021	BCR	C38-C26-C25	-2.33	121.94	124.48
14	B	1232	CLA	CAC-C3C-C4C	2.33	127.83	124.79
14	B	1231	CLA	CHB-C1B-C2B	-2.33	120.66	127.43
18	l	4019	BCR	C3-C4-C5	-2.33	109.90	114.06
18	L	4022	BCR	C35-C13-C12	2.33	121.65	118.09
14	G	1128	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
18	G	4001	BCR	C34-C9-C8	2.33	121.65	118.09
14	b	1221	CLA	C1-C2-C3	-2.33	122.38	126.20
14	H	1229	CLA	O2A-C1-C2	2.33	117.08	108.11
14	B	1220	CLA	C3C-C4C-NC	2.33	113.42	110.43
14	B	1214	CLA	CMB-C2B-C1B	2.33	128.97	125.42
15	b	1237	F6C	CAC-C3C-C4C	2.33	128.12	124.91
14	A	1108	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
14	H	1235	CLA	C3C-C4C-NC	2.33	113.42	110.43
14	G	1108	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
14	a	1128	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
14	B	1217	CLA	C3D-C4D-ND	2.33	113.77	109.99
14	A	1131	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	A	1102	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	a	1119	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	G	1127	CLA	C11-C10-C8	-2.33	108.23	115.97
14	H	1236	CLA	C4D-C3D-CAD	2.33	110.63	108.11
14	B	1228	CLA	OBD-CAD-C3D	-2.33	122.98	128.42
14	H	1217	CLA	C4-C3-C5	2.33	119.27	115.23
14	A	1133	CLA	C3C-C4C-NC	2.33	113.41	110.43
14	A	1132	CLA	C3D-C4D-ND	2.33	113.77	109.99
14	b	1229	CLA	O2A-C1-C2	2.32	117.06	108.11
14	B	1217	CLA	C4-C3-C5	2.32	119.26	115.23
14	H	1208	CLA	CAA-CBA-CGA	-2.32	106.61	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1231	CLA	CHB-C1B-C2B	-2.32	120.68	127.43
18	L	4019	BCR	C3-C4-C5	-2.32	109.91	114.06
14	b	1204	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	H	1231	CLA	CHB-C1B-C2B	-2.32	120.68	127.43
15	b	1230	F6C	CMD-C2D-C3D	-2.32	122.36	127.69
14	a	1126	CLA	C4D-C3D-CAD	2.32	110.63	108.11
14	b	1232	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	A	1114	CLA	C3D-C4D-ND	2.32	113.76	109.99
18	l	4022	BCR	C35-C13-C12	2.32	121.64	118.09
14	A	1119	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	A	1126	CLA	C4D-C3D-CAD	2.32	110.63	108.11
14	G	1116	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
14	B	1213	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	H	1217	CLA	C3D-C4D-ND	2.32	113.76	109.99
14	a	1117	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	G	1131	CLA	C4-C3-C5	2.32	119.26	115.23
14	H	1220	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	A	1133	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
14	H	1220	CLA	C3C-C4C-NC	2.32	113.40	110.43
18	U	4019	BCR	C3-C4-C5	-2.32	109.92	114.06
14	b	1214	CLA	CMA-C3A-C4A	2.32	118.01	111.77
18	A	4001	BCR	C34-C9-C8	2.32	121.63	118.09
15	a	1120	F6C	CHA-C1A-C2A	-2.32	124.18	130.41
14	b	1206	CLA	C3D-C4D-ND	2.32	113.75	109.99
14	A	1131	CLA	C4-C3-C5	2.32	119.25	115.23
14	A	1138	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	G	1109	CLA	CMC-C2C-C1C	2.32	128.66	125.03
14	B	1229	CLA	O2A-C1-C2	2.32	117.03	108.11
14	a	1105	CLA	C3C-C4C-NC	2.32	113.40	110.43
14	a	1127	CLA	C11-C10-C8	-2.32	108.26	115.97
14	H	1221	CLA	CAC-C3C-C4C	2.32	127.81	124.79
14	G	1104	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
14	A	1127	CLA	C11-C10-C8	-2.32	108.26	115.97
14	a	1103	CLA	CHB-C4A-NA	2.32	127.74	124.40
14	B	1232	CLA	CMC-C2C-C1C	2.32	128.65	125.03
14	H	1214	CLA	CMA-C3A-C4A	2.32	118.00	111.77
14	b	1228	CLA	OBD-CAD-C3D	-2.32	123.00	128.42
14	b	1214	CLA	CHC-C1C-C2C	-2.32	120.37	126.95
14	G	1117	CLA	CAC-C3C-C4C	2.32	127.80	124.79
15	G	1120	F6C	CHA-C1A-C2A	-2.32	124.19	130.41
14	A	1127	CLA	C4-C3-C5	2.31	119.25	115.23
14	A	1136	CLA	C3D-C4D-ND	2.31	113.75	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	U	1501	CLA	C3D-C4D-ND	2.31	113.75	109.99
14	b	1235	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	G	1128	CLA	CMB-C2B-C1B	-2.31	121.89	125.42
15	B	1230	F6C	CMA-C3A-C2A	-2.31	119.89	126.15
14	G	1131	CLA	C1-O2A-CGA	2.31	122.25	116.65
14	A	1109	CLA	CMC-C2C-C1C	2.31	128.65	125.03
14	H	1223	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
14	A	1128	CLA	CHC-C1C-C2C	-2.31	120.37	126.95
14	H	1239	CLA	CMA-C3A-C4A	2.31	117.99	111.77
14	b	1227	CLA	CMC-C2C-C1C	2.31	128.65	125.03
14	B	1220	CLA	CAC-C3C-C4C	2.31	127.80	124.79
14	a	1112	CLA	C3D-C4D-ND	2.31	113.75	109.99
14	B	1221	CLA	C1-C2-C3	-2.31	122.41	126.20
14	b	1217	CLA	C4-C3-C5	2.31	119.24	115.23
15	H	1230	F6C	CMD-C2D-C3D	-2.31	122.39	127.69
14	A	1116	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
14	B	1227	CLA	CMC-C2C-C1C	2.31	128.64	125.03
15	A	1120	F6C	CHA-C1A-C2A	-2.31	124.20	130.41
14	H	1213	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	a	1012	CLA	C11-C10-C8	-2.31	108.30	115.97
14	B	1208	CLA	CAA-CBA-CGA	-2.31	106.66	113.21
15	H	1230	F6C	CMA-C3A-C2A	-2.31	119.91	126.15
14	B	1205	CLA	CMB-C2B-C3B	2.31	131.98	126.55
14	b	1202	CLA	C3D-C4D-ND	2.31	113.74	109.99
14	B	1239	CLA	CMA-C3A-C4A	2.31	117.97	111.77
14	b	1239	CLA	CMA-C3A-C4A	2.31	117.97	111.77
14	G	1112	CLA	C3D-C4D-ND	2.31	113.73	109.99
14	a	1103	CLA	C3D-C4D-ND	2.31	113.73	109.99
14	b	1213	CLA	C3C-C4C-NC	2.31	113.38	110.43
18	V	4021	BCR	C8-C9-C10	2.31	122.64	119.01
14	G	1012	CLA	C11-C10-C8	-2.31	108.30	115.97
18	H	4014	BCR	C36-C18-C17	-2.31	119.08	122.82
18	b	4005	BCR	C3-C4-C5	-2.31	109.94	114.06
14	A	1109	CLA	CMB-C2B-C1B	2.30	128.93	125.42
14	a	1109	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	b	1232	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	B	1214	CLA	CMA-C3A-C4A	2.30	117.97	111.77
14	G	1133	CLA	C3C-C4C-NC	2.30	113.38	110.43
14	B	1206	CLA	C3D-C4D-ND	2.30	113.73	109.99
14	a	1114	CLA	C3D-C4D-ND	2.30	113.73	109.99
14	A	1131	CLA	C1-O2A-CGA	2.30	122.23	116.65
14	H	1227	CLA	CMC-C2C-C1C	2.30	128.63	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1138	CLA	CAC-C3C-C4C	2.30	127.79	124.79
14	G	1116	CLA	C3C-C4C-NC	2.30	113.38	110.43
18	m	4021	BCR	C8-C9-C10	2.30	122.63	119.01
14	G	1133	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
14	H	1214	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
14	b	1208	CLA	CAA-CBA-CGA	-2.30	106.67	113.21
14	b	1214	CLA	CMC-C2C-C3C	2.30	132.37	126.15
14	a	1131	CLA	C1-O2A-CGA	2.30	122.22	116.65
18	m	4021	BCR	C40-C30-C25	2.30	113.85	110.24
14	B	1204	CLA	CAC-C3C-C4C	2.30	127.78	124.79
14	a	1138	CLA	CAC-C3C-C4C	2.30	127.78	124.79
14	W	1701	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	a	1131	CLA	C3C-C4C-NC	2.30	113.38	110.43
14	b	1205	CLA	CMB-C2B-C3B	2.30	131.96	126.55
14	G	1112	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
18	A	4001	BCR	C34-C9-C10	-2.30	119.09	122.82
14	A	1104	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
14	a	1133	CLA	C3C-C4C-NC	2.30	113.38	110.43
14	A	1012	CLA	C11-C10-C8	-2.30	108.32	115.97
14	B	1214	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
18	A	4001	BCR	C35-C13-C12	2.30	121.60	118.09
14	b	1220	CLA	CAC-C3C-C4C	2.30	127.78	124.79
14	H	1218	CLA	C4D-C3D-CAD	2.30	110.60	108.11
14	A	1112	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
14	a	1133	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
14	G	1131	CLA	C3C-C4C-NC	2.30	113.37	110.43
14	a	1128	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
14	b	1223	CLA	CHA-C1A-NA	-2.30	121.19	126.39
18	a	4001	BCR	C34-C9-C10	-2.30	119.09	122.82
14	G	1128	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
14	b	1227	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
14	H	1216	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
14	A	1128	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
14	H	1223	CLA	OBD-CAD-C3D	-2.30	123.05	128.42
14	a	1112	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
14	B	1232	CLA	C3C-C4C-NC	2.29	113.37	110.43
15	a	1120	F6C	O1D-CGD-CBD	-2.29	119.99	124.52
14	B	1202	CLA	C3D-C4D-ND	2.29	113.72	109.99
14	A	1138	CLA	O2A-C1-C2	2.29	116.93	108.11
14	A	1107	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	B	4005	BCR	C3-C4-C5	-2.29	109.97	114.06
14	B	1214	CLA	CMC-C2C-C3C	2.29	132.35	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1223	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
14	G	1107	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
18	G	4001	BCR	C34-C9-C10	-2.29	119.10	122.82
14	A	1116	CLA	C3C-C4C-NC	2.29	113.36	110.43
14	H	1232	CLA	C3C-C4C-NC	2.29	113.36	110.43
14	A	1104	CLA	CHB-C4A-NA	2.29	127.71	124.40
14	H	1234	CLA	C4-C3-C2	-2.29	117.75	123.63
14	G	1119	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	H	1227	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
14	A	1132	CLA	CMA-C3A-C4A	2.29	117.93	111.77
14	b	1201	CLA	CMB-C2B-C3B	2.29	131.94	126.55
14	B	1216	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
14	G	1113	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
14	B	1235	CLA	C3C-C4C-NC	2.29	113.36	110.43
14	H	1205	CLA	CMB-C2B-C3B	2.29	131.94	126.55
14	A	1112	CLA	CMB-C2B-C1B	2.29	128.91	125.42
18	a	4001	BCR	C35-C13-C12	2.29	121.58	118.09
20	b	5002	LMG	C8-O7-C10	-2.29	112.32	117.80
14	B	1223	CLA	CHA-C1A-NA	-2.29	121.21	126.39
18	H	4004	BCR	C33-C5-C6	-2.29	121.99	124.48
18	b	4016	BCR	C3-C4-C5	-2.29	109.97	114.06
18	H	4005	BCR	C3-C4-C5	-2.29	109.98	114.06
13	A	1011	CL0	C4C-CHD-C1D	2.29	124.25	116.07
14	a	1132	CLA	CMA-C3A-C4A	2.29	117.92	111.77
14	A	1123	CLA	C3D-C4D-ND	2.29	113.70	109.99
14	a	1115	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
14	H	1214	CLA	CMC-C2C-C3C	2.29	132.33	126.15
14	B	1219	CLA	C4D-C3D-CAD	2.29	110.59	108.11
14	B	1021	CLA	CMA-C3A-C2A	-2.29	105.14	113.98
14	a	1107	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
18	H	4004	BCR	C37-C22-C21	-2.29	119.11	122.82
14	G	1112	CLA	CMB-C2B-C1B	2.29	128.90	125.42
14	a	1127	CLA	C4-C3-C5	2.29	119.19	115.23
14	A	1117	CLA	CAC-C3C-C4C	2.29	127.76	124.79
14	B	1223	CLA	OBD-CAD-C3D	-2.29	123.08	128.42
14	G	1114	CLA	C3D-C4D-ND	2.29	113.70	109.99
14	B	1239	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
14	G	1138	CLA	O2A-C1-C2	2.28	116.90	108.11
14	a	1138	CLA	O2A-C1-C2	2.28	116.90	108.11
14	L	1501	CLA	C3D-C4D-ND	2.28	113.70	109.99
18	B	4016	BCR	C3-C4-C5	-2.28	109.98	114.06
18	B	4014	BCR	C36-C18-C17	-2.28	119.12	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1109	CLA	CMB-C2B-C1B	2.28	128.90	125.42
14	G	1138	CLA	CMA-C3A-C4A	2.28	117.91	111.77
18	b	4004	BCR	C37-C22-C21	-2.28	119.12	122.82
18	b	4014	BCR	C36-C18-C17	-2.28	119.12	122.82
14	A	1107	CLA	CMA-C3A-C4A	2.28	117.91	111.77
20	H	5002	LMG	C8-O7-C10	-2.28	112.34	117.80
14	b	1212	CLA	CAC-C3C-C4C	2.28	127.76	124.79
14	H	1201	CLA	CMB-C2B-C3B	2.28	131.91	126.55
14	B	1223	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
14	H	1021	CLA	CMA-C3A-C2A	-2.28	105.17	113.98
14	H	1236	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	b	1232	CLA	C3C-C4C-NC	2.28	113.35	110.43
20	B	5002	LMG	C8-O7-C10	-2.28	112.34	117.80
14	b	1021	CLA	CMA-C3A-C2A	-2.28	105.17	113.98
14	b	1216	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
14	b	1223	CLA	OBD-CAD-C3D	-2.28	123.09	128.42
14	B	1236	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	B	1227	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
14	H	1212	CLA	CAC-C3C-C4C	2.28	127.75	124.79
14	H	1223	CLA	CHA-C1A-NA	-2.28	121.23	126.39
14	H	1239	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
14	a	1116	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
13	G	1011	CL0	C4C-CHD-C1D	2.28	124.22	116.07
18	M	4021	BCR	C8-C9-C10	2.28	122.59	119.01
13	a	1011	CL0	C4C-CHD-C1D	2.28	124.22	116.07
18	M	4021	BCR	C2-C1-C6	2.28	113.75	110.44
14	A	1128	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
14	G	1127	CLA	C4-C3-C5	2.28	119.18	115.23
14	W	1701	CLA	C3D-C4D-ND	2.27	113.68	109.99
14	a	1123	CLA	C3D-C4D-ND	2.27	113.68	109.99
14	H	1201	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
14	b	1210	CLA	C4D-C3D-CAD	2.27	110.58	108.11
18	b	4014	BCR	C4-C5-C6	-2.27	119.63	122.70
14	H	1219	CLA	C4D-C3D-CAD	2.27	110.58	108.11
18	B	4006	BCR	C2-C1-C6	-2.27	107.14	110.44
18	b	4006	BCR	C2-C1-C6	-2.27	107.14	110.44
18	V	4021	BCR	C40-C30-C25	2.27	113.81	110.24
14	A	1104	CLA	C7-C6-C5	-2.27	107.20	113.26
14	a	1138	CLA	CMA-C3A-C4A	2.27	117.88	111.77
14	A	1104	CLA	CMC-C2C-C1C	2.27	128.59	125.03
14	b	1218	CLA	C4D-C3D-CAD	2.27	110.57	108.11
18	G	4001	BCR	C35-C13-C12	2.27	121.56	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1201	CLA	CMB-C2B-C3B	2.27	131.89	126.55
14	G	1132	CLA	CMA-C3A-C4A	2.27	117.88	111.77
18	V	4021	BCR	C2-C1-C6	2.27	113.74	110.44
14	a	1116	CLA	C3C-C4C-NC	2.27	113.34	110.43
14	b	1220	CLA	C3C-C4C-NC	2.27	113.34	110.43
18	B	4004	BCR	C37-C22-C21	-2.27	119.14	122.82
14	A	1101	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
14	a	1104	CLA	C7-C6-C5	-2.27	107.21	113.26
14	A	1113	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
14	b	1234	CLA	C4-C3-C2	-2.27	117.80	123.63
18	G	4008	BCR	C36-C18-C17	-2.27	119.14	122.82
14	a	1111	CLA	CHA-C1A-NA	-2.27	121.25	126.39
14	B	1212	CLA	C3D-C4D-ND	2.27	113.67	109.99
14	A	1012	CLA	C3D-C4D-ND	2.27	113.67	109.99
18	m	4021	BCR	C2-C1-C6	2.27	113.73	110.44
14	B	1224	CLA	CMB-C2B-C3B	2.27	131.88	126.55
14	b	1023	CLA	CAC-C3C-C2C	-2.27	123.39	127.56
21	G	6001	LMT	O5'-C5'-C4'	2.27	114.41	109.72
14	b	1231	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
14	H	1012	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
14	b	1201	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
14	a	1104	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	A	1140	CLA	C1-O2A-CGA	2.27	122.14	116.65
18	A	4008	BCR	C36-C18-C17	-2.27	119.14	122.82
21	a	6001	LMT	O5'-C5'-C4'	2.27	114.41	109.72
14	b	1206	CLA	CHC-C1C-C2C	-2.27	120.51	126.95
21	A	6001	LMT	O5'-C5'-C4'	2.27	114.41	109.72
14	G	1130	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
14	a	1113	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
14	a	1116	CLA	CMA-C3A-C4A	2.27	117.86	111.77
15	G	1121	F6C	CHC-C1C-C2C	-2.27	120.85	127.43
18	a	4008	BCR	C36-C18-C17	-2.26	119.15	122.82
18	B	4014	BCR	C4-C5-C6	-2.26	119.64	122.70
14	B	1214	CLA	CBB-CAB-C3B	-2.26	116.22	127.53
18	l	4019	BCR	C34-C9-C10	-2.26	119.15	122.82
14	b	1214	CLA	CBB-CAB-C3B	-2.26	116.22	127.53
14	a	1128	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
15	G	1120	F6C	O1D-CGD-CBD	-2.26	120.05	124.52
14	B	1210	CLA	C4D-C3D-CAD	2.26	110.56	108.11
14	H	1238	CLA	C11-C12-C13	-2.26	108.44	115.97
18	H	4014	BCR	C4-C5-C6	-2.26	119.65	122.70
14	b	1236	CLA	C3C-C4C-NC	2.26	113.33	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1133	CLA	C3D-C4D-ND	2.26	113.67	109.99
14	G	1104	CLA	C7-C6-C5	-2.26	107.23	113.26
14	G	1125	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
14	A	1111	CLA	CHA-C1A-NA	-2.26	121.27	126.39
14	G	1101	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
14	b	1214	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
14	B	1208	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	B	1023	CLA	CAC-C3C-C2C	-2.26	123.40	127.56
14	b	1239	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
14	a	1133	CLA	C3D-C4D-ND	2.26	113.66	109.99
14	b	1238	CLA	C11-C12-C13	-2.26	108.45	115.97
18	H	4016	BCR	C3-C4-C5	-2.26	110.02	114.06
14	a	1107	CLA	CMA-C3A-C4A	2.26	117.85	111.77
14	a	1130	CLA	CHB-C1B-C2B	-2.26	120.86	127.43
14	X	1701	CLA	C3D-C4D-ND	2.26	113.66	109.99
18	b	4012	BCR	C34-C9-C10	-2.26	119.15	122.82
14	A	1130	CLA	CHB-C1B-C2B	-2.26	120.86	127.43
15	A	1120	F6C	O1D-CGD-CBD	-2.26	120.06	124.52
18	B	4004	BCR	C33-C5-C6	-2.26	122.02	124.48
14	a	1104	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
14	A	1138	CLA	CMA-C3A-C4A	2.26	117.85	111.77
14	a	1140	CLA	C1-O2A-CGA	2.26	122.12	116.65
14	G	1105	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	H	1228	CLA	CMB-C2B-C3B	2.26	131.87	126.55
14	H	1214	CLA	CBB-CAB-C3B	-2.26	116.23	127.53
18	M	4021	BCR	C40-C30-C25	2.26	113.79	110.24
14	G	1114	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
14	G	1104	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	a	1104	CLA	CMC-C2C-C1C	2.26	128.56	125.03
14	B	1238	CLA	C11-C12-C13	-2.26	108.46	115.97
14	G	1104	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
14	b	1216	CLA	CMC-C2C-C3C	2.26	132.26	126.15
14	a	1103	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
14	a	1012	CLA	C3D-C4D-ND	2.26	113.66	109.99
14	A	1105	CLA	C3C-C4C-NC	2.26	113.32	110.43
14	x	1701	CLA	C3D-C4D-ND	2.26	113.65	109.99
14	B	1234	CLA	C4-C3-C2	-2.26	117.83	123.63
14	G	1115	CLA	CMD-C2D-C3D	-2.26	122.52	127.69
20	R	5006	LMG	C8-O7-C10	-2.26	112.40	117.80
14	G	1140	CLA	C1-O2A-CGA	2.26	122.11	116.65
14	A	1117	CLA	CMD-C2D-C3D	-2.26	122.52	127.69
14	B	1231	CLA	CAA-C2A-C3A	-2.26	106.91	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1123	CLA	C3D-C4D-ND	2.25	113.65	109.99
14	b	1214	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
14	B	1022	CLA	C4C-C3C-C2C	-2.25	103.61	106.89
14	A	1125	CLA	CHC-C1C-C2C	-2.25	120.54	126.95
14	b	1238	CLA	C16-C15-C13	-2.25	108.47	115.97
14	A	1137	CLA	CAC-C3C-C4C	2.25	127.72	124.79
18	b	4004	BCR	C33-C5-C6	-2.25	122.03	124.48
14	H	1023	CLA	CAC-C3C-C2C	-2.25	123.42	127.56
14	A	1103	CLA	CHC-C1C-C2C	-2.25	120.54	126.95
14	H	1206	CLA	CHC-C1C-C2C	-2.25	120.54	126.95
14	a	1109	CLA	CMB-C2B-C1B	2.25	128.85	125.42
14	G	1111	CLA	CHA-C1A-NA	-2.25	121.29	126.39
14	A	1140	CLA	C4D-C3D-CAD	2.25	110.55	108.11
14	G	1107	CLA	CMA-C3A-C4A	2.25	117.83	111.77
13	A	1011	CL0	CMC-C2C-C1C	2.25	128.79	124.73
14	B	1201	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
14	U	1502	CLA	CMB-C2B-C1B	2.25	128.85	125.42
14	G	1135	CLA	CMC-C2C-C1C	2.25	128.55	125.03
14	B	1022	CLA	C3D-C4D-ND	2.25	113.65	109.99
14	G	1118	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
14	b	1023	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
14	G	1140	CLA	C4B-CHC-C1C	2.25	131.54	126.25
14	H	1209	CLA	C3C-C4C-NC	2.25	113.31	110.43
14	B	1206	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
14	a	1119	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
14	B	1023	CLA	CAA-CBA-CGA	-2.25	106.82	113.21
14	a	1114	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
14	G	1117	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
15	A	1121	F6C	CHC-C1C-C2C	-2.25	120.90	127.43
14	B	1209	CLA	C3C-C4C-NC	2.25	113.31	110.43
14	b	1212	CLA	C3D-C4D-ND	2.25	113.64	109.99
14	A	1114	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
14	H	1224	CLA	CMB-C2B-C3B	2.25	131.84	126.55
14	B	1215	CLA	C1-O2A-CGA	2.25	122.09	116.65
14	a	1140	CLA	C4B-CHC-C1C	2.25	131.53	126.25
14	b	1208	CLA	C3C-C4C-NC	2.25	113.31	110.43
13	a	1011	CL0	C2C-C1C-NC	2.25	116.82	110.46
18	B	4012	BCR	C24-C25-C26	-2.25	116.38	121.56
13	G	1011	CL0	C2C-C1C-NC	2.25	116.82	110.46
18	A	4011	BCR	C35-C13-C12	2.25	121.52	118.09
14	G	1114	CLA	CHB-C1B-C2B	-2.25	120.91	127.43
14	H	1231	CLA	CAA-C2A-C3A	-2.25	106.93	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1228	CLA	CMB-C2B-C3B	2.25	131.83	126.55
14	a	1125	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
14	B	1212	CLA	C4D-C3D-CAD	2.25	110.55	108.11
14	b	1209	CLA	C3C-C4C-NC	2.25	113.31	110.43
15	H	1230	F6C	O1D-CGD-CBD	-2.25	120.09	124.52
14	a	1137	CLA	OBD-CAD-C3D	-2.24	123.17	128.42
18	b	4012	BCR	C24-C25-C26	-2.24	116.39	121.56
18	B	4005	BCR	C27-C26-C25	-2.24	119.67	122.70
14	a	1101	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
14	b	1228	CLA	CMB-C2B-C3B	2.24	131.83	126.55
14	G	1140	CLA	CMA-C3A-C4A	2.24	117.81	111.77
14	A	1114	CLA	CHB-C1B-C2B	-2.24	120.91	127.43
18	B	4009	BCR	C31-C1-C6	-2.24	106.72	110.24
14	a	1137	CLA	CAC-C3C-C4C	2.24	127.71	124.79
14	B	1203	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
14	b	1224	CLA	CMB-C2B-C3B	2.24	131.83	126.55
18	H	4012	BCR	C24-C25-C26	-2.24	116.39	121.56
13	G	1011	CL0	OBD-CAD-C3D	-2.24	124.39	127.89
14	B	1216	CLA	CMC-C2C-C3C	2.24	132.22	126.15
14	H	1216	CLA	CMC-C2C-C3C	2.24	132.22	126.15
13	A	1011	CL0	C2C-C1C-NC	2.24	116.81	110.46
14	G	1132	CLA	C11-C10-C8	-2.24	108.51	115.97
14	b	1022	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
14	H	1012	CLA	C3D-C4D-ND	2.24	113.63	109.99
13	a	1011	CL0	OBD-CAD-C3D	-2.24	124.39	127.89
14	A	1140	CLA	C4B-CHC-C1C	2.24	131.52	126.25
14	b	1210	CLA	C4B-CHC-C1C	2.24	131.52	126.25
14	a	1114	CLA	CHB-C1B-C2B	-2.24	120.92	127.43
14	a	1112	CLA	CMB-C2B-C1B	2.24	128.83	125.42
20	I	5006	LMG	C8-O7-C10	-2.24	112.44	117.80
18	G	4002	BCR	C33-C5-C6	-2.24	122.04	124.48
14	A	1115	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
14	G	1012	CLA	C3D-C4D-ND	2.24	113.63	109.99
18	b	4005	BCR	C27-C26-C25	-2.24	119.68	122.70
14	A	1116	CLA	CMA-C3A-C4A	2.24	117.79	111.77
14	B	1218	CLA	C4D-C3D-CAD	2.24	110.54	108.11
15	a	1121	F6C	CHC-C1C-C2C	-2.24	120.93	127.43
14	A	1137	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
14	H	1208	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	H	1224	CLA	C4C-C3C-C2C	-2.24	103.63	106.89
14	a	1106	CLA	CMC-C2C-C1C	2.24	128.53	125.03
14	H	1238	CLA	C16-C15-C13	-2.24	108.53	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1103	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
13	a	1011	CL0	CMC-C2C-C1C	2.24	128.76	124.73
14	G	1104	CLA	CMC-C2C-C1C	2.24	128.53	125.03
14	B	1238	CLA	C16-C15-C13	-2.24	108.53	115.97
14	G	1116	CLA	CMA-C3A-C4A	2.24	117.78	111.77
14	H	1214	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
15	B	1230	F6C	CAA-CBA-CGA	-2.24	107.74	113.67
14	b	1022	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
14	a	1103	CLA	CMC-C2C-C1C	2.24	128.53	125.03
14	L	1502	CLA	CMB-C2B-C1B	2.23	128.82	125.42
14	H	1023	CLA	CAA-CBA-CGA	-2.23	106.86	113.21
14	a	1140	CLA	C4D-C3D-CAD	2.23	110.53	108.11
20	i	5006	LMG	C8-O7-C10	-2.23	112.45	117.80
18	A	4002	BCR	C33-C5-C6	-2.23	122.05	124.48
14	H	1210	CLA	C4B-CHC-C1C	2.23	131.50	126.25
14	B	1210	CLA	C4B-CHC-C1C	2.23	131.50	126.25
14	A	1111	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
14	l	1502	CLA	C3C-C4C-NC	2.23	113.29	110.43
14	H	1232	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
14	A	1131	CLA	CMB-C2B-C1B	2.23	128.82	125.42
15	H	1237	F6C	C1C-CHC-C4B	2.23	131.50	126.25
18	L	4019	BCR	C34-C9-C10	-2.23	119.20	122.82
14	B	1214	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
14	H	1212	CLA	C3D-C4D-ND	2.23	113.61	109.99
14	H	1201	CLA	C4-C3-C2	-2.23	117.89	123.63
14	b	1203	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
18	b	4009	BCR	C31-C1-C6	-2.23	106.74	110.24
14	A	1119	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
14	a	1104	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
18	L	4022	BCR	C31-C1-C6	-2.23	106.75	110.24
14	G	1131	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
14	b	1022	CLA	C3D-C4D-ND	2.23	113.61	109.99
15	G	1121	F6C	CMC-C2C-C1C	2.23	128.81	125.42
14	a	1138	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
14	a	1111	CLA	OBD-CAD-C3D	-2.23	123.20	128.42
21	G	6002	LMT	C3B-C4B-C5B	-2.23	106.19	110.23
18	H	4006	BCR	C2-C1-C6	-2.23	107.20	110.44
14	H	1215	CLA	C1-O2A-CGA	2.23	122.05	116.65
14	A	1132	CLA	C11-C10-C8	-2.23	108.56	115.97
14	a	1118	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
14	b	1201	CLA	C4-C3-C2	-2.23	117.90	123.63
14	A	1137	CLA	CAA-C2A-C3A	-2.23	106.98	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1011	CL0	CMC-C2C-C1C	2.23	128.74	124.73
14	G	1137	CLA	OBD-CAD-C3D	-2.23	123.21	128.42
15	B	1237	F6C	C1C-CHC-C4B	2.23	131.48	126.25
14	G	1119	CLA	C4C-C3C-C2C	-2.23	103.65	106.89
14	A	1138	CLA	CHB-C1B-C2B	-2.23	120.97	127.43
14	A	1133	CLA	C3D-C4D-ND	2.23	113.60	109.99
18	H	4012	BCR	C34-C9-C10	-2.23	119.21	122.82
14	b	1021	CLA	C7-C6-C5	-2.22	107.33	113.26
14	H	1209	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
14	b	1215	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
18	B	4012	BCR	C35-C13-C12	2.22	121.49	118.09
14	b	1209	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
14	b	1232	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
14	a	1132	CLA	C11-C10-C8	-2.22	108.58	115.97
14	H	1224	CLA	CAC-C3C-C4C	2.22	127.68	124.79
14	H	1222	CLA	C11-C12-C13	-2.22	108.58	115.97
18	a	4011	BCR	C35-C13-C12	2.22	121.48	118.09
14	G	1137	CLA	CAC-C3C-C4C	2.22	127.68	124.79
14	B	1232	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
14	B	1229	CLA	CMA-C3A-C4A	2.22	117.75	111.77
14	b	1212	CLA	C4D-C3D-CAD	2.22	110.52	108.11
14	H	1203	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
14	B	1232	CLA	C3D-C4D-ND	2.22	113.60	109.99
14	G	1137	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
21	a	6002	LMT	C3B-C4B-C5B	-2.22	106.20	110.23
14	a	1111	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
14	A	1140	CLA	CMA-C3A-C4A	2.22	117.74	111.77
14	A	1118	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
14	b	1224	CLA	C4D-C3D-CAD	2.22	110.52	108.11
18	a	4001	BCR	C38-C26-C25	-2.22	122.06	124.48
18	U	4019	BCR	C34-C9-C10	-2.22	119.22	122.82
14	a	1117	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
13	A	1011	CL0	OBD-CAD-C3D	-2.22	124.43	127.89
14	G	1106	CLA	CMC-C2C-C1C	2.22	128.50	125.03
14	l	1502	CLA	CMB-C2B-C1B	2.22	128.80	125.42
14	b	1021	CLA	C11-C10-C8	-2.22	108.59	115.97
14	H	1232	CLA	C3D-C4D-ND	2.22	113.59	109.99
14	B	1209	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
14	b	1224	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
14	H	1224	CLA	C4D-C3D-CAD	2.22	110.52	108.11
14	a	1137	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
14	G	1104	CLA	O1D-CGD-CBD	-2.22	120.14	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1222	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	A	1111	CLA	OBD-CAD-C3D	-2.22	123.23	128.42
14	B	1021	CLA	C7-C6-C5	-2.22	107.35	113.26
14	B	1222	CLA	C4-C3-C2	-2.22	117.94	123.63
14	G	1140	CLA	C4D-C3D-CAD	2.22	110.51	108.11
14	B	1222	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
14	B	1205	CLA	CHB-C1B-C2B	-2.22	120.99	127.43
14	H	1210	CLA	C1-C2-C3	-2.22	122.57	126.20
14	B	1212	CLA	C4C-C3C-C2C	-2.22	103.67	106.89
14	A	1129	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
14	B	1215	CLA	CHC-C1C-C2C	-2.21	120.65	126.95
14	A	1103	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	b	1222	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
18	H	4009	BCR	C31-C1-C6	-2.21	106.77	110.24
14	b	1238	CLA	CED-O2D-CGD	2.21	120.94	115.92
14	H	1021	CLA	C7-C6-C5	-2.21	107.36	113.26
14	A	1106	CLA	CMA-C3A-C4A	2.21	117.72	111.77
18	l	4022	BCR	C31-C1-C6	-2.21	106.77	110.24
14	B	1238	CLA	CED-O2D-CGD	2.21	120.94	115.92
14	A	1106	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	G	1111	CLA	OBD-CAD-C3D	-2.21	123.24	128.42
14	a	1140	CLA	CMA-C3A-C4A	2.21	117.72	111.77
14	H	1214	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
14	B	1222	CLA	C11-C12-C13	-2.21	108.61	115.97
14	b	1229	CLA	CMA-C3A-C4A	2.21	117.72	111.77
21	G	6002	LMT	O5B-C5B-C6B	2.21	111.92	106.44
14	B	1201	CLA	C4-C3-C2	-2.21	117.95	123.63
14	B	1224	CLA	C4C-C3C-C2C	-2.21	103.67	106.89
14	A	1131	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
14	a	1129	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
18	H	4005	BCR	C27-C26-C25	-2.21	119.72	122.70
15	b	1237	F6C	C1C-CHC-C4B	2.21	131.44	126.25
14	H	1217	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
18	l	4019	BCR	C37-C22-C21	-2.21	119.23	122.82
14	A	1135	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	a	1106	CLA	CMA-C3A-C4A	2.21	117.71	111.77
14	A	1101	CLA	CAC-C3C-C4C	2.21	127.66	124.79
14	G	1103	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	A	1126	CLA	CMB-C2B-C1B	2.21	128.78	125.42
14	b	1023	CLA	CMC-C2C-C3C	2.21	132.12	126.15
18	G	4011	BCR	C35-C13-C12	2.21	121.46	118.09
18	b	4012	BCR	C35-C13-C12	2.21	121.46	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1210	CLA	CMB-C2B-C3B	2.21	131.74	126.55
14	b	1222	CLA	C11-C12-C13	-2.21	108.63	115.97
14	H	1210	CLA	CMB-C2B-C3B	2.21	131.74	126.55
18	G	4002	BCR	C35-C13-C12	2.21	121.46	118.09
14	B	1023	CLA	CMC-C2C-C3C	2.21	132.12	126.15
14	a	1135	CLA	CMC-C2C-C1C	2.21	128.48	125.03
14	b	1226	CLA	C4-C3-C5	2.21	119.06	115.23
14	b	1219	CLA	C4D-C3D-CAD	2.21	110.50	108.11
14	B	1214	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
14	G	1138	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
14	G	1123	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
18	G	4011	BCR	C8-C9-C10	2.21	122.48	119.01
14	a	1116	CLA	CMB-C2B-C1B	2.21	128.78	125.42
14	b	1205	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
14	b	1215	CLA	C3D-C4D-ND	2.21	113.57	109.99
18	L	4019	BCR	C37-C22-C21	-2.21	119.24	122.82
14	B	1217	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
18	B	4012	BCR	C34-C9-C10	-2.20	119.24	122.82
14	A	1118	CLA	OBD-CAD-C3D	-2.20	123.26	128.42
14	b	1222	CLA	C4-C3-C2	-2.20	117.97	123.63
14	B	1224	CLA	CAC-C3C-C4C	2.20	127.66	124.79
14	b	1220	CLA	CHC-C1C-C2C	-2.20	120.68	126.95
14	G	1129	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
14	G	1115	CLA	CMB-C2B-C3B	2.20	131.74	126.55
14	b	1210	CLA	CMB-C2B-C3B	2.20	131.74	126.55
18	G	4003	BCR	C36-C18-C17	-2.20	119.25	122.82
14	B	1021	CLA	C11-C10-C8	-2.20	108.64	115.97
18	a	4002	BCR	C33-C5-C6	-2.20	122.08	124.48
14	A	1124	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
14	H	1012	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
15	A	1121	F6C	CMC-C2C-C1C	2.20	128.77	125.42
18	U	4019	BCR	C37-C22-C21	-2.20	119.25	122.82
14	B	1220	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
14	H	1226	CLA	C4-C3-C5	2.20	119.05	115.23
14	H	1023	CLA	CMC-C2C-C3C	2.20	132.10	126.15
18	b	4005	BCR	C1-C6-C5	-2.20	119.63	122.64
14	b	1210	CLA	C1-C2-C3	-2.20	122.59	126.20
14	G	1106	CLA	CMA-C3A-C4A	2.20	117.69	111.77
18	A	4002	BCR	C35-C13-C12	2.20	121.45	118.09
14	A	1013	CLA	CAC-C3C-C4C	2.20	127.65	124.79
14	A	1118	CLA	CMC-C2C-C1C	2.20	128.47	125.03
14	B	1239	CLA	C4-C3-C5	2.20	119.05	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1021	CLA	C11-C10-C8	-2.20	108.65	115.97
18	U	4022	BCR	C31-C1-C6	-2.20	106.79	110.24
14	H	1215	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
18	H	4013	BCR	C36-C18-C17	-2.20	119.25	122.82
14	B	1210	CLA	C1-C2-C3	-2.20	122.59	126.20
14	b	1215	CLA	C1-O2A-CGA	2.20	121.98	116.65
15	b	1230	F6C	CAA-CBA-CGA	-2.20	107.83	113.67
14	a	1126	CLA	CMB-C2B-C1B	2.20	128.77	125.42
18	b	4005	BCR	C36-C18-C17	-2.20	119.25	122.82
14	H	1212	CLA	C4D-C3D-CAD	2.20	110.49	108.11
14	G	1118	CLA	OBD-CAD-C3D	-2.20	123.28	128.42
14	b	1217	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	a	1124	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
14	G	1118	CLA	CMC-C2C-C1C	2.20	128.47	125.03
14	H	1238	CLA	CED-O2D-CGD	2.20	120.90	115.92
14	B	1218	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
15	B	1230	F6C	O1D-CGD-CBD	-2.20	120.18	124.52
14	G	1111	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	G	1117	CLA	CMC-C2C-C3C	2.20	132.09	126.15
14	A	1115	CLA	CMB-C2B-C3B	2.20	131.72	126.55
21	A	6002	LMT	C3B-C4B-C5B	-2.20	106.25	110.23
14	L	1502	CLA	C3C-C4C-NC	2.20	113.24	110.43
14	H	1215	CLA	C3D-C4D-ND	2.20	113.56	109.99
18	B	4009	BCR	C1-C6-C5	-2.20	119.64	122.64
14	H	1229	CLA	CMA-C3A-C4A	2.20	117.67	111.77
14	A	1123	CLA	CMD-C2D-C3D	-2.20	122.66	127.69
14	H	1215	CLA	C4D-C3D-CAD	2.20	110.49	108.11
18	G	4007	BCR	C35-C13-C12	2.19	121.44	118.09
14	H	1221	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
18	A	4011	BCR	C8-C9-C10	2.19	122.46	119.01
14	a	1131	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
14	U	1502	CLA	C3C-C4C-NC	2.19	113.24	110.43
14	H	1222	CLA	C4-C3-C2	-2.19	117.99	123.63
14	a	1110	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
14	a	1126	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
14	b	1238	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
14	A	1116	CLA	CMB-C2B-C1B	2.19	128.76	125.42
14	G	1126	CLA	CMB-C2B-C1B	2.19	128.76	125.42
18	H	4012	BCR	C35-C13-C12	2.19	121.44	118.09
14	G	1110	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
14	b	1214	CLA	C3D-C4D-ND	2.19	113.55	109.99
14	b	1221	CLA	CAA-CBA-CGA	-2.19	106.98	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	6002	LMT	O5B-C5B-C6B	2.19	111.87	106.44
14	a	1111	CLA	C3D-C4D-ND	2.19	113.55	109.99
18	b	4013	BCR	C36-C18-C17	-2.19	119.27	122.82
14	l	1503	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
14	G	1124	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
18	b	4005	BCR	C28-C27-C26	-2.19	110.15	114.06
14	a	1118	CLA	OBD-CAD-C3D	-2.19	123.30	128.42
14	H	1205	CLA	CHB-C1B-C2B	-2.19	121.07	127.43
14	U	1503	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
14	G	1131	CLA	CMB-C2B-C1B	2.19	128.75	125.42
14	A	1104	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
14	a	1131	CLA	CMB-C2B-C1B	2.19	128.75	125.42
14	H	1218	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
14	A	1111	CLA	C3D-C4D-ND	2.19	113.54	109.99
21	A	6002	LMT	O5B-C5B-C6B	2.19	111.86	106.44
18	H	4009	BCR	C1-C6-C5	-2.19	119.65	122.64
18	a	4002	BCR	C35-C13-C12	2.19	121.43	118.09
14	b	1227	CLA	CAC-C3C-C4C	2.19	127.64	124.79
14	A	1119	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
14	a	1132	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
15	a	1121	F6C	CMC-C2C-C1C	2.19	128.75	125.42
15	B	1237	F6C	OMB-CMB-C2B	-2.19	120.69	125.62
14	b	1224	CLA	CAC-C3C-C4C	2.19	127.64	124.79
14	b	1218	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
14	A	1102	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
14	B	1221	CLA	CAA-CBA-CGA	-2.19	107.00	113.21
14	a	1123	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
14	a	1127	CLA	CMA-C3A-C4A	2.19	117.65	111.77
14	a	1126	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
14	b	1210	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
18	B	4005	BCR	C1-C6-C5	-2.19	119.65	122.64
14	b	1210	CLA	CMC-C2C-C1C	2.19	128.45	125.03
18	b	4012	BCR	C4-C5-C6	-2.19	119.75	122.70
14	b	1212	CLA	C4C-C3C-C2C	-2.19	103.71	106.89
14	H	1220	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
14	U	1503	CLA	CHC-C1C-C2C	-2.18	120.74	126.95
18	B	4005	BCR	C28-C27-C26	-2.18	110.16	114.06
14	G	1126	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
14	H	1239	CLA	C4-C3-C5	2.18	119.02	115.23
14	H	1211	CLA	C3C-C4C-NC	2.18	113.23	110.43
14	a	1125	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
14	A	1126	CLA	O2D-CGD-O1D	-2.18	119.60	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	1503	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
14	A	1117	CLA	CMC-C2C-C3C	2.18	132.05	126.15
16	a	2001	PQN	C12-C11-C3	-2.18	106.70	112.08
14	a	1102	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
14	b	1239	CLA	C4-C3-C5	2.18	119.02	115.23
14	G	1130	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
18	H	4005	BCR	C1-C6-C5	-2.18	119.66	122.64
14	G	1127	CLA	CMA-C3A-C4A	2.18	117.64	111.77
14	B	1210	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
18	G	4001	BCR	C38-C26-C25	-2.18	122.11	124.48
14	b	1232	CLA	C3D-C4D-ND	2.18	113.53	109.99
15	H	1237	F6C	OMB-CMB-C2B	-2.18	120.70	125.62
14	l	1503	CLA	C3C-C4C-NC	2.18	113.22	110.43
14	l	1503	CLA	C6-C5-C3	-2.18	108.16	113.47
15	H	1230	F6C	CAA-CBA-CGA	-2.18	107.89	113.67
14	G	1116	CLA	CMB-C2B-C1B	2.18	128.74	125.42
14	b	1220	CLA	C4D-C3D-CAD	2.18	110.47	108.11
18	a	4011	BCR	C8-C9-C10	2.18	122.44	119.01
14	B	1238	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
18	B	4004	BCR	C31-C1-C6	-2.18	106.83	110.24
14	b	1215	CLA	C4D-C3D-CAD	2.18	110.47	108.11
14	A	1128	CLA	C3D-C4D-ND	2.18	113.53	109.99
14	G	1118	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
14	B	1022	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
14	U	1503	CLA	C6-C5-C3	-2.18	108.17	113.47
14	G	1013	CLA	CAC-C3C-C4C	2.18	127.62	124.79
14	A	1118	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
14	H	1238	CLA	O2D-CGD-O1D	-2.18	119.61	123.85
18	H	4005	BCR	C28-C27-C26	-2.18	110.18	114.06
14	b	1022	CLA	CHA-C1A-NA	-2.17	121.47	126.39
14	L	1503	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
14	a	1115	CLA	CMB-C2B-C3B	2.17	131.66	126.55
14	B	1227	CLA	CAC-C3C-C4C	2.17	127.62	124.79
14	G	1102	CLA	CHB-C1B-C2B	-2.17	121.11	127.43
14	A	1126	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
14	A	1118	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
14	b	1211	CLA	C3C-C4C-NC	2.17	113.22	110.43
14	a	1119	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
20	R	5006	LMG	O8-C28-O10	-2.17	118.19	123.63
14	A	1132	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
14	L	1503	CLA	C6-C5-C3	-2.17	108.18	113.47
14	A	1110	CLA	CMD-C2D-C3D	-2.17	122.71	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1131	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
14	B	1226	CLA	C4-C3-C5	2.17	119.00	115.23
18	b	4009	BCR	C1-C6-C5	-2.17	119.67	122.64
14	a	1013	CLA	CAC-C3C-C4C	2.17	127.61	124.79
14	a	1131	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
14	A	1127	CLA	CMA-C3A-C4A	2.17	117.61	111.77
14	A	1126	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
14	A	1136	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
14	B	1225	CLA	C3D-C4D-ND	2.17	113.52	109.99
18	B	4012	BCR	C4-C5-C6	-2.17	119.77	122.70
14	G	1119	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
14	G	1131	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
14	H	1210	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
14	G	1132	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
14	A	1113	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
14	H	1205	CLA	C16-C15-C13	-2.17	108.75	115.97
14	G	1136	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
14	H	1225	CLA	C3D-C4D-ND	2.17	113.51	109.99
14	H	1210	CLA	CMC-C2C-C1C	2.17	128.42	125.03
14	l	1503	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
14	a	1113	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
14	G	1126	CLA	C4C-C3C-C2C	-2.17	103.74	106.89
18	H	4004	BCR	C31-C1-C6	-2.17	106.84	110.24
18	H	4014	BCR	C34-C9-C10	-2.17	119.31	122.82
16	A	2001	PQN	C12-C11-C3	-2.17	106.75	112.08
14	a	1113	CLA	C3D-C4D-ND	2.17	113.51	109.99
18	a	4003	BCR	C36-C18-C17	-2.17	119.31	122.82
20	I	5006	LMG	O8-C28-O10	-2.17	118.21	123.63
14	G	1113	CLA	C3D-C4D-ND	2.17	113.51	109.99
14	H	1203	CLA	C3D-C4D-ND	2.17	113.51	109.99
14	a	1130	CLA	CMD-C2D-C3D	-2.16	122.72	127.69
14	b	1228	CLA	CMD-C2D-C3D	-2.16	122.72	127.69
14	a	1101	CLA	CAC-C3C-C4C	2.16	127.61	124.79
14	B	1215	CLA	C3D-C4D-ND	2.16	113.50	109.99
14	H	1220	CLA	C4D-C3D-CAD	2.16	110.46	108.11
14	b	1222	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
14	a	1118	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
14	H	1227	CLA	CAC-C3C-C4C	2.16	127.60	124.79
14	B	1210	CLA	CMC-C2C-C1C	2.16	128.41	125.03
14	H	1202	CLA	CMC-C2C-C1C	2.16	128.41	125.03
14	b	1205	CLA	C16-C15-C13	-2.16	108.78	115.97
14	a	1117	CLA	CMC-C2C-C3C	2.16	132.00	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1237	F6C	OMB-CMB-C2B	-2.16	120.74	125.62
14	G	1101	CLA	CAC-C3C-C4C	2.16	127.60	124.79
14	G	1113	CLA	CHC-C1C-C2C	-2.16	120.80	126.95
18	a	4007	BCR	C35-C13-C12	2.16	121.39	118.09
18	G	4002	BCR	C30-C25-C26	-2.16	119.68	122.64
14	B	1215	CLA	C4D-C3D-CAD	2.16	110.45	108.11
14	a	1118	CLA	CMC-C2C-C1C	2.16	128.41	125.03
18	b	4012	BCR	C38-C26-C27	2.16	118.20	113.60
14	A	1123	CLA	CMB-C2B-C3B	2.16	131.63	126.55
14	A	1140	CLA	C4C-C3C-C2C	-2.16	103.75	106.89
18	B	4005	BCR	C36-C18-C17	-2.16	119.32	122.82
14	b	1213	CLA	C1-O2A-CGA	2.16	121.88	116.65
18	H	4012	BCR	C4-C5-C6	-2.16	119.79	122.70
14	G	1118	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
14	H	1216	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
14	B	1203	CLA	CHD-C4C-C3C	-2.16	121.63	124.77
14	B	1022	CLA	CHA-C1A-NA	-2.16	121.50	126.39
14	H	1214	CLA	C3D-C4D-ND	2.16	113.49	109.99
14	a	1128	CLA	C3D-C4D-ND	2.16	113.49	109.99
14	A	1130	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
18	B	4013	BCR	C36-C18-C17	-2.16	119.32	122.82
20	i	5006	LMG	O8-C28-O10	-2.16	118.23	123.63
14	a	1136	CLA	OBD-CAD-C3D	-2.16	123.37	128.42
14	B	1205	CLA	C16-C15-C13	-2.16	108.80	115.97
14	K	1401	CLA	CMC-C2C-C1C	2.16	128.40	125.03
14	B	1213	CLA	C1-O2A-CGA	2.16	121.87	116.65
14	A	1106	CLA	CHB-C4A-NA	2.16	127.51	124.40
14	a	1126	CLA	C4C-C3C-C2C	-2.16	103.75	106.89
14	A	1105	CLA	CMB-C2B-C3B	2.16	131.62	126.55
14	H	1213	CLA	C1-O2A-CGA	2.15	121.87	116.65
14	A	1128	CLA	C6-C5-C3	-2.15	108.22	113.47
18	B	4012	BCR	C36-C18-C17	-2.15	119.33	122.82
18	A	4001	BCR	C38-C26-C25	-2.15	122.13	124.48
14	B	1220	CLA	C4D-C3D-CAD	2.15	110.45	108.11
14	H	1212	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
14	B	1211	CLA	C3C-C4C-NC	2.15	113.19	110.43
18	b	4012	BCR	C36-C18-C17	-2.15	119.33	122.82
14	H	1012	CLA	CHA-C1A-NA	-2.15	121.52	126.39
14	G	1125	CLA	CHA-C4D-ND	2.15	136.99	132.55
18	A	4007	BCR	C35-C13-C12	2.15	121.38	118.09
14	H	1232	CLA	CHA-C1A-NA	-2.15	121.52	126.39
14	G	1128	CLA	C3D-C4D-ND	2.15	113.49	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1223	CLA	CMA-C3A-C4A	2.15	117.56	111.77
14	b	1202	CLA	CMC-C2C-C1C	2.15	128.40	125.03
14	A	1130	CLA	CHA-C4D-ND	2.15	136.99	132.55
14	b	1225	CLA	C3D-C4D-ND	2.15	113.48	109.99
18	A	4002	BCR	C30-C25-C26	-2.15	119.69	122.64
18	A	4003	BCR	C36-C18-C17	-2.15	119.33	122.82
14	G	1140	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
15	b	1230	F6C	CHC-C1C-C2C	-2.15	121.18	127.43
14	B	1224	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	a	1118	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
14	A	1125	CLA	CHA-C4D-ND	2.15	136.99	132.55
14	G	1111	CLA	C3D-C4D-ND	2.15	113.48	109.99
14	G	1122	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
14	T	1401	CLA	CMC-C2C-C1C	2.15	128.39	125.03
18	R	4018	BCR	C23-C22-C21	2.15	122.39	119.01
18	H	4009	BCR	C4-C5-C6	-2.15	119.80	122.70
14	G	1126	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
14	A	1113	CLA	C3D-C4D-ND	2.15	113.48	109.99
14	H	1202	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
14	A	1103	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	A	1119	CLA	C4-C3-C5	2.15	118.96	115.23
14	B	1222	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
14	b	1202	CLA	CHA-C1A-NA	-2.15	121.53	126.39
14	G	1103	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	G	1128	CLA	C6-C5-C3	-2.15	108.24	113.47
14	a	1125	CLA	CHA-C4D-ND	2.15	136.98	132.55
18	H	4012	BCR	C38-C26-C27	2.15	118.17	113.60
18	i	4018	BCR	C23-C24-C25	-2.15	121.26	127.00
14	H	1222	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
14	H	1236	CLA	C4B-CHC-C1C	2.15	131.29	126.25
14	B	1214	CLA	C3D-C4D-ND	2.15	113.48	109.99
14	G	1123	CLA	CMB-C2B-C3B	2.15	131.60	126.55
14	a	1126	CLA	CHB-C1B-C2B	-2.15	121.20	127.43
14	a	1103	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	H	1228	CLA	CMD-C2D-C3D	-2.15	122.77	127.69
18	I	4018	BCR	C23-C24-C25	-2.14	121.27	127.00
18	H	4009	BCR	C1-C6-C7	2.14	121.47	115.65
14	L	1503	CLA	C3C-C4C-NC	2.14	113.18	110.43
18	H	4005	BCR	C36-C18-C17	-2.14	119.34	122.82
14	a	1128	CLA	C6-C5-C3	-2.14	108.25	113.47
14	a	1130	CLA	CHA-C4D-ND	2.14	136.97	132.55
14	H	1223	CLA	CMA-C3A-C4A	2.14	117.53	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1105	CLA	CMB-C2B-C3B	2.14	131.59	126.55
14	b	1202	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
14	G	1126	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
18	G	4003	BCR	C38-C26-C27	2.14	118.16	113.60
14	G	1106	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	A	1119	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
14	G	1119	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
14	a	1122	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
14	B	1202	CLA	CMC-C2C-C1C	2.14	128.38	125.03
14	k	1401	CLA	CMC-C2C-C1C	2.14	128.38	125.03
14	b	1202	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
14	B	1223	CLA	CMA-C3A-C4A	2.14	117.53	111.77
14	B	1228	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
14	H	1219	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	G	1111	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
14	G	1114	CLA	CHA-C1A-NA	-2.14	121.55	126.39
18	B	4009	BCR	C1-C6-C7	2.14	121.45	115.65
14	B	1204	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
14	B	1216	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
14	a	1139	CLA	CMB-C2B-C1B	2.14	128.68	125.42
14	b	1203	CLA	CHD-C4C-C3C	-2.14	121.66	124.77
18	R	4018	BCR	C23-C24-C25	-2.14	121.28	127.00
14	a	1106	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	b	1219	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	B	1202	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
18	H	4004	BCR	C34-C9-C10	-2.14	119.35	122.82
14	H	1229	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	b	1220	CLA	CMB-C2B-C3B	2.14	131.58	126.55
14	b	1204	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
14	G	1119	CLA	C4-C3-C5	2.14	118.94	115.23
18	b	4009	BCR	C1-C6-C7	2.14	121.45	115.65
16	G	2001	PQN	C12-C11-C3	-2.14	106.82	112.08
14	G	1129	CLA	CAC-C3C-C4C	2.14	127.57	124.79
14	a	1123	CLA	CMB-C2B-C3B	2.14	131.58	126.55
14	a	1132	CLA	C4-C3-C5	2.14	118.94	115.23
14	b	1216	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
14	H	1202	CLA	CHC-C1C-C2C	-2.14	120.88	126.95
14	H	1204	CLA	O1D-CGD-CBD	-2.14	120.31	124.52
18	a	4003	BCR	C38-C26-C27	2.14	118.15	113.60
14	G	1128	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
14	B	1203	CLA	C3D-C4D-ND	2.14	113.46	109.99
14	G	1105	CLA	CMB-C2B-C3B	2.14	131.57	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1139	CLA	CMB-C2B-C1B	2.14	128.67	125.42
14	a	1112	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
14	B	1206	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
14	b	1232	CLA	CHA-C1A-NA	-2.13	121.56	126.39
18	b	4009	BCR	C4-C5-C6	-2.13	119.82	122.70
14	a	1119	CLA	CHC-C1C-C2C	-2.13	120.88	126.95
14	b	1236	CLA	C4B-CHC-C1C	2.13	131.26	126.25
14	A	1102	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
18	b	4014	BCR	C34-C9-C10	-2.13	119.36	122.82
14	a	1102	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
14	G	1108	CLA	O2D-CGD-O1D	-2.13	119.70	123.85
14	B	1202	CLA	CHA-C1A-NA	-2.13	121.56	126.39
14	B	1222	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
18	B	4012	BCR	C38-C26-C27	2.13	118.14	113.60
14	B	1202	CLA	CHC-C1C-C2C	-2.13	120.89	126.95
14	A	1122	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
18	b	4010	BCR	C35-C13-C12	2.13	121.34	118.09
14	L	1501	CLA	CMA-C3A-C4A	2.13	117.50	111.77
14	l	1501	CLA	CMA-C3A-C4A	2.13	117.50	111.77
18	A	4003	BCR	C38-C26-C27	2.13	118.14	113.60
14	A	1125	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
14	a	1130	CLA	CMC-C2C-C1C	2.13	128.36	125.03
14	H	1203	CLA	CHD-C4C-C3C	-2.13	121.67	124.77
14	A	1126	CLA	CHB-C1B-C2B	-2.13	121.24	127.43
14	b	1203	CLA	C3D-C4D-ND	2.13	113.45	109.99
14	H	1228	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
14	a	1140	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
18	b	4004	BCR	C31-C1-C6	-2.13	106.90	110.24
14	G	1133	CLA	CHC-C1C-C2C	-2.13	120.90	126.95
14	A	1111	CLA	C4C-C3C-C2C	-2.13	103.79	106.89
14	G	1138	CLA	C3C-C4C-NC	2.13	113.16	110.43
18	I	4018	BCR	C23-C22-C21	2.13	122.36	119.01
13	a	1011	CL0	C4C-C3C-C2C	-2.13	104.97	113.37
18	B	4010	BCR	C35-C13-C12	2.13	121.34	118.09
14	H	1220	CLA	CMB-C2B-C3B	2.13	131.55	126.55
14	B	1219	CLA	CHB-C4A-NA	2.13	127.47	124.40
18	i	4018	BCR	C23-C22-C21	2.13	122.36	119.01
14	G	1140	CLA	C1-C2-C3	-2.13	122.71	126.20
14	G	1125	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
14	A	1128	CLA	C4C-C3C-C2C	-2.13	103.80	106.89
14	b	1206	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
14	b	1215	CLA	O1D-CGD-CBD	-2.13	120.33	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	U	1501	CLA	CMA-C3A-C4A	2.13	117.48	111.77
14	H	1206	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
14	U	1503	CLA	C3C-C4C-NC	2.12	113.15	110.43
14	G	1102	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
18	G	4007	BCR	C30-C25-C24	2.12	121.41	115.65
14	a	1133	CLA	CHC-C1C-C2C	-2.12	120.91	126.95
18	B	4013	BCR	C29-C30-C25	2.12	113.52	110.44
13	A	1011	CL0	C4C-C3C-C2C	-2.12	104.98	113.37
14	A	1102	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
14	G	1130	CLA	CHA-C4D-ND	2.12	136.93	132.55
14	B	1236	CLA	C4B-CHC-C1C	2.12	131.24	126.25
14	a	1114	CLA	CHA-C1A-NA	-2.12	121.58	126.39
14	G	1130	CLA	CMC-C2C-C1C	2.12	128.35	125.03
14	L	1503	CLA	C1-O2A-CGA	2.12	121.79	116.65
18	B	4004	BCR	C34-C9-C10	-2.12	119.38	122.82
18	H	4012	BCR	C36-C18-C17	-2.12	119.38	122.82
14	G	1112	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
18	b	4004	BCR	C34-C9-C10	-2.12	119.38	122.82
14	A	1133	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	A	1130	CLA	CMC-C2C-C1C	2.12	128.35	125.03
14	G	1132	CLA	C4-C3-C5	2.12	118.91	115.23
14	B	1232	CLA	CHA-C1A-NA	-2.12	121.59	126.39
14	A	1124	CLA	CMA-C3A-C4A	2.12	117.47	111.77
13	G	1011	CL0	C4C-C3C-C2C	-2.12	105.00	113.37
14	A	1133	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
14	H	1222	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
15	H	1230	F6C	CHC-C1C-C2C	-2.12	121.27	127.43
14	b	1206	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	G	1133	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	B	1220	CLA	CMB-C2B-C3B	2.12	131.53	126.55
14	H	1202	CLA	CHA-C1A-NA	-2.12	121.60	126.39
21	a	6002	LMT	O1B-C4'-C5'	-2.12	103.92	109.48
14	a	1132	CLA	C4D-C3D-CAD	2.12	110.41	108.11
14	b	1226	CLA	C3D-C4D-ND	2.12	113.43	109.99
14	a	1128	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
14	a	1111	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
14	A	1128	CLA	C4-C3-C5	2.11	118.90	115.23
14	H	1207	CLA	C3C-C4C-NC	2.11	113.14	110.43
14	G	1124	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	A	1114	CLA	CHA-C1A-NA	-2.11	121.61	126.39
18	a	4001	BCR	C15-C14-C13	-2.11	124.31	127.28
14	a	1119	CLA	C4-C3-C5	2.11	118.89	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1138	CLA	C3C-C4C-NC	2.11	113.14	110.43
21	A	6002	LMT	O1B-C4'-C5'	-2.11	103.94	109.48
14	a	1124	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	B	1217	CLA	CBA-CAA-C2A	2.11	120.07	113.79
14	b	1228	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
18	A	4007	BCR	C30-C25-C24	2.11	121.38	115.65
21	a	6001	LMT	O1'-C1'-C2'	2.11	111.48	108.27
14	b	1217	CLA	CBA-CAA-C2A	2.11	120.07	113.79
18	H	4005	BCR	C33-C5-C4	2.11	118.09	113.60
14	B	1223	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
14	B	1206	CLA	CMA-C3A-C4A	2.11	117.44	111.77
14	B	1228	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
14	a	1128	CLA	C4-C3-C5	2.11	118.89	115.23
14	H	1217	CLA	CBA-CAA-C2A	2.11	120.07	113.79
18	b	4005	BCR	C33-C5-C4	2.11	118.09	113.60
14	A	1128	CLA	CMC-C2C-C3C	2.11	131.85	126.15
14	a	1129	CLA	CAC-C3C-C4C	2.11	127.53	124.79
14	x	1701	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
18	B	4014	BCR	C34-C9-C10	-2.11	119.40	122.82
18	b	4013	BCR	C29-C30-C25	2.11	113.50	110.44
18	a	4007	BCR	C30-C25-C24	2.11	121.36	115.65
14	b	1207	CLA	C3C-C4C-NC	2.11	113.13	110.43
14	U	1503	CLA	C1-O2A-CGA	2.11	121.75	116.65
14	U	1503	CLA	C11-C10-C8	-2.11	108.96	115.97
18	A	4011	BCR	C31-C1-C6	-2.11	106.94	110.24
18	B	4009	BCR	C4-C5-C6	-2.11	119.86	122.70
14	A	1112	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
14	b	1021	CLA	CMB-C2B-C3B	2.11	131.50	126.55
14	G	1136	CLA	C1-C2-C3	-2.11	122.75	126.20
14	l	1503	CLA	C1-O2A-CGA	2.10	121.75	116.65
14	H	1215	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
14	H	1226	CLA	C3D-C4D-ND	2.10	113.41	109.99
14	A	1111	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
14	a	1133	CLA	CMA-C3A-C4A	2.10	117.42	111.77
18	A	4001	BCR	C15-C14-C13	-2.10	124.33	127.28
14	a	1102	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
21	G	6002	LMT	O1B-C4'-C5'	-2.10	103.96	109.48
14	a	1128	CLA	CMC-C2C-C3C	2.10	131.83	126.15
14	A	1129	CLA	CMB-C2B-C3B	2.10	131.49	126.55
14	H	1221	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	A	1132	CLA	C4-C3-C5	2.10	118.87	115.23
18	H	4013	BCR	C29-C30-C25	2.10	113.49	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1225	CLA	CHD-C1D-ND	-2.10	121.85	124.80
18	b	4014	BCR	C39-C30-C25	-2.10	106.95	110.24
14	b	1222	CLA	C4C-C3C-C2C	-2.10	103.84	106.89
14	b	1204	CLA	CBB-CAB-C3B	-2.10	117.04	127.53
14	a	1104	CLA	C4-C3-C5	2.10	118.87	115.23
14	G	1111	CLA	CMB-C2B-C3B	2.10	131.49	126.55
18	H	4010	BCR	C35-C13-C12	2.10	121.29	118.09
14	A	1139	CLA	CMB-C2B-C1B	2.10	128.61	125.42
18	b	4014	BCR	C12-C13-C14	-2.10	115.71	119.01
14	H	1238	CLA	CAA-CBA-CGA	-2.10	107.25	113.21
14	B	1021	CLA	CMB-C2B-C3B	2.10	131.48	126.55
14	l	1503	CLA	C11-C10-C8	-2.10	109.00	115.97
14	b	1204	CLA	OBD-CAD-C3D	-2.10	123.52	128.42
14	G	1136	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
14	b	1202	CLA	C1-C2-C3	-2.10	122.76	126.20
14	B	1215	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
14	B	1225	CLA	CHD-C1D-ND	-2.10	121.85	124.80
14	X	1701	CLA	C4C-C3C-C2C	-2.10	103.84	106.89
14	G	1109	CLA	CHC-C1C-C2C	-2.10	120.99	126.95
14	G	1131	CLA	C3D-C4D-ND	2.09	113.39	109.99
14	b	1221	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	a	1125	CLA	C1D-CHD-C4C	-2.09	121.57	126.02
14	H	1234	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
18	B	4005	BCR	C33-C5-C4	2.09	118.06	113.60
14	L	1503	CLA	C11-C10-C8	-2.09	109.00	115.97
14	b	1238	CLA	CAA-CBA-CGA	-2.09	107.26	113.21
14	b	1215	CLA	C11-C10-C8	-2.09	109.01	115.97
14	B	1229	CLA	C3C-C4C-NC	2.09	113.11	110.43
18	G	4001	BCR	C15-C14-C13	-2.09	124.34	127.28
14	B	1221	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	H	1021	CLA	CMB-C2B-C3B	2.09	131.47	126.55
14	U	1502	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
15	a	1121	F6C	CMD-C2D-C3D	-2.09	122.89	127.69
14	B	1238	CLA	CAA-CBA-CGA	-2.09	107.27	113.21
14	H	1204	CLA	CBB-CAB-C3B	-2.09	117.07	127.53
14	k	1401	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
14	G	1128	CLA	CMC-C2C-C3C	2.09	131.81	126.15
14	B	1204	CLA	CBB-CAB-C3B	-2.09	117.07	127.53
14	B	1215	CLA	CMC-C2C-C3C	2.09	131.81	126.15
18	a	4002	BCR	C30-C25-C26	-2.09	119.78	122.64
14	B	1215	CLA	C11-C10-C8	-2.09	109.01	115.97
14	G	1102	CLA	O1D-CGD-CBD	-2.09	120.39	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1222	CLA	CAC-C3C-C4C	2.09	127.51	124.79
14	A	1110	CLA	C3D-C4D-ND	2.09	113.39	109.99
14	A	1140	CLA	C1-C2-C3	-2.09	122.77	126.20
14	H	1215	CLA	C11-C10-C8	-2.09	109.02	115.97
18	H	4014	BCR	C12-C13-C14	-2.09	115.72	119.01
15	B	1230	F6C	CHC-C1C-C2C	-2.09	121.36	127.43
14	A	1108	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
15	b	1230	F6C	CAC-C3C-C4C	2.09	127.79	124.91
14	A	1129	CLA	CAC-C3C-C4C	2.09	127.51	124.79
14	H	1202	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
18	B	4012	BCR	C23-C22-C21	2.09	122.30	119.01
18	G	4011	BCR	C31-C1-C6	-2.09	106.97	110.24
14	a	1114	CLA	CMC-C2C-C3C	2.09	131.80	126.15
14	A	1104	CLA	C4-C3-C5	2.09	118.85	115.23
14	A	1136	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
14	B	1216	CLA	C3C-C4C-NC	2.09	113.11	110.43
14	H	1206	CLA	CMA-C3A-C4A	2.09	117.38	111.77
14	B	1234	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
19	a	5001	LHG	O7-C7-O9	-2.09	118.83	123.70
14	B	1207	CLA	C3C-C4C-NC	2.09	113.10	110.43
14	a	1136	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
18	H	4010	BCR	C28-C27-C26	-2.09	110.33	114.06
14	l	1502	CLA	CBC-CAC-C3C	-2.09	106.76	112.42
14	G	1013	CLA	C4D-C3D-CAD	2.09	110.37	108.11
15	H	1237	F6C	CED-O2D-CGD	2.09	120.65	115.92
18	B	4014	BCR	C12-C13-C14	-2.09	115.73	119.01
14	A	1109	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
14	A	1131	CLA	C3D-C4D-ND	2.09	113.38	109.99
14	H	1225	CLA	CHD-C1D-ND	-2.09	121.87	124.80
14	a	1136	CLA	CHB-C1B-C2B	-2.08	121.37	127.43
15	B	1237	F6C	CHC-C1C-C2C	-2.08	121.37	127.43
14	G	1104	CLA	C4-C3-C5	2.08	118.85	115.23
14	B	1206	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
14	a	1136	CLA	C1-C2-C3	-2.08	122.78	126.20
15	G	1121	F6C	CMD-C2D-C3D	-2.08	122.91	127.69
14	B	1211	CLA	C1-O2A-CGA	2.08	121.70	116.65
14	H	1215	CLA	CMC-C2C-C3C	2.08	131.79	126.15
14	a	1138	CLA	C3C-C4C-NC	2.08	113.10	110.43
14	a	1108	CLA	O2D-CGD-O1D	-2.08	119.79	123.85
14	A	1140	CLA	CMB-C2B-C1B	2.08	128.59	125.42
14	G	1101	CLA	CMD-C2D-C3D	-2.08	122.91	127.69
14	B	1221	CLA	CGD-CBD-CAD	-2.08	104.10	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1229	CLA	C3C-C4C-NC	2.08	113.10	110.43
14	G	1125	CLA	C1D-CHD-C4C	-2.08	121.59	126.02
18	b	4010	BCR	C28-C27-C26	-2.08	110.34	114.06
14	T	1401	CLA	CHC-C1C-C2C	-2.08	121.03	126.95
14	a	1114	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
14	A	1136	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
14	b	1215	CLA	CMC-C2C-C3C	2.08	131.78	126.15
14	B	1202	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
14	B	1202	CLA	C1-C2-C3	-2.08	122.79	126.20
14	b	1214	CLA	CHA-C1A-NA	-2.08	121.68	126.39
14	L	1502	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
14	G	1117	CLA	C4D-C3D-CAD	2.08	110.36	108.11
14	B	1216	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
14	B	1226	CLA	C3D-C4D-ND	2.08	113.37	109.99
19	A	5001	LHG	O7-C7-O9	-2.08	118.84	123.70
14	H	1216	CLA	C3C-C4C-NC	2.08	113.09	110.43
18	a	4003	BCR	C33-C5-C4	2.08	118.03	113.60
14	a	1130	CLA	CHA-C1A-NA	-2.08	121.68	126.39
14	b	1202	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
14	a	1109	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
14	A	1112	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
14	a	1112	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
14	G	1132	CLA	C4D-C3D-CAD	2.08	110.36	108.11
14	G	1136	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
14	H	1223	CLA	C4C-C3C-C2C	-2.08	103.87	106.89
14	A	1125	CLA	C1D-CHD-C4C	-2.08	121.60	126.02
14	a	1129	CLA	CMB-C2B-C3B	2.08	131.44	126.55
14	B	1214	CLA	CHA-C1A-NA	-2.08	121.69	126.39
14	G	1129	CLA	CMB-C2B-C3B	2.08	131.44	126.55
18	A	4003	BCR	C33-C5-C4	2.08	118.02	113.60
14	b	1211	CLA	CHB-C4A-NA	2.08	127.40	124.40
14	b	1211	CLA	C1-O2A-CGA	2.08	121.68	116.65
14	G	1103	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
14	H	1202	CLA	C1-C2-C3	-2.08	122.80	126.20
14	A	1103	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
14	a	1111	CLA	CMB-C2B-C3B	2.08	131.43	126.55
18	l	4022	BCR	C1-C6-C7	2.08	121.28	115.65
14	H	1211	CLA	C1-O2A-CGA	2.08	121.67	116.65
14	a	1140	CLA	C1-C2-C3	-2.08	122.80	126.20
14	G	1114	CLA	CMC-C2C-C3C	2.07	131.76	126.15
15	b	1237	F6C	CED-O2D-CGD	2.07	120.62	115.92
18	G	4003	BCR	C33-C5-C4	2.07	118.02	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	U	4022	BCR	C1-C6-C7	2.07	121.28	115.65
14	H	1214	CLA	CHA-C1A-NA	-2.07	121.69	126.39
14	A	1136	CLA	C1-C2-C3	-2.07	122.80	126.20
14	b	1223	CLA	C4C-C3C-C2C	-2.07	103.87	106.89
18	H	4014	BCR	C39-C30-C25	-2.07	106.99	110.24
14	a	1131	CLA	C3D-C4D-ND	2.07	113.36	109.99
14	G	1128	CLA	C4-C3-C5	2.07	118.83	115.23
14	H	1206	CLA	C4B-C3B-C2B	-2.07	104.72	107.30
14	b	1221	CLA	C4C-C3C-C2C	-2.07	103.87	106.89
14	A	1111	CLA	CMB-C2B-C3B	2.07	131.43	126.55
14	B	1204	CLA	OBD-CAD-C3D	-2.07	123.57	128.42
14	A	1101	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
18	H	4012	BCR	C23-C22-C21	2.07	122.27	119.01
14	A	1124	CLA	C4-C3-C5	2.07	118.83	115.23
14	G	1111	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
14	G	1114	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
18	B	4010	BCR	C28-C27-C26	-2.07	110.36	114.06
14	K	1401	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
14	a	1137	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
14	B	1228	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
15	H	1237	F6C	CHC-C1C-C2C	-2.07	121.42	127.43
14	A	1114	CLA	CMC-C2C-C3C	2.07	131.75	126.15
15	A	1121	F6C	CMD-C2D-C3D	-2.07	122.94	127.69
14	W	1701	CLA	C4C-C3C-C2C	-2.07	103.88	106.89
19	G	5001	LHG	O7-C7-O9	-2.07	118.86	123.70
14	G	1123	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	B	1215	CLA	CHA-C4D-ND	2.07	136.82	132.55
14	H	1215	CLA	CHA-C4D-ND	2.07	136.82	132.55
15	B	1237	F6C	CED-O2D-CGD	2.07	120.61	115.92
14	A	1137	CLA	CHC-C1C-C2C	-2.07	121.07	126.95
14	H	1221	CLA	CGD-CBD-CAD	-2.07	104.15	110.85
14	b	1206	CLA	C4B-C3B-C2B	-2.07	104.73	107.30
14	G	1102	CLA	C1-O2A-CGA	2.07	121.66	116.65
14	a	1111	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
14	a	1136	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
14	G	1130	CLA	C4D-C3D-CAD	2.07	110.35	108.11
14	B	1211	CLA	CHB-C4A-NA	2.07	127.38	124.40
14	b	1234	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
14	G	1110	CLA	C3D-C4D-ND	2.07	113.35	109.99
14	b	1239	CLA	C4C-C3C-C2C	-2.07	103.88	106.89
14	b	1216	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
14	b	1221	CLA	CGD-CBD-CAD	-2.07	104.16	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1237	F6C	CHC-C1C-C2C	-2.07	121.43	127.43
14	G	1130	CLA	CHA-C1A-NA	-2.07	121.71	126.39
14	G	1129	CLA	CMA-C3A-C4A	2.07	117.33	111.77
21	A	6002	LMT	C2'-C3'-C4'	2.07	114.37	109.68
14	G	1137	CLA	CHC-C1C-C2C	-2.07	121.08	126.95
14	a	1140	CLA	CMB-C2B-C1B	2.07	128.56	125.42
14	a	1101	CLA	CMD-C2D-C3D	-2.06	122.95	127.69
14	B	1222	CLA	CAC-C3C-C4C	2.06	127.48	124.79
18	H	4004	BCR	C33-C5-C4	2.06	118.00	113.60
14	A	1129	CLA	CMA-C3A-C4A	2.06	117.32	111.77
14	b	1233	CLA	CHC-C1C-C2C	-2.06	121.08	126.95
18	a	4011	BCR	C31-C1-C6	-2.06	107.01	110.24
14	a	1129	CLA	CMA-C3A-C4A	2.06	117.32	111.77
14	H	1228	CLA	CHB-C1B-C2B	-2.06	121.44	127.43
14	G	1136	CLA	C1-O2A-CGA	2.06	121.64	116.65
14	G	1012	CLA	CHA-C4D-ND	2.06	136.80	132.55
14	B	1210	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
14	B	1239	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
14	a	1103	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
18	L	4022	BCR	C1-C6-C7	2.06	121.24	115.65
14	H	1204	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
14	A	1130	CLA	CHA-C1A-NA	-2.06	121.72	126.39
18	G	4007	BCR	C8-C7-C6	-2.06	121.49	127.00
18	R	4018	BCR	C27-C26-C25	-2.06	119.92	122.70
14	A	1136	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
21	a	6002	LMT	C2'-C3'-C4'	2.06	114.35	109.68
18	A	4007	BCR	C8-C7-C6	-2.06	121.50	127.00
14	A	1136	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
14	b	1232	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
14	A	1136	CLA	C1-O2A-CGA	2.06	121.63	116.65
14	a	1012	CLA	CHA-C4D-ND	2.06	136.79	132.55
18	B	4004	BCR	C33-C5-C4	2.06	117.98	113.60
21	A	6001	LMT	O1'-C1'-C2'	2.06	111.40	108.27
14	a	1110	CLA	C3D-C4D-ND	2.06	113.33	109.99
14	B	1215	CLA	CHB-C1B-C2B	-2.06	121.46	127.43
14	H	1216	CLA	O2D-CGD-O1D	-2.06	119.85	123.85
14	G	1112	CLA	CHC-C1C-C2C	-2.06	121.11	126.95
14	H	1227	CLA	CHC-C1C-C2C	-2.06	121.11	126.95
18	b	4004	BCR	C33-C5-C4	2.06	117.98	113.60
21	G	6001	LMT	O1'-C1'-C2'	2.05	111.39	108.27
14	A	1114	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
14	b	1215	CLA	CMD-C2D-C3D	-2.05	122.98	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1135	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
14	b	1227	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
14	A	1123	CLA	CHA-C1A-NA	-2.05	121.74	126.39
14	H	1215	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
14	B	1227	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
14	B	1233	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
14	b	1210	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
14	H	1214	CLA	C11-C10-C8	-2.05	109.14	115.97
14	a	1135	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
14	B	1215	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
14	b	1215	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
14	b	1216	CLA	C3C-C4C-NC	2.05	113.06	110.43
14	a	1123	CLA	CHA-C1A-NA	-2.05	121.75	126.39
14	G	1136	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
14	A	1109	CLA	CAC-C3C-C4C	2.05	127.46	124.79
14	B	1214	CLA	C11-C10-C8	-2.05	109.15	115.97
14	b	1236	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
18	b	4012	BCR	C23-C22-C21	2.05	122.23	119.01
14	G	1135	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
18	B	4014	BCR	C39-C30-C25	-2.05	107.03	110.24
14	B	1202	CLA	CAC-C3C-C4C	2.05	127.46	124.79
14	A	1013	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	a	1013	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	a	1117	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	b	1228	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
14	l	1503	CLA	C11-C12-C13	-2.05	109.15	115.97
14	a	1136	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
14	G	1109	CLA	CAC-C3C-C4C	2.05	127.46	124.79
14	b	1214	CLA	C11-C10-C8	-2.05	109.15	115.97
18	U	4019	BCR	C35-C13-C12	2.05	121.22	118.09
14	b	1023	CLA	CMA-C3A-C4A	2.05	117.28	111.77
14	G	1117	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
14	B	1221	CLA	CMB-C2B-C3B	2.05	131.37	126.55
14	B	1232	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
14	A	1117	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
14	b	1222	CLA	CAC-C3C-C4C	2.05	127.45	124.79
18	B	4016	BCR	C34-C9-C10	-2.05	119.50	122.82
14	B	1216	CLA	C4D-C3D-CAD	2.05	110.33	108.11
15	b	1237	F6C	O1D-CGD-CBD	-2.05	120.48	124.52
14	A	1102	CLA	C1-O2A-CGA	2.05	121.60	116.65
14	H	1233	CLA	CHC-C1C-C2C	-2.05	121.14	126.95
14	W	1701	CLA	CMD-C2D-C3D	-2.05	123.00	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1203	CLA	CHA-C4D-ND	2.04	136.77	132.55
19	a	5001	LHG	O8-C23-O10	-2.04	118.51	123.63
18	a	4007	BCR	C8-C7-C6	-2.04	121.54	127.00
14	H	1221	CLA	CMB-C2B-C3B	2.04	131.36	126.55
14	A	1132	CLA	C4D-C3D-CAD	2.04	110.33	108.11
14	H	1215	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
14	B	1222	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
14	b	1221	CLA	CMB-C2B-C3B	2.04	131.36	126.55
14	A	1130	CLA	C4D-C3D-CAD	2.04	110.33	108.11
18	H	4016	BCR	C34-C9-C10	-2.04	119.51	122.82
14	L	1503	CLA	C11-C12-C13	-2.04	109.17	115.97
14	B	1228	CLA	CMC-C2C-C3C	2.04	131.67	126.15
14	a	1102	CLA	C1-O2A-CGA	2.04	121.59	116.65
21	G	6002	LMT	C2'-C3'-C4'	2.04	114.32	109.68
14	H	1204	CLA	CMD-C2D-C3D	-2.04	123.00	127.69
14	b	1202	CLA	CAC-C3C-C4C	2.04	127.45	124.79
14	b	1204	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
14	a	1136	CLA	C1-O2A-CGA	2.04	121.59	116.65
14	A	1117	CLA	C4D-C3D-CAD	2.04	110.32	108.11
14	H	1210	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
14	b	1215	CLA	CHA-C4D-ND	2.04	136.76	132.55
14	H	1232	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
14	G	1140	CLA	CMB-C2B-C1B	2.04	128.52	125.42
14	A	1012	CLA	CHA-C4D-ND	2.04	136.76	132.55
19	A	5001	LHG	O8-C23-O10	-2.04	118.53	123.63
14	H	1211	CLA	CHB-C4A-NA	2.04	127.34	124.40
14	G	1135	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
15	B	1237	F6C	O1D-CGD-CBD	-2.04	120.50	124.52
14	U	1503	CLA	C11-C12-C13	-2.04	109.19	115.97
14	a	1117	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
14	b	1228	CLA	C3C-C4C-NC	2.04	113.04	110.43
14	A	1123	CLA	CAC-C3C-C4C	2.04	127.44	124.79
14	B	1221	CLA	C4C-C3C-C2C	-2.04	103.93	106.89
14	B	1206	CLA	C4C-C3C-C2C	-2.04	103.93	106.89
14	B	1023	CLA	CMA-C3A-C4A	2.04	117.25	111.77
14	B	1228	CLA	C3C-C4C-NC	2.04	113.04	110.43
14	G	1140	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
18	b	4016	BCR	C34-C9-C10	-2.04	119.52	122.82
14	G	1124	CLA	C4-C3-C5	2.03	118.76	115.23
14	a	1124	CLA	C4-C3-C5	2.03	118.76	115.23
14	H	1239	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
19	G	5001	LHG	O8-C23-O10	-2.03	118.54	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1203	CLA	CHA-C4D-ND	2.03	136.75	132.55
14	b	1228	CLA	CMC-C2C-C3C	2.03	131.65	126.15
14	b	1222	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
14	B	1205	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
14	B	1204	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
14	b	1209	CLA	CAC-C3C-C4C	2.03	127.44	124.79
14	A	1129	CLA	OBD-CAD-C3D	-2.03	123.66	128.42
14	b	1203	CLA	CHA-C4D-ND	2.03	136.74	132.55
14	G	1012	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
14	H	1228	CLA	CMC-C2C-C3C	2.03	131.65	126.15
14	A	1140	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
14	G	1136	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
18	l	4019	BCR	C35-C13-C12	2.03	121.19	118.09
14	G	1101	CLA	C4C-C3C-C2C	-2.03	103.93	106.89
14	B	1236	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
14	X	1701	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
14	B	1209	CLA	CAC-C3C-C4C	2.03	127.43	124.79
18	G	4002	BCR	C23-C24-C25	-2.03	121.57	127.00
14	G	1130	CLA	C3D-C4D-ND	2.03	113.29	109.99
14	H	1209	CLA	CAC-C3C-C4C	2.03	127.43	124.79
18	L	4019	BCR	C35-C13-C12	2.03	121.19	118.09
14	H	1221	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
14	a	1012	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
14	x	1701	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
18	I	4018	BCR	C27-C26-C25	-2.03	119.96	122.70
18	B	4014	BCR	C1-C6-C5	-2.03	119.86	122.64
14	a	1106	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
14	H	1216	CLA	C4D-C3D-CAD	2.03	110.31	108.11
18	G	4003	BCR	C37-C22-C21	-2.03	119.53	122.82
14	H	1202	CLA	CAC-C3C-C4C	2.03	127.43	124.79
14	b	1205	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
14	G	1137	CLA	CMB-C2B-C1B	2.03	128.50	125.42
14	H	1229	CLA	CHB-C1B-C2B	-2.03	121.55	127.43
14	H	1023	CLA	CMA-C3A-C4A	2.03	117.22	111.77
15	H	1237	F6C	O1D-CGD-CBD	-2.02	120.52	124.52
14	a	1103	CLA	C4D-C3D-CAD	2.02	110.31	108.11
18	i	4018	BCR	C27-C26-C25	-2.02	119.97	122.70
14	a	1102	CLA	C4D-C3D-CAD	2.02	110.30	108.11
14	B	1214	CLA	CHA-C4D-ND	2.02	136.72	132.55
14	A	1012	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
14	H	1214	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
14	a	1101	CLA	C4C-C3C-C2C	-2.02	103.95	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	4008	BCR	C37-C22-C21	-2.02	119.54	122.82
14	b	1214	CLA	CAA-CBA-CGA	-2.02	107.47	113.21
15	B	1230	F6C	CAC-C3C-C4C	2.02	127.69	124.91
18	a	4008	BCR	C37-C22-C21	-2.02	119.54	122.82
14	G	1123	CLA	CAC-C3C-C4C	2.02	127.42	124.79
14	G	1132	CLA	CMC-C2C-C1C	2.02	128.19	125.03
14	H	1224	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
14	A	1106	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
14	l	1503	CLA	CAC-C3C-C4C	2.02	127.42	124.79
14	a	1132	CLA	CMC-C2C-C1C	2.02	128.19	125.03
18	B	4006	BCR	C8-C7-C6	2.02	132.39	127.00
14	A	1101	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
14	H	1206	CLA	C4D-C3D-CAD	2.02	110.30	108.11
14	b	1206	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
18	b	4004	BCR	C4-C5-C6	-2.02	119.98	122.70
13	a	1011	CL0	C1-C2-C3	-2.02	122.89	126.20
14	a	1140	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
14	a	1122	CLA	CMC-C2C-C1C	2.02	128.19	125.03
14	b	1234	CLA	CHA-C1A-NA	-2.02	121.82	126.39
18	b	4006	BCR	C8-C7-C6	2.02	132.39	127.00
14	H	1222	CLA	CHB-C1B-C2B	-2.02	121.57	127.43
14	H	1214	CLA	CHA-C4D-ND	2.02	136.71	132.55
18	B	4004	BCR	C4-C5-C6	-2.02	119.98	122.70
14	b	1202	CLA	CHB-C4A-NA	2.02	127.31	124.40
14	H	1228	CLA	C3C-C4C-NC	2.02	113.01	110.43
14	a	1137	CLA	CMB-C2B-C1B	2.02	128.49	125.42
14	H	1205	CLA	C4C-C3C-C2C	-2.02	103.96	106.89
18	A	4008	BCR	C37-C22-C21	-2.02	119.55	122.82
14	a	1135	CLA	CGD-CBD-CAD	-2.02	104.32	110.85
14	A	1137	CLA	CMB-C2B-C1B	2.02	128.49	125.42
14	G	1135	CLA	CGD-CBD-CAD	-2.02	104.32	110.85
18	H	4005	BCR	C31-C1-C6	-2.02	107.08	110.24
18	a	4003	BCR	C37-C22-C21	-2.01	119.55	122.82
14	A	1103	CLA	C4D-C3D-CAD	2.01	110.29	108.11
14	b	1214	CLA	CHA-C4D-ND	2.01	136.71	132.55
14	a	1129	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
15	A	1120	F6C	OBD-CAD-C3D	-2.01	123.71	128.42
14	H	1236	CLA	CMD-C2D-C3D	-2.01	123.07	127.69
14	A	1135	CLA	CHC-C1C-C2C	-2.01	121.22	126.95
14	G	1106	CLA	C4C-C3C-C2C	-2.01	103.96	106.89
14	B	1214	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
14	H	1207	CLA	CHC-C1C-C2C	-2.01	121.23	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1129	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
14	a	1135	CLA	C5-C3-C4	2.01	119.22	114.59
18	b	4014	BCR	C1-C6-C5	-2.01	119.89	122.64
18	A	4003	BCR	C37-C22-C21	-2.01	119.56	122.82
14	G	1103	CLA	C4D-C3D-CAD	2.01	110.29	108.11
14	H	1023	CLA	C4D-C3D-CAD	2.01	110.29	108.11
14	A	1128	CLA	CAC-C3C-C4C	2.01	127.41	124.79
14	G	1118	CLA	C3C-C4C-NC	2.01	113.01	110.43
14	B	1022	CLA	CHD-C4C-C3C	-2.01	121.84	124.77
14	G	1124	CLA	CMC-C2C-C1C	2.01	128.18	125.03
14	a	1123	CLA	CAC-C3C-C4C	2.01	127.41	124.79
14	b	1229	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
14	A	1124	CLA	CMC-C2C-C1C	2.01	128.18	125.03
14	l	1501	CLA	CHA-C1A-NA	-2.01	121.84	126.39
14	H	1206	CLA	C4C-C3C-C2C	-2.01	103.97	106.89
18	b	4004	BCR	C23-C22-C21	2.01	122.17	119.01
14	B	1234	CLA	CHA-C1A-NA	-2.01	121.84	126.39
18	L	4022	BCR	C34-C9-C10	-2.01	119.56	122.82
14	b	1214	CLA	C4-C3-C2	-2.01	118.47	123.63
14	A	1132	CLA	CMC-C2C-C1C	2.01	128.17	125.03
14	a	1118	CLA	C3C-C4C-NC	2.01	113.00	110.43
14	G	1106	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
14	A	1135	CLA	CGD-CBD-CAD	-2.01	104.34	110.85
14	B	1202	CLA	CHB-C4A-NA	2.01	127.30	124.40
18	b	4005	BCR	C31-C1-C6	-2.01	107.09	110.24
13	A	1011	CL0	C1-C2-C3	-2.01	122.91	126.20
14	H	1012	CLA	CHD-C4C-C3C	-2.01	121.84	124.77
15	a	1121	F6C	CMC-C2C-C3C	2.01	129.88	125.62
14	B	1207	CLA	CHA-C1A-NA	-2.01	121.84	126.39
14	b	1224	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
14	A	1135	CLA	C5-C3-C4	2.01	119.21	114.59
14	b	1206	CLA	C4D-C3D-CAD	2.01	110.29	108.11
18	B	4004	BCR	C35-C13-C12	2.01	121.16	118.09
14	a	1119	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
18	i	4018	BCR	C1-C6-C7	2.01	121.09	115.65
15	G	1120	F6C	OBD-CAD-C3D	-2.01	123.72	128.42
14	B	1229	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
18	G	4011	BCR	C30-C25-C24	2.01	121.09	115.65
14	b	1207	CLA	CHC-C1C-C2C	-2.01	121.25	126.95
14	B	1214	CLA	C4-C3-C2	-2.01	118.47	123.63
14	B	1224	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
13	G	1011	CL0	C1-C2-C3	-2.01	122.91	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4004	BCR	C4-C5-C6	-2.01	119.99	122.70
14	l	1502	CLA	C4-C3-C5	2.01	118.71	115.23
14	B	1219	CLA	CMB-C2B-C1B	2.01	128.47	125.42
14	B	1207	CLA	CHC-C1C-C2C	-2.00	121.25	126.95
14	G	1119	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
14	B	1216	CLA	C4C-C3C-C2C	-2.00	103.97	106.89
18	I	4018	BCR	C1-C6-C7	2.00	121.09	115.65
15	H	1230	F6C	CAC-C3C-C4C	2.00	127.67	124.91
14	H	1214	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
14	a	1106	CLA	C4C-C3C-C2C	-2.00	103.97	106.89
18	R	4018	BCR	C1-C6-C7	2.00	121.08	115.65
18	H	4010	BCR	C29-C28-C27	-2.00	106.87	111.28
18	a	4002	BCR	C23-C24-C25	-2.00	121.65	127.00
14	a	1135	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
14	a	1130	CLA	C4D-C3D-CAD	2.00	110.28	108.11
20	G	5005	LMG	O7-C10-O9	-2.00	119.03	123.70
14	H	1214	CLA	C4-C3-C2	-2.00	118.49	123.63
20	a	5005	LMG	O7-C10-O9	-2.00	119.03	123.70
14	a	1126	CLA	CBA-CAA-C2A	2.00	119.74	113.79

All (273) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
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	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	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
14	B	1203	CLA	ND
14	B	1204	CLA	ND
14	B	1205	CLA	ND
14	B	1206	CLA	ND
14	B	1207	CLA	ND
14	B	1208	CLA	ND
14	B	1209	CLA	ND
14	B	1210	CLA	ND

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Mol	Chain	Res	Type	Atom
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	1238	CLA	ND
14	B	1239	CLA	ND
14	G	1012	CLA	ND
14	G	1013	CLA	ND
14	G	1101	CLA	ND
14	G	1102	CLA	ND
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

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Mol	Chain	Res	Type	Atom
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	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	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	1012	CLA	ND
14	H	1021	CLA	ND
14	H	1023	CLA	ND
14	H	1201	CLA	ND
14	H	1202	CLA	ND
14	H	1203	CLA	ND
14	H	1204	CLA	ND
14	H	1205	CLA	ND
14	H	1206	CLA	ND
14	H	1207	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

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Mol	Chain	Res	Type	Atom
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	1238	CLA	ND
14	H	1239	CLA	ND
14	K	1401	CLA	ND
14	L	1501	CLA	ND
14	L	1502	CLA	ND
14	L	1503	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	X	1701	CLA	ND
14	a	1012	CLA	ND
14	a	1013	CLA	ND
14	a	1101	CLA	ND
14	a	1102	CLA	ND
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

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Mol	Chain	Res	Type	Atom
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	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	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
14	b	1203	CLA	ND
14	b	1204	CLA	ND
14	b	1205	CLA	ND
14	b	1206	CLA	ND
14	b	1207	CLA	ND
14	b	1208	CLA	ND
14	b	1209	CLA	ND
14	b	1210	CLA	ND

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Mol	Chain	Res	Type	Atom
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	1238	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
15	A	1120	F6C	NA
15	A	1121	F6C	NA
15	B	1230	F6C	NA
15	B	1237	F6C	NA
15	G	1120	F6C	NA
15	G	1121	F6C	NA
15	H	1230	F6C	NA
15	H	1237	F6C	NA
15	a	1120	F6C	NA
15	a	1121	F6C	NA

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Mol	Chain	Res	Type	Atom
15	b	1230	F6C	NA
15	b	1237	F6C	NA

All (4098) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	1011	CL0	C2-C1-O2A-CGA
13	A	1011	CL0	CHA-CBD-CGD-O1D
13	G	1011	CL0	C2-C1-O2A-CGA
13	G	1011	CL0	CHA-CBD-CGD-O1D
13	a	1011	CL0	C2-C1-O2A-CGA
13	a	1011	CL0	CHA-CBD-CGD-O1D
14	A	1012	CLA	C2B-C3B-CAB-CBB
14	A	1012	CLA	C4B-C3B-CAB-CBB
14	A	1013	CLA	C2-C1-O2A-CGA
14	A	1101	CLA	C2B-C3B-CAB-CBB
14	A	1101	CLA	C4B-C3B-CAB-CBB
14	A	1101	CLA	CHA-CBD-CGD-O1D
14	A	1101	CLA	CHA-CBD-CGD-O2D
14	A	1102	CLA	C1A-C2A-CAA-CBA
14	A	1103	CLA	C2-C3-C5-C6
14	A	1103	CLA	C4-C3-C5-C6
14	A	1106	CLA	C3A-C2A-CAA-CBA
14	A	1106	CLA	CHA-CBD-CGD-O1D
14	A	1106	CLA	CHA-CBD-CGD-O2D
14	A	1107	CLA	C2B-C3B-CAB-CBB
14	A	1107	CLA	C4B-C3B-CAB-CBB
14	A	1108	CLA	C4B-C3B-CAB-CBB
14	A	1110	CLA	C2B-C3B-CAB-CBB
14	A	1110	CLA	C4B-C3B-CAB-CBB
14	A	1110	CLA	CHA-CBD-CGD-O1D
14	A	1110	CLA	CHA-CBD-CGD-O2D
14	A	1111	CLA	C2-C3-C5-C6
14	A	1111	CLA	C4-C3-C5-C6
14	A	1113	CLA	CAD-CBD-CGD-O1D
14	A	1113	CLA	CAD-CBD-CGD-O2D
14	A	1115	CLA	C1A-C2A-CAA-CBA
14	A	1115	CLA	C3A-C2A-CAA-CBA
14	A	1115	CLA	CBD-CGD-O2D-CED
14	A	1116	CLA	C1A-C2A-CAA-CBA
14	A	1116	CLA	C3A-C2A-CAA-CBA
14	A	1117	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	1117	CLA	C3A-C2A-CAA-CBA
14	A	1118	CLA	C2-C1-O2A-CGA
14	A	1118	CLA	C2B-C3B-CAB-CBB
14	A	1118	CLA	C4B-C3B-CAB-CBB
14	A	1122	CLA	CBA-CGA-O2A-C1
14	A	1122	CLA	C2B-C3B-CAB-CBB
14	A	1122	CLA	C4B-C3B-CAB-CBB
14	A	1126	CLA	CBD-CGD-O2D-CED
14	A	1128	CLA	CHA-CBD-CGD-O1D
14	A	1128	CLA	CHA-CBD-CGD-O2D
14	A	1130	CLA	C4-C3-C5-C6
14	A	1131	CLA	C2B-C3B-CAB-CBB
14	A	1131	CLA	C4B-C3B-CAB-CBB
14	A	1132	CLA	C2B-C3B-CAB-CBB
14	A	1132	CLA	C4B-C3B-CAB-CBB
14	A	1132	CLA	CHA-CBD-CGD-O1D
14	A	1132	CLA	CHA-CBD-CGD-O2D
14	A	1133	CLA	C1A-C2A-CAA-CBA
14	A	1133	CLA	C3A-C2A-CAA-CBA
14	A	1133	CLA	CHA-CBD-CGD-O1D
14	A	1133	CLA	CHA-CBD-CGD-O2D
14	A	1137	CLA	CHA-CBD-CGD-O1D
14	A	1137	CLA	CHA-CBD-CGD-O2D
14	A	1138	CLA	C1A-C2A-CAA-CBA
14	A	1138	CLA	CBD-CGD-O2D-CED
14	A	1139	CLA	CBD-CGD-O2D-CED
14	A	1140	CLA	C2-C3-C5-C6
14	A	1140	CLA	C4-C3-C5-C6
14	B	1021	CLA	C2-C1-O2A-CGA
14	B	1021	CLA	CBD-CGD-O2D-CED
14	B	1201	CLA	CHA-CBD-CGD-O1D
14	B	1201	CLA	CHA-CBD-CGD-O2D
14	B	1201	CLA	C4-C3-C5-C6
14	B	1203	CLA	C1A-C2A-CAA-CBA
14	B	1203	CLA	O1A-CGA-O2A-C1
14	B	1203	CLA	CBD-CGD-O2D-CED
14	B	1204	CLA	C2B-C3B-CAB-CBB
14	B	1204	CLA	C4B-C3B-CAB-CBB
14	B	1205	CLA	CHA-CBD-CGD-O1D
14	B	1205	CLA	CHA-CBD-CGD-O2D
14	B	1206	CLA	C1A-C2A-CAA-CBA
14	B	1206	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	1207	CLA	C1A-C2A-CAA-CBA
14	B	1207	CLA	C3A-C2A-CAA-CBA
14	B	1207	CLA	CBD-CGD-O2D-CED
14	B	1209	CLA	C2B-C3B-CAB-CBB
14	B	1209	CLA	C4B-C3B-CAB-CBB
14	B	1210	CLA	C1A-C2A-CAA-CBA
14	B	1211	CLA	CBD-CGD-O2D-CED
14	B	1212	CLA	CHA-CBD-CGD-O1D
14	B	1212	CLA	CHA-CBD-CGD-O2D
14	B	1213	CLA	C1A-C2A-CAA-CBA
14	B	1213	CLA	CBA-CGA-O2A-C1
14	B	1213	CLA	O1A-CGA-O2A-C1
14	B	1214	CLA	CBA-CGA-O2A-C1
14	B	1214	CLA	O1A-CGA-O2A-C1
14	B	1214	CLA	C2B-C3B-CAB-CBB
14	B	1214	CLA	C4B-C3B-CAB-CBB
14	B	1215	CLA	C3A-C2A-CAA-CBA
14	B	1215	CLA	CBD-CGD-O2D-CED
14	B	1216	CLA	C4B-C3B-CAB-CBB
14	B	1217	CLA	C3A-C2A-CAA-CBA
14	B	1217	CLA	C2B-C3B-CAB-CBB
14	B	1217	CLA	C4B-C3B-CAB-CBB
14	B	1217	CLA	CBD-CGD-O2D-CED
14	B	1218	CLA	CHA-CBD-CGD-O1D
14	B	1218	CLA	CHA-CBD-CGD-O2D
14	B	1222	CLA	CHA-CBD-CGD-O1D
14	B	1222	CLA	CHA-CBD-CGD-O2D
14	B	1222	CLA	C6-C7-C8-C9
14	B	1224	CLA	CBD-CGD-O2D-CED
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	1228	CLA	CBD-CGD-O2D-CED
14	B	1229	CLA	C3A-C2A-CAA-CBA
14	B	1229	CLA	C2-C1-O2A-CGA
14	B	1229	CLA	CBD-CGD-O2D-CED
14	B	1232	CLA	CBD-CGD-O2D-CED
14	B	1233	CLA	C2B-C3B-CAB-CBB
14	B	1233	CLA	C4B-C3B-CAB-CBB
14	B	1233	CLA	CBD-CGD-O2D-CED
14	B	1234	CLA	C2B-C3B-CAB-CBB
14	B	1234	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	B	1239	CLA	C2-C1-O2A-CGA
14	B	1239	CLA	C2B-C3B-CAB-CBB
14	B	1239	CLA	C4B-C3B-CAB-CBB
14	G	1012	CLA	C2B-C3B-CAB-CBB
14	G	1012	CLA	C4B-C3B-CAB-CBB
14	G	1013	CLA	C2-C1-O2A-CGA
14	G	1101	CLA	C2B-C3B-CAB-CBB
14	G	1101	CLA	C4B-C3B-CAB-CBB
14	G	1101	CLA	CHA-CBD-CGD-O1D
14	G	1101	CLA	CHA-CBD-CGD-O2D
14	G	1102	CLA	C1A-C2A-CAA-CBA
14	G	1103	CLA	C2-C3-C5-C6
14	G	1103	CLA	C4-C3-C5-C6
14	G	1106	CLA	C3A-C2A-CAA-CBA
14	G	1106	CLA	CHA-CBD-CGD-O1D
14	G	1106	CLA	CHA-CBD-CGD-O2D
14	G	1107	CLA	C2B-C3B-CAB-CBB
14	G	1107	CLA	C4B-C3B-CAB-CBB
14	G	1108	CLA	C4B-C3B-CAB-CBB
14	G	1110	CLA	C2B-C3B-CAB-CBB
14	G	1110	CLA	C4B-C3B-CAB-CBB
14	G	1110	CLA	CHA-CBD-CGD-O1D
14	G	1110	CLA	CHA-CBD-CGD-O2D
14	G	1111	CLA	C2-C3-C5-C6
14	G	1111	CLA	C4-C3-C5-C6
14	G	1113	CLA	CAD-CBD-CGD-O1D
14	G	1113	CLA	CAD-CBD-CGD-O2D
14	G	1115	CLA	C1A-C2A-CAA-CBA
14	G	1115	CLA	C3A-C2A-CAA-CBA
14	G	1115	CLA	CBD-CGD-O2D-CED
14	G	1116	CLA	C1A-C2A-CAA-CBA
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	1118	CLA	C2-C1-O2A-CGA
14	G	1118	CLA	C2B-C3B-CAB-CBB
14	G	1118	CLA	C4B-C3B-CAB-CBB
14	G	1122	CLA	CBA-CGA-O2A-C1
14	G	1122	CLA	C2B-C3B-CAB-CBB
14	G	1122	CLA	C4B-C3B-CAB-CBB
14	G	1126	CLA	CBD-CGD-O2D-CED
14	G	1128	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	G	1128	CLA	CHA-CBD-CGD-O2D
14	G	1131	CLA	C2B-C3B-CAB-CBB
14	G	1131	CLA	C4B-C3B-CAB-CBB
14	G	1132	CLA	C2B-C3B-CAB-CBB
14	G	1132	CLA	C4B-C3B-CAB-CBB
14	G	1132	CLA	CHA-CBD-CGD-O1D
14	G	1132	CLA	CHA-CBD-CGD-O2D
14	G	1133	CLA	C1A-C2A-CAA-CBA
14	G	1133	CLA	C3A-C2A-CAA-CBA
14	G	1133	CLA	CHA-CBD-CGD-O1D
14	G	1133	CLA	CHA-CBD-CGD-O2D
14	G	1137	CLA	CHA-CBD-CGD-O1D
14	G	1137	CLA	CHA-CBD-CGD-O2D
14	G	1138	CLA	C1A-C2A-CAA-CBA
14	G	1138	CLA	CBD-CGD-O2D-CED
14	G	1139	CLA	CBD-CGD-O2D-CED
14	G	1140	CLA	C2-C3-C5-C6
14	G	1140	CLA	C4-C3-C5-C6
14	H	1021	CLA	C2-C1-O2A-CGA
14	H	1021	CLA	CBD-CGD-O2D-CED
14	H	1201	CLA	CHA-CBD-CGD-O1D
14	H	1201	CLA	CHA-CBD-CGD-O2D
14	H	1201	CLA	C4-C3-C5-C6
14	H	1203	CLA	C1A-C2A-CAA-CBA
14	H	1203	CLA	CBD-CGD-O2D-CED
14	H	1204	CLA	C2B-C3B-CAB-CBB
14	H	1204	CLA	C4B-C3B-CAB-CBB
14	H	1205	CLA	CHA-CBD-CGD-O1D
14	H	1205	CLA	CHA-CBD-CGD-O2D
14	H	1206	CLA	C1A-C2A-CAA-CBA
14	H	1206	CLA	C3A-C2A-CAA-CBA
14	H	1207	CLA	C1A-C2A-CAA-CBA
14	H	1207	CLA	C3A-C2A-CAA-CBA
14	H	1207	CLA	CBD-CGD-O2D-CED
14	H	1209	CLA	C2B-C3B-CAB-CBB
14	H	1209	CLA	C4B-C3B-CAB-CBB
14	H	1210	CLA	C1A-C2A-CAA-CBA
14	H	1211	CLA	CBD-CGD-O2D-CED
14	H	1212	CLA	CHA-CBD-CGD-O1D
14	H	1212	CLA	CHA-CBD-CGD-O2D
14	H	1213	CLA	C1A-C2A-CAA-CBA
14	H	1213	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	H	1213	CLA	O1A-CGA-O2A-C1
14	H	1214	CLA	CBA-CGA-O2A-C1
14	H	1214	CLA	O1A-CGA-O2A-C1
14	H	1214	CLA	C2B-C3B-CAB-CBB
14	H	1214	CLA	C4B-C3B-CAB-CBB
14	H	1215	CLA	C3A-C2A-CAA-CBA
14	H	1215	CLA	CBD-CGD-O2D-CED
14	H	1216	CLA	C4B-C3B-CAB-CBB
14	H	1217	CLA	C3A-C2A-CAA-CBA
14	H	1217	CLA	C2B-C3B-CAB-CBB
14	H	1217	CLA	C4B-C3B-CAB-CBB
14	H	1217	CLA	CBD-CGD-O2D-CED
14	H	1218	CLA	CHA-CBD-CGD-O1D
14	H	1218	CLA	CHA-CBD-CGD-O2D
14	H	1222	CLA	CHA-CBD-CGD-O1D
14	H	1222	CLA	CHA-CBD-CGD-O2D
14	H	1222	CLA	C6-C7-C8-C9
14	H	1224	CLA	CBD-CGD-O2D-CED
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	1228	CLA	CBD-CGD-O2D-CED
14	H	1229	CLA	C3A-C2A-CAA-CBA
14	H	1229	CLA	C2-C1-O2A-CGA
14	H	1229	CLA	CBD-CGD-O2D-CED
14	H	1232	CLA	CBD-CGD-O2D-CED
14	H	1233	CLA	C2B-C3B-CAB-CBB
14	H	1233	CLA	C4B-C3B-CAB-CBB
14	H	1233	CLA	CBD-CGD-O2D-CED
14	H	1234	CLA	C2B-C3B-CAB-CBB
14	H	1234	CLA	C4B-C3B-CAB-CBB
14	H	1239	CLA	C2-C1-O2A-CGA
14	H	1239	CLA	C2B-C3B-CAB-CBB
14	H	1239	CLA	C4B-C3B-CAB-CBB
14	K	1401	CLA	C2B-C3B-CAB-CBB
14	K	1401	CLA	C4B-C3B-CAB-CBB
14	K	1401	CLA	CBD-CGD-O2D-CED
14	L	1501	CLA	C1A-C2A-CAA-CBA
14	L	1501	CLA	CHA-CBD-CGD-O1D
14	L	1501	CLA	CHA-CBD-CGD-O2D
14	L	1502	CLA	C2B-C3B-CAB-CBB
14	L	1502	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	T	1401	CLA	C2B-C3B-CAB-CBB
14	T	1401	CLA	C4B-C3B-CAB-CBB
14	T	1401	CLA	CBD-CGD-O2D-CED
14	U	1501	CLA	C1A-C2A-CAA-CBA
14	U	1501	CLA	CHA-CBD-CGD-O1D
14	U	1501	CLA	CHA-CBD-CGD-O2D
14	U	1502	CLA	C2B-C3B-CAB-CBB
14	U	1502	CLA	C4B-C3B-CAB-CBB
14	W	1701	CLA	C2B-C3B-CAB-CBB
14	W	1701	CLA	C4B-C3B-CAB-CBB
14	X	1701	CLA	C2B-C3B-CAB-CBB
14	X	1701	CLA	C4B-C3B-CAB-CBB
14	a	1012	CLA	C2B-C3B-CAB-CBB
14	a	1012	CLA	C4B-C3B-CAB-CBB
14	a	1013	CLA	C2-C1-O2A-CGA
14	a	1101	CLA	C2B-C3B-CAB-CBB
14	a	1101	CLA	C4B-C3B-CAB-CBB
14	a	1101	CLA	CHA-CBD-CGD-O1D
14	a	1101	CLA	CHA-CBD-CGD-O2D
14	a	1102	CLA	C1A-C2A-CAA-CBA
14	a	1103	CLA	C2-C3-C5-C6
14	a	1103	CLA	C4-C3-C5-C6
14	a	1106	CLA	C3A-C2A-CAA-CBA
14	a	1106	CLA	CHA-CBD-CGD-O1D
14	a	1106	CLA	CHA-CBD-CGD-O2D
14	a	1107	CLA	C2B-C3B-CAB-CBB
14	a	1107	CLA	C4B-C3B-CAB-CBB
14	a	1108	CLA	C4B-C3B-CAB-CBB
14	a	1110	CLA	C2B-C3B-CAB-CBB
14	a	1110	CLA	C4B-C3B-CAB-CBB
14	a	1110	CLA	CHA-CBD-CGD-O1D
14	a	1110	CLA	CHA-CBD-CGD-O2D
14	a	1111	CLA	C2-C3-C5-C6
14	a	1111	CLA	C4-C3-C5-C6
14	a	1113	CLA	CAD-CBD-CGD-O1D
14	a	1113	CLA	CAD-CBD-CGD-O2D
14	a	1115	CLA	C1A-C2A-CAA-CBA
14	a	1115	CLA	C3A-C2A-CAA-CBA
14	a	1115	CLA	CBD-CGD-O2D-CED
14	a	1116	CLA	C1A-C2A-CAA-CBA
14	a	1116	CLA	C3A-C2A-CAA-CBA
14	a	1117	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	a	1117	CLA	C3A-C2A-CAA-CBA
14	a	1118	CLA	C2-C1-O2A-CGA
14	a	1118	CLA	C2B-C3B-CAB-CBB
14	a	1118	CLA	C4B-C3B-CAB-CBB
14	a	1122	CLA	CBA-CGA-O2A-C1
14	a	1122	CLA	C2B-C3B-CAB-CBB
14	a	1122	CLA	C4B-C3B-CAB-CBB
14	a	1126	CLA	CBD-CGD-O2D-CED
14	a	1128	CLA	CHA-CBD-CGD-O1D
14	a	1128	CLA	CHA-CBD-CGD-O2D
14	a	1131	CLA	C2B-C3B-CAB-CBB
14	a	1131	CLA	C4B-C3B-CAB-CBB
14	a	1132	CLA	C2B-C3B-CAB-CBB
14	a	1132	CLA	C4B-C3B-CAB-CBB
14	a	1132	CLA	CHA-CBD-CGD-O1D
14	a	1132	CLA	CHA-CBD-CGD-O2D
14	a	1133	CLA	C1A-C2A-CAA-CBA
14	a	1133	CLA	C3A-C2A-CAA-CBA
14	a	1133	CLA	CHA-CBD-CGD-O1D
14	a	1133	CLA	CHA-CBD-CGD-O2D
14	a	1137	CLA	CHA-CBD-CGD-O1D
14	a	1137	CLA	CHA-CBD-CGD-O2D
14	a	1138	CLA	C1A-C2A-CAA-CBA
14	a	1138	CLA	CBD-CGD-O2D-CED
14	a	1139	CLA	CBD-CGD-O2D-CED
14	a	1140	CLA	C2-C3-C5-C6
14	a	1140	CLA	C4-C3-C5-C6
14	b	1021	CLA	C2-C1-O2A-CGA
14	b	1021	CLA	CBD-CGD-O2D-CED
14	b	1201	CLA	CHA-CBD-CGD-O1D
14	b	1201	CLA	CHA-CBD-CGD-O2D
14	b	1201	CLA	C4-C3-C5-C6
14	b	1203	CLA	C1A-C2A-CAA-CBA
14	b	1203	CLA	CBD-CGD-O2D-CED
14	b	1204	CLA	C2B-C3B-CAB-CBB
14	b	1204	CLA	C4B-C3B-CAB-CBB
14	b	1205	CLA	CHA-CBD-CGD-O1D
14	b	1205	CLA	CHA-CBD-CGD-O2D
14	b	1206	CLA	C1A-C2A-CAA-CBA
14	b	1206	CLA	C3A-C2A-CAA-CBA
14	b	1207	CLA	C1A-C2A-CAA-CBA
14	b	1207	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	1207	CLA	CBD-CGD-O2D-CED
14	b	1209	CLA	C2B-C3B-CAB-CBB
14	b	1209	CLA	C4B-C3B-CAB-CBB
14	b	1210	CLA	C1A-C2A-CAA-CBA
14	b	1211	CLA	CBD-CGD-O2D-CED
14	b	1212	CLA	CHA-CBD-CGD-O1D
14	b	1212	CLA	CHA-CBD-CGD-O2D
14	b	1213	CLA	C1A-C2A-CAA-CBA
14	b	1213	CLA	CBA-CGA-O2A-C1
14	b	1213	CLA	O1A-CGA-O2A-C1
14	b	1214	CLA	CBA-CGA-O2A-C1
14	b	1214	CLA	O1A-CGA-O2A-C1
14	b	1214	CLA	C2B-C3B-CAB-CBB
14	b	1214	CLA	C4B-C3B-CAB-CBB
14	b	1215	CLA	C3A-C2A-CAA-CBA
14	b	1215	CLA	CBD-CGD-O2D-CED
14	b	1216	CLA	C4B-C3B-CAB-CBB
14	b	1217	CLA	C3A-C2A-CAA-CBA
14	b	1217	CLA	C2B-C3B-CAB-CBB
14	b	1217	CLA	C4B-C3B-CAB-CBB
14	b	1217	CLA	CBD-CGD-O2D-CED
14	b	1218	CLA	CHA-CBD-CGD-O1D
14	b	1218	CLA	CHA-CBD-CGD-O2D
14	b	1222	CLA	CHA-CBD-CGD-O1D
14	b	1222	CLA	CHA-CBD-CGD-O2D
14	b	1222	CLA	C6-C7-C8-C9
14	b	1224	CLA	CBD-CGD-O2D-CED
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	1228	CLA	CBD-CGD-O2D-CED
14	b	1229	CLA	C3A-C2A-CAA-CBA
14	b	1229	CLA	C2-C1-O2A-CGA
14	b	1229	CLA	CBD-CGD-O2D-CED
14	b	1232	CLA	CBD-CGD-O2D-CED
14	b	1233	CLA	C2B-C3B-CAB-CBB
14	b	1233	CLA	C4B-C3B-CAB-CBB
14	b	1233	CLA	CBD-CGD-O2D-CED
14	b	1234	CLA	C2B-C3B-CAB-CBB
14	b	1234	CLA	C4B-C3B-CAB-CBB
14	b	1239	CLA	C2-C1-O2A-CGA
14	b	1239	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	1239	CLA	C4B-C3B-CAB-CBB
14	k	1401	CLA	C2B-C3B-CAB-CBB
14	k	1401	CLA	C4B-C3B-CAB-CBB
14	k	1401	CLA	CBD-CGD-O2D-CED
14	l	1501	CLA	C1A-C2A-CAA-CBA
14	l	1501	CLA	CHA-CBD-CGD-O1D
14	l	1501	CLA	CHA-CBD-CGD-O2D
14	l	1502	CLA	C2B-C3B-CAB-CBB
14	l	1502	CLA	C4B-C3B-CAB-CBB
14	x	1701	CLA	C2B-C3B-CAB-CBB
14	x	1701	CLA	C4B-C3B-CAB-CBB
15	A	1120	F6C	C1B-C2B-CMB-OMB
15	A	1121	F6C	C1A-C2A-CAA-CBA
15	A	1121	F6C	C1B-C2B-CMB-OMB
15	B	1230	F6C	CHA-CBD-CGD-O1D
15	B	1230	F6C	CHA-CBD-CGD-O2D
15	B	1230	F6C	C3B-C2B-CMB-OMB
15	B	1237	F6C	C3B-C2B-CMB-OMB
15	G	1120	F6C	C1B-C2B-CMB-OMB
15	G	1121	F6C	C1A-C2A-CAA-CBA
15	G	1121	F6C	C1B-C2B-CMB-OMB
15	H	1230	F6C	CHA-CBD-CGD-O1D
15	H	1230	F6C	CHA-CBD-CGD-O2D
15	H	1237	F6C	C3B-C2B-CMB-OMB
15	a	1120	F6C	C1B-C2B-CMB-OMB
15	a	1121	F6C	C1A-C2A-CAA-CBA
15	a	1121	F6C	C1B-C2B-CMB-OMB
15	b	1230	F6C	CHA-CBD-CGD-O1D
15	b	1230	F6C	CHA-CBD-CGD-O2D
15	b	1237	F6C	C3B-C2B-CMB-OMB
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	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	C9-C10-C11-C12
18	A	4003	BCR	C10-C11-C12-C13
18	A	4003	BCR	C21-C22-C23-C24
18	A	4003	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	A	4007	BCR	C11-C10-C9-C8
18	A	4007	BCR	C11-C10-C9-C34
18	A	4007	BCR	C10-C11-C12-C13
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	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	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	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	4012	BCR	C7-C8-C9-C34
18	B	4012	BCR	C11-C10-C9-C8
18	B	4012	BCR	C11-C10-C9-C34
18	B	4012	BCR	C10-C11-C12-C13
18	B	4012	BCR	C11-C12-C13-C14
18	B	4012	BCR	C11-C12-C13-C35
18	B	4012	BCR	C17-C18-C19-C20
18	B	4012	BCR	C36-C18-C19-C20
18	B	4012	BCR	C19-C20-C21-C22
18	B	4012	BCR	C21-C22-C23-C24
18	B	4012	BCR	C37-C22-C23-C24
18	B	4012	BCR	C23-C24-C25-C26
18	B	4012	BCR	C23-C24-C25-C30
18	B	4013	BCR	C11-C10-C9-C8
18	B	4013	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	B	4013	BCR	C10-C11-C12-C13
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	C21-C22-C23-C24
18	B	4013	BCR	C23-C24-C25-C26
18	B	4014	BCR	C11-C10-C9-C8
18	B	4014	BCR	C11-C10-C9-C34
18	B	4014	BCR	C10-C11-C12-C13
18	B	4014	BCR	C11-C12-C13-C14
18	B	4014	BCR	C11-C12-C13-C35
18	B	4014	BCR	C17-C18-C19-C20
18	B	4016	BCR	C11-C10-C9-C34
18	B	4016	BCR	C17-C18-C19-C20
18	B	4016	BCR	C36-C18-C19-C20
18	B	4017	BCR	C11-C10-C9-C8
18	B	4017	BCR	C11-C10-C9-C34
18	B	4017	BCR	C10-C11-C12-C13
18	B	4017	BCR	C21-C22-C23-C24
18	B	4017	BCR	C37-C22-C23-C24
18	G	4001	BCR	C11-C10-C9-C8
18	G	4001	BCR	C11-C10-C9-C34
18	G	4001	BCR	C17-C18-C19-C20
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	C9-C10-C11-C12
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	C10-C11-C12-C13
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

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Mol	Chain	Res	Type	Atoms
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	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	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	4012	BCR	C7-C8-C9-C34
18	H	4012	BCR	C11-C10-C9-C8
18	H	4012	BCR	C11-C10-C9-C34
18	H	4012	BCR	C10-C11-C12-C13
18	H	4012	BCR	C11-C12-C13-C14
18	H	4012	BCR	C11-C12-C13-C35
18	H	4012	BCR	C17-C18-C19-C20
18	H	4012	BCR	C36-C18-C19-C20
18	H	4012	BCR	C19-C20-C21-C22
18	H	4012	BCR	C21-C22-C23-C24
18	H	4012	BCR	C37-C22-C23-C24
18	H	4012	BCR	C23-C24-C25-C26
18	H	4012	BCR	C23-C24-C25-C30
18	H	4013	BCR	C11-C10-C9-C8
18	H	4013	BCR	C11-C10-C9-C34
18	H	4013	BCR	C10-C11-C12-C13
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	C21-C22-C23-C24
18	H	4013	BCR	C23-C24-C25-C26
18	H	4014	BCR	C11-C10-C9-C8
18	H	4014	BCR	C11-C10-C9-C34
18	H	4014	BCR	C10-C11-C12-C13
18	H	4014	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	H	4014	BCR	C11-C12-C13-C35
18	H	4014	BCR	C17-C18-C19-C20
18	H	4016	BCR	C11-C10-C9-C34
18	H	4016	BCR	C17-C18-C19-C20
18	H	4016	BCR	C36-C18-C19-C20
18	H	4017	BCR	C11-C10-C9-C8
18	H	4017	BCR	C11-C10-C9-C34
18	H	4017	BCR	C10-C11-C12-C13
18	H	4017	BCR	C21-C22-C23-C24
18	H	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	C11-C10-C9-C8
18	I	4018	BCR	C11-C10-C9-C34
18	I	4018	BCR	C19-C20-C21-C22
18	I	4020	BCR	C11-C10-C9-C34
18	L	4019	BCR	C21-C22-C23-C24
18	L	4019	BCR	C37-C22-C23-C24
18	L	4019	BCR	C23-C24-C25-C26
18	L	4019	BCR	C23-C24-C25-C30
18	L	4022	BCR	C11-C10-C9-C8
18	L	4022	BCR	C11-C10-C9-C34
18	M	4021	BCR	C7-C8-C9-C10
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	C17-C18-C19-C20
18	M	4021	BCR	C36-C18-C19-C20
18	R	4018	BCR	C7-C8-C9-C10
18	R	4018	BCR	C7-C8-C9-C34
18	R	4018	BCR	C11-C10-C9-C8
18	R	4018	BCR	C11-C10-C9-C34
18	R	4020	BCR	C11-C10-C9-C34
18	U	4019	BCR	C21-C22-C23-C24
18	U	4019	BCR	C37-C22-C23-C24
18	U	4019	BCR	C23-C24-C25-C26
18	U	4019	BCR	C23-C24-C25-C30
18	U	4022	BCR	C11-C10-C9-C8
18	U	4022	BCR	C11-C10-C9-C34
18	V	4021	BCR	C7-C8-C9-C10
18	V	4021	BCR	C7-C8-C9-C34
18	V	4021	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	V	4021	BCR	C11-C10-C9-C34
18	V	4021	BCR	C17-C18-C19-C20
18	V	4021	BCR	C36-C18-C19-C20
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	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	C9-C10-C11-C12
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	C10-C11-C12-C13
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	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	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	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

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Mol	Chain	Res	Type	Atoms
18	b	4012	BCR	C7-C8-C9-C34
18	b	4012	BCR	C11-C10-C9-C8
18	b	4012	BCR	C11-C10-C9-C34
18	b	4012	BCR	C10-C11-C12-C13
18	b	4012	BCR	C11-C12-C13-C14
18	b	4012	BCR	C11-C12-C13-C35
18	b	4012	BCR	C17-C18-C19-C20
18	b	4012	BCR	C36-C18-C19-C20
18	b	4012	BCR	C19-C20-C21-C22
18	b	4012	BCR	C21-C22-C23-C24
18	b	4012	BCR	C37-C22-C23-C24
18	b	4012	BCR	C23-C24-C25-C26
18	b	4012	BCR	C23-C24-C25-C30
18	b	4013	BCR	C11-C10-C9-C8
18	b	4013	BCR	C11-C10-C9-C34
18	b	4013	BCR	C10-C11-C12-C13
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	C21-C22-C23-C24
18	b	4013	BCR	C23-C24-C25-C26
18	b	4014	BCR	C11-C10-C9-C8
18	b	4014	BCR	C11-C10-C9-C34
18	b	4014	BCR	C10-C11-C12-C13
18	b	4014	BCR	C11-C12-C13-C14
18	b	4014	BCR	C11-C12-C13-C35
18	b	4014	BCR	C17-C18-C19-C20
18	b	4016	BCR	C11-C10-C9-C34
18	b	4016	BCR	C17-C18-C19-C20
18	b	4016	BCR	C36-C18-C19-C20
18	b	4017	BCR	C11-C10-C9-C8
18	b	4017	BCR	C11-C10-C9-C34
18	b	4017	BCR	C10-C11-C12-C13
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	C11-C10-C9-C8
18	i	4018	BCR	C11-C10-C9-C34
18	i	4018	BCR	C19-C20-C21-C22
18	i	4020	BCR	C11-C10-C9-C34
18	l	4019	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	l	4019	BCR	C37-C22-C23-C24
18	l	4019	BCR	C23-C24-C25-C26
18	l	4019	BCR	C23-C24-C25-C30
18	l	4022	BCR	C11-C10-C9-C8
18	l	4022	BCR	C11-C10-C9-C34
18	m	4021	BCR	C7-C8-C9-C10
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	C17-C18-C19-C20
18	m	4021	BCR	C36-C18-C19-C20
19	A	5001	LHG	O1-C1-C2-C3
19	A	5001	LHG	C4-O6-P-O3
19	A	5001	LHG	C4-O6-P-O4
19	A	5001	LHG	C4-O6-P-O5
19	B	5004	LHG	O1-C1-C2-C3
19	B	5004	LHG	C3-O3-P-O6
19	B	5004	LHG	C4-O6-P-O3
19	B	5004	LHG	C4-O6-P-O4
19	G	5001	LHG	O1-C1-C2-C3
19	G	5001	LHG	C4-O6-P-O3
19	G	5001	LHG	C4-O6-P-O4
19	G	5001	LHG	C4-O6-P-O5
19	H	5004	LHG	O1-C1-C2-C3
19	H	5004	LHG	C3-O3-P-O6
19	H	5004	LHG	C4-O6-P-O3
19	H	5004	LHG	C4-O6-P-O4
19	a	5001	LHG	O1-C1-C2-C3
19	a	5001	LHG	C4-O6-P-O3
19	a	5001	LHG	C4-O6-P-O4
19	a	5001	LHG	C4-O6-P-O5
19	b	5004	LHG	O1-C1-C2-C3
19	b	5004	LHG	C3-O3-P-O6
19	b	5004	LHG	C4-O6-P-O3
19	b	5004	LHG	C4-O6-P-O4
20	A	5005	LMG	O10-C28-O8-C9
20	B	5002	LMG	O6-C1-O1-C7
20	G	5005	LMG	O10-C28-O8-C9
20	H	5002	LMG	O6-C1-O1-C7
20	a	5005	LMG	O10-C28-O8-C9
20	b	5002	LMG	O6-C1-O1-C7
14	A	1119	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	1216	CLA	O1D-CGD-O2D-CED
14	G	1119	CLA	O1D-CGD-O2D-CED
14	H	1216	CLA	O1D-CGD-O2D-CED
14	a	1119	CLA	O1D-CGD-O2D-CED
14	b	1216	CLA	O1D-CGD-O2D-CED
14	B	1023	CLA	C2C-C3C-CAC-CBC
14	H	1023	CLA	C2C-C3C-CAC-CBC
14	b	1023	CLA	C2C-C3C-CAC-CBC
14	A	1139	CLA	O1D-CGD-O2D-CED
14	B	1021	CLA	O1D-CGD-O2D-CED
14	B	1203	CLA	O1D-CGD-O2D-CED
14	B	1217	CLA	O1D-CGD-O2D-CED
14	G	1139	CLA	O1D-CGD-O2D-CED
14	H	1021	CLA	O1D-CGD-O2D-CED
14	H	1203	CLA	O1D-CGD-O2D-CED
14	H	1217	CLA	O1D-CGD-O2D-CED
14	K	1401	CLA	O1D-CGD-O2D-CED
14	T	1401	CLA	O1D-CGD-O2D-CED
14	W	1701	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
14	a	1139	CLA	O1D-CGD-O2D-CED
14	b	1203	CLA	O1D-CGD-O2D-CED
14	b	1217	CLA	O1D-CGD-O2D-CED
14	k	1401	CLA	O1D-CGD-O2D-CED
14	x	1701	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	CBD-CGD-O2D-CED
14	A	1107	CLA	CBD-CGD-O2D-CED
14	A	1108	CLA	CBD-CGD-O2D-CED
14	A	1109	CLA	CBD-CGD-O2D-CED
14	A	1111	CLA	CBD-CGD-O2D-CED
14	A	1114	CLA	CBD-CGD-O2D-CED
14	A	1116	CLA	CBD-CGD-O2D-CED
14	A	1119	CLA	CBD-CGD-O2D-CED
14	A	1124	CLA	CBD-CGD-O2D-CED
14	A	1131	CLA	CBD-CGD-O2D-CED
14	A	1132	CLA	CBD-CGD-O2D-CED
14	A	1137	CLA	CBD-CGD-O2D-CED
14	B	1206	CLA	CBD-CGD-O2D-CED
14	B	1213	CLA	CBD-CGD-O2D-CED
14	B	1216	CLA	CBD-CGD-O2D-CED
14	B	1227	CLA	CBD-CGD-O2D-CED
14	B	1239	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	G	1102	CLA	CBD-CGD-O2D-CED
14	G	1107	CLA	CBD-CGD-O2D-CED
14	G	1108	CLA	CBD-CGD-O2D-CED
14	G	1109	CLA	CBD-CGD-O2D-CED
14	G	1111	CLA	CBD-CGD-O2D-CED
14	G	1114	CLA	CBD-CGD-O2D-CED
14	G	1116	CLA	CBD-CGD-O2D-CED
14	G	1119	CLA	CBD-CGD-O2D-CED
14	G	1124	CLA	CBD-CGD-O2D-CED
14	G	1131	CLA	CBD-CGD-O2D-CED
14	G	1132	CLA	CBD-CGD-O2D-CED
14	G	1137	CLA	CBD-CGD-O2D-CED
14	H	1206	CLA	CBD-CGD-O2D-CED
14	H	1213	CLA	CBD-CGD-O2D-CED
14	H	1216	CLA	CBD-CGD-O2D-CED
14	H	1227	CLA	CBD-CGD-O2D-CED
14	H	1239	CLA	CBD-CGD-O2D-CED
14	L	1501	CLA	CBD-CGD-O2D-CED
14	U	1501	CLA	CBD-CGD-O2D-CED
14	W	1701	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
14	a	1102	CLA	CBD-CGD-O2D-CED
14	a	1107	CLA	CBD-CGD-O2D-CED
14	a	1108	CLA	CBD-CGD-O2D-CED
14	a	1109	CLA	CBD-CGD-O2D-CED
14	a	1111	CLA	CBD-CGD-O2D-CED
14	a	1114	CLA	CBD-CGD-O2D-CED
14	a	1116	CLA	CBD-CGD-O2D-CED
14	a	1119	CLA	CBD-CGD-O2D-CED
14	a	1124	CLA	CBD-CGD-O2D-CED
14	a	1131	CLA	CBD-CGD-O2D-CED
14	a	1132	CLA	CBD-CGD-O2D-CED
14	a	1137	CLA	CBD-CGD-O2D-CED
14	b	1206	CLA	CBD-CGD-O2D-CED
14	b	1213	CLA	CBD-CGD-O2D-CED
14	b	1216	CLA	CBD-CGD-O2D-CED
14	b	1227	CLA	CBD-CGD-O2D-CED
14	b	1239	CLA	CBD-CGD-O2D-CED
14	l	1501	CLA	CBD-CGD-O2D-CED
14	x	1701	CLA	CBD-CGD-O2D-CED
15	A	1121	F6C	CBD-CGD-O2D-CED
15	G	1121	F6C	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	a	1121	F6C	CBD-CGD-O2D-CED
14	A	1102	CLA	O1A-CGA-O2A-C1
14	A	1118	CLA	O1A-CGA-O2A-C1
14	A	1122	CLA	O1A-CGA-O2A-C1
14	A	1127	CLA	O1A-CGA-O2A-C1
14	A	1133	CLA	O1A-CGA-O2A-C1
14	A	1138	CLA	O1A-CGA-O2A-C1
14	B	1222	CLA	O1A-CGA-O2A-C1
14	G	1102	CLA	O1A-CGA-O2A-C1
14	G	1118	CLA	O1A-CGA-O2A-C1
14	G	1122	CLA	O1A-CGA-O2A-C1
14	G	1127	CLA	O1A-CGA-O2A-C1
14	G	1133	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	a	1102	CLA	O1A-CGA-O2A-C1
14	a	1118	CLA	O1A-CGA-O2A-C1
14	a	1122	CLA	O1A-CGA-O2A-C1
14	a	1127	CLA	O1A-CGA-O2A-C1
14	a	1133	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	A	1138	CLA	O1D-CGD-O2D-CED
14	G	1138	CLA	O1D-CGD-O2D-CED
14	a	1138	CLA	O1D-CGD-O2D-CED
14	b	1021	CLA	O1D-CGD-O2D-CED
21	A	6002	LMT	O5B-C1B-O1B-C4'
21	G	6002	LMT	O5B-C1B-O1B-C4'
21	a	6002	LMT	O5B-C1B-O1B-C4'
14	B	1023	CLA	C4C-C3C-CAC-CBC
14	H	1023	CLA	C4C-C3C-CAC-CBC
14	b	1023	CLA	C4C-C3C-CAC-CBC
14	A	1108	CLA	O1D-CGD-O2D-CED
14	G	1108	CLA	O1D-CGD-O2D-CED
14	a	1108	CLA	O1D-CGD-O2D-CED
15	A	1121	F6C	O1D-CGD-O2D-CED
15	G	1121	F6C	O1D-CGD-O2D-CED
15	a	1121	F6C	O1D-CGD-O2D-CED
14	A	1127	CLA	CBA-CGA-O2A-C1
14	A	1133	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1203	CLA	CBA-CGA-O2A-C1
14	B	1222	CLA	CBA-CGA-O2A-C1
14	B	1224	CLA	CBA-CGA-O2A-C1
14	B	1235	CLA	CBA-CGA-O2A-C1
14	G	1127	CLA	CBA-CGA-O2A-C1
14	G	1133	CLA	CBA-CGA-O2A-C1
14	H	1203	CLA	CBA-CGA-O2A-C1
14	H	1222	CLA	CBA-CGA-O2A-C1
14	H	1224	CLA	CBA-CGA-O2A-C1
14	H	1235	CLA	CBA-CGA-O2A-C1
14	a	1127	CLA	CBA-CGA-O2A-C1
14	a	1133	CLA	CBA-CGA-O2A-C1
14	b	1203	CLA	CBA-CGA-O2A-C1
14	b	1222	CLA	CBA-CGA-O2A-C1
14	b	1224	CLA	CBA-CGA-O2A-C1
14	b	1235	CLA	CBA-CGA-O2A-C1
20	B	5002	LMG	C29-C28-O8-C9
20	H	5002	LMG	C29-C28-O8-C9
20	b	5002	LMG	C29-C28-O8-C9
14	A	1118	CLA	CBD-CGD-O2D-CED
14	G	1118	CLA	CBD-CGD-O2D-CED
14	a	1118	CLA	CBD-CGD-O2D-CED
15	B	1237	F6C	CBD-CGD-O2D-CED
15	b	1237	F6C	CBD-CGD-O2D-CED
14	A	1111	CLA	O1A-CGA-O2A-C1
14	A	1131	CLA	O1A-CGA-O2A-C1
14	B	1202	CLA	O1A-CGA-O2A-C1
14	B	1204	CLA	O1A-CGA-O2A-C1
14	B	1221	CLA	O1A-CGA-O2A-C1
14	B	1224	CLA	O1A-CGA-O2A-C1
14	B	1226	CLA	O1A-CGA-O2A-C1
14	B	1235	CLA	O1A-CGA-O2A-C1
14	G	1111	CLA	O1A-CGA-O2A-C1
14	G	1131	CLA	O1A-CGA-O2A-C1
14	H	1202	CLA	O1A-CGA-O2A-C1
14	H	1204	CLA	O1A-CGA-O2A-C1
14	H	1221	CLA	O1A-CGA-O2A-C1
14	H	1224	CLA	O1A-CGA-O2A-C1
14	H	1226	CLA	O1A-CGA-O2A-C1
14	H	1235	CLA	O1A-CGA-O2A-C1
14	a	1111	CLA	O1A-CGA-O2A-C1
14	a	1131	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	1202	CLA	O1A-CGA-O2A-C1
14	b	1204	CLA	O1A-CGA-O2A-C1
14	b	1221	CLA	O1A-CGA-O2A-C1
14	b	1224	CLA	O1A-CGA-O2A-C1
14	b	1226	CLA	O1A-CGA-O2A-C1
14	b	1235	CLA	O1A-CGA-O2A-C1
15	B	1237	F6C	O1A-CGA-O2A-C1
15	H	1237	F6C	O1A-CGA-O2A-C1
15	b	1237	F6C	O1A-CGA-O2A-C1
20	B	5002	LMG	O10-C28-O8-C9
20	H	5002	LMG	O10-C28-O8-C9
20	I	5006	LMG	O10-C28-O8-C9
20	R	5006	LMG	O10-C28-O8-C9
20	b	5002	LMG	O10-C28-O8-C9
20	i	5006	LMG	O10-C28-O8-C9
14	B	1207	CLA	O1D-CGD-O2D-CED
14	B	1211	CLA	O1D-CGD-O2D-CED
14	B	1215	CLA	O1D-CGD-O2D-CED
14	B	1224	CLA	O1D-CGD-O2D-CED
14	B	1228	CLA	O1D-CGD-O2D-CED
14	B	1229	CLA	O1D-CGD-O2D-CED
14	B	1232	CLA	O1D-CGD-O2D-CED
14	B	1233	CLA	O1D-CGD-O2D-CED
14	H	1207	CLA	O1D-CGD-O2D-CED
14	H	1211	CLA	O1D-CGD-O2D-CED
14	H	1215	CLA	O1D-CGD-O2D-CED
14	H	1224	CLA	O1D-CGD-O2D-CED
14	H	1228	CLA	O1D-CGD-O2D-CED
14	H	1229	CLA	O1D-CGD-O2D-CED
14	H	1232	CLA	O1D-CGD-O2D-CED
14	H	1233	CLA	O1D-CGD-O2D-CED
14	b	1207	CLA	O1D-CGD-O2D-CED
14	b	1211	CLA	O1D-CGD-O2D-CED
14	b	1215	CLA	O1D-CGD-O2D-CED
14	b	1224	CLA	O1D-CGD-O2D-CED
14	b	1228	CLA	O1D-CGD-O2D-CED
14	b	1229	CLA	O1D-CGD-O2D-CED
14	b	1232	CLA	O1D-CGD-O2D-CED
14	b	1233	CLA	O1D-CGD-O2D-CED
15	H	1237	F6C	CBD-CGD-O2D-CED
14	A	1126	CLA	O1D-CGD-O2D-CED
14	G	1126	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	1126	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	C3-C5-C6-C7
14	A	1118	CLA	C3-C5-C6-C7
14	A	1127	CLA	C3-C5-C6-C7
14	A	1128	CLA	C3-C5-C6-C7
14	A	1130	CLA	C3-C5-C6-C7
14	A	1131	CLA	C3-C5-C6-C7
14	A	1140	CLA	C3-C5-C6-C7
14	B	1204	CLA	C3-C5-C6-C7
14	B	1208	CLA	C3-C5-C6-C7
14	B	1210	CLA	C3-C5-C6-C7
14	B	1234	CLA	C3-C5-C6-C7
14	B	1235	CLA	C3-C5-C6-C7
14	B	1239	CLA	C3-C5-C6-C7
14	G	1102	CLA	C3-C5-C6-C7
14	G	1118	CLA	C3-C5-C6-C7
14	G	1127	CLA	C3-C5-C6-C7
14	G	1128	CLA	C3-C5-C6-C7
14	G	1130	CLA	C3-C5-C6-C7
14	G	1131	CLA	C3-C5-C6-C7
14	G	1140	CLA	C3-C5-C6-C7
14	H	1204	CLA	C3-C5-C6-C7
14	H	1208	CLA	C3-C5-C6-C7
14	H	1210	CLA	C3-C5-C6-C7
14	H	1234	CLA	C3-C5-C6-C7
14	H	1235	CLA	C3-C5-C6-C7
14	H	1239	CLA	C3-C5-C6-C7
14	a	1102	CLA	C3-C5-C6-C7
14	a	1118	CLA	C3-C5-C6-C7
14	a	1127	CLA	C3-C5-C6-C7
14	a	1128	CLA	C3-C5-C6-C7
14	a	1130	CLA	C3-C5-C6-C7
14	a	1131	CLA	C3-C5-C6-C7
14	a	1140	CLA	C3-C5-C6-C7
14	b	1204	CLA	C3-C5-C6-C7
14	b	1208	CLA	C3-C5-C6-C7
14	b	1210	CLA	C3-C5-C6-C7
14	b	1234	CLA	C3-C5-C6-C7
14	b	1235	CLA	C3-C5-C6-C7
14	b	1239	CLA	C3-C5-C6-C7
15	B	1237	F6C	C3-C5-C6-C7
15	H	1237	F6C	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
15	b	1237	F6C	C3-C5-C6-C7
14	A	1115	CLA	O1D-CGD-O2D-CED
14	G	1115	CLA	O1D-CGD-O2D-CED
14	a	1115	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	CBA-CGA-O2A-C1
14	A	1118	CLA	CBA-CGA-O2A-C1
14	A	1131	CLA	CBA-CGA-O2A-C1
14	A	1138	CLA	CBA-CGA-O2A-C1
14	G	1102	CLA	CBA-CGA-O2A-C1
14	G	1118	CLA	CBA-CGA-O2A-C1
14	G	1131	CLA	CBA-CGA-O2A-C1
14	G	1138	CLA	CBA-CGA-O2A-C1
14	a	1102	CLA	CBA-CGA-O2A-C1
14	a	1118	CLA	CBA-CGA-O2A-C1
14	a	1131	CLA	CBA-CGA-O2A-C1
14	a	1138	CLA	CBA-CGA-O2A-C1
20	A	5005	LMG	C29-C28-O8-C9
20	G	5005	LMG	C29-C28-O8-C9
20	a	5005	LMG	C29-C28-O8-C9
14	A	1012	CLA	CBD-CGD-O2D-CED
14	A	1013	CLA	CBD-CGD-O2D-CED
14	A	1101	CLA	CBD-CGD-O2D-CED
14	A	1105	CLA	CBD-CGD-O2D-CED
14	A	1106	CLA	CBD-CGD-O2D-CED
14	A	1112	CLA	CBD-CGD-O2D-CED
14	A	1128	CLA	CBD-CGD-O2D-CED
14	B	1023	CLA	CBD-CGD-O2D-CED
14	B	1201	CLA	CBD-CGD-O2D-CED
14	B	1212	CLA	CBD-CGD-O2D-CED
14	B	1214	CLA	CBD-CGD-O2D-CED
14	B	1218	CLA	CBD-CGD-O2D-CED
14	B	1219	CLA	CBD-CGD-O2D-CED
14	B	1222	CLA	CBD-CGD-O2D-CED
14	B	1223	CLA	CBD-CGD-O2D-CED
14	B	1235	CLA	CBD-CGD-O2D-CED
14	B	1236	CLA	CBD-CGD-O2D-CED
14	B	1238	CLA	CBD-CGD-O2D-CED
14	G	1012	CLA	CBD-CGD-O2D-CED
14	G	1013	CLA	CBD-CGD-O2D-CED
14	G	1101	CLA	CBD-CGD-O2D-CED
14	G	1105	CLA	CBD-CGD-O2D-CED
14	G	1106	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	G	1112	CLA	CBD-CGD-O2D-CED
14	G	1128	CLA	CBD-CGD-O2D-CED
14	H	1023	CLA	CBD-CGD-O2D-CED
14	H	1201	CLA	CBD-CGD-O2D-CED
14	H	1212	CLA	CBD-CGD-O2D-CED
14	H	1214	CLA	CBD-CGD-O2D-CED
14	H	1218	CLA	CBD-CGD-O2D-CED
14	H	1219	CLA	CBD-CGD-O2D-CED
14	H	1222	CLA	CBD-CGD-O2D-CED
14	H	1223	CLA	CBD-CGD-O2D-CED
14	H	1235	CLA	CBD-CGD-O2D-CED
14	H	1236	CLA	CBD-CGD-O2D-CED
14	H	1238	CLA	CBD-CGD-O2D-CED
14	L	1503	CLA	CBD-CGD-O2D-CED
14	U	1503	CLA	CBD-CGD-O2D-CED
14	a	1012	CLA	CBD-CGD-O2D-CED
14	a	1013	CLA	CBD-CGD-O2D-CED
14	a	1101	CLA	CBD-CGD-O2D-CED
14	a	1105	CLA	CBD-CGD-O2D-CED
14	a	1106	CLA	CBD-CGD-O2D-CED
14	a	1112	CLA	CBD-CGD-O2D-CED
14	a	1128	CLA	CBD-CGD-O2D-CED
14	b	1023	CLA	CBD-CGD-O2D-CED
14	b	1201	CLA	CBD-CGD-O2D-CED
14	b	1212	CLA	CBD-CGD-O2D-CED
14	b	1214	CLA	CBD-CGD-O2D-CED
14	b	1218	CLA	CBD-CGD-O2D-CED
14	b	1219	CLA	CBD-CGD-O2D-CED
14	b	1222	CLA	CBD-CGD-O2D-CED
14	b	1223	CLA	CBD-CGD-O2D-CED
14	b	1235	CLA	CBD-CGD-O2D-CED
14	b	1236	CLA	CBD-CGD-O2D-CED
14	b	1238	CLA	CBD-CGD-O2D-CED
14	l	1503	CLA	CBD-CGD-O2D-CED
15	A	1120	F6C	CBD-CGD-O2D-CED
15	G	1120	F6C	CBD-CGD-O2D-CED
15	a	1120	F6C	CBD-CGD-O2D-CED
14	A	1131	CLA	O1D-CGD-O2D-CED
14	G	1131	CLA	O1D-CGD-O2D-CED
14	a	1131	CLA	O1D-CGD-O2D-CED
14	A	1128	CLA	O1A-CGA-O2A-C1
14	G	1128	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1128	CLA	O1A-CGA-O2A-C1
14	A	1116	CLA	C4-C3-C5-C6
14	A	1118	CLA	C4-C3-C5-C6
14	A	1136	CLA	C4-C3-C5-C6
14	B	1214	CLA	C4-C3-C5-C6
14	B	1216	CLA	C4-C3-C5-C6
14	B	1229	CLA	C4-C3-C5-C6
14	G	1116	CLA	C4-C3-C5-C6
14	G	1118	CLA	C4-C3-C5-C6
14	G	1130	CLA	C4-C3-C5-C6
14	G	1136	CLA	C4-C3-C5-C6
14	H	1214	CLA	C4-C3-C5-C6
14	H	1216	CLA	C4-C3-C5-C6
14	H	1229	CLA	C4-C3-C5-C6
14	a	1116	CLA	C4-C3-C5-C6
14	a	1118	CLA	C4-C3-C5-C6
14	a	1130	CLA	C4-C3-C5-C6
14	a	1136	CLA	C4-C3-C5-C6
14	b	1214	CLA	C4-C3-C5-C6
14	b	1216	CLA	C4-C3-C5-C6
14	b	1229	CLA	C4-C3-C5-C6
15	B	1237	F6C	C4-C3-C5-C6
15	H	1237	F6C	C4-C3-C5-C6
15	b	1237	F6C	C4-C3-C5-C6
14	A	1116	CLA	C2-C3-C5-C6
14	A	1118	CLA	C2-C3-C5-C6
14	A	1130	CLA	C2-C3-C5-C6
14	A	1136	CLA	C2-C3-C5-C6
14	B	1201	CLA	C2-C3-C5-C6
14	B	1214	CLA	C2-C3-C5-C6
14	B	1216	CLA	C2-C3-C5-C6
14	B	1229	CLA	C2-C3-C5-C6
14	G	1116	CLA	C2-C3-C5-C6
14	G	1118	CLA	C2-C3-C5-C6
14	G	1130	CLA	C2-C3-C5-C6
14	G	1136	CLA	C2-C3-C5-C6
14	H	1201	CLA	C2-C3-C5-C6
14	H	1214	CLA	C2-C3-C5-C6
14	H	1216	CLA	C2-C3-C5-C6
14	H	1229	CLA	C2-C3-C5-C6
14	a	1116	CLA	C2-C3-C5-C6
14	a	1118	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	a	1130	CLA	C2-C3-C5-C6
14	a	1136	CLA	C2-C3-C5-C6
14	b	1201	CLA	C2-C3-C5-C6
14	b	1214	CLA	C2-C3-C5-C6
14	b	1216	CLA	C2-C3-C5-C6
14	b	1229	CLA	C2-C3-C5-C6
15	B	1237	F6C	C2-C3-C5-C6
15	H	1237	F6C	C2-C3-C5-C6
15	b	1237	F6C	C2-C3-C5-C6
14	B	1206	CLA	O1D-CGD-O2D-CED
14	H	1206	CLA	O1D-CGD-O2D-CED
14	b	1206	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	C2A-CAA-CBA-CGA
14	A	1131	CLA	C2A-CAA-CBA-CGA
14	G	1102	CLA	C2A-CAA-CBA-CGA
14	G	1131	CLA	C2A-CAA-CBA-CGA
14	a	1102	CLA	C2A-CAA-CBA-CGA
14	a	1131	CLA	C2A-CAA-CBA-CGA
14	A	1013	CLA	C3-C5-C6-C7
14	A	1138	CLA	C3-C5-C6-C7
14	B	1022	CLA	C3-C5-C6-C7
14	B	1202	CLA	C3-C5-C6-C7
14	B	1213	CLA	C3-C5-C6-C7
14	G	1013	CLA	C3-C5-C6-C7
14	G	1138	CLA	C3-C5-C6-C7
14	H	1012	CLA	C3-C5-C6-C7
14	H	1202	CLA	C3-C5-C6-C7
14	H	1213	CLA	C3-C5-C6-C7
14	a	1013	CLA	C3-C5-C6-C7
14	a	1138	CLA	C3-C5-C6-C7
14	b	1022	CLA	C3-C5-C6-C7
14	b	1202	CLA	C3-C5-C6-C7
14	b	1213	CLA	C3-C5-C6-C7
14	A	1111	CLA	CBA-CGA-O2A-C1
14	B	1202	CLA	CBA-CGA-O2A-C1
14	B	1204	CLA	CBA-CGA-O2A-C1
14	B	1208	CLA	CBA-CGA-O2A-C1
14	B	1221	CLA	CBA-CGA-O2A-C1
14	B	1226	CLA	CBA-CGA-O2A-C1
14	G	1111	CLA	CBA-CGA-O2A-C1
14	H	1202	CLA	CBA-CGA-O2A-C1
14	H	1204	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	H	1208	CLA	CBA-CGA-O2A-C1
14	H	1221	CLA	CBA-CGA-O2A-C1
14	H	1226	CLA	CBA-CGA-O2A-C1
14	a	1111	CLA	CBA-CGA-O2A-C1
14	b	1202	CLA	CBA-CGA-O2A-C1
14	b	1204	CLA	CBA-CGA-O2A-C1
14	b	1208	CLA	CBA-CGA-O2A-C1
14	b	1221	CLA	CBA-CGA-O2A-C1
14	b	1226	CLA	CBA-CGA-O2A-C1
15	B	1237	F6C	CBA-CGA-O2A-C1
15	H	1237	F6C	CBA-CGA-O2A-C1
15	b	1237	F6C	CBA-CGA-O2A-C1
20	I	5006	LMG	C29-C28-O8-C9
20	R	5006	LMG	C29-C28-O8-C9
20	i	5006	LMG	C29-C28-O8-C9
18	B	4013	BCR	C15-C16-C17-C18
18	B	4017	BCR	C9-C10-C11-C12
18	B	4017	BCR	C19-C20-C21-C22
18	H	4013	BCR	C15-C16-C17-C18
18	H	4017	BCR	C9-C10-C11-C12
18	H	4017	BCR	C19-C20-C21-C22
18	I	4018	BCR	C9-C10-C11-C12
18	I	4018	BCR	C15-C16-C17-C18
18	I	4020	BCR	C19-C20-C21-C22
18	R	4018	BCR	C9-C10-C11-C12
18	R	4018	BCR	C15-C16-C17-C18
18	R	4018	BCR	C19-C20-C21-C22
18	R	4020	BCR	C19-C20-C21-C22
18	b	4013	BCR	C15-C16-C17-C18
18	b	4017	BCR	C9-C10-C11-C12
18	b	4017	BCR	C19-C20-C21-C22
18	i	4018	BCR	C9-C10-C11-C12
18	i	4018	BCR	C15-C16-C17-C18
18	i	4020	BCR	C19-C20-C21-C22
14	A	1130	CLA	O1A-CGA-O2A-C1
14	G	1130	CLA	O1A-CGA-O2A-C1
14	a	1130	CLA	O1A-CGA-O2A-C1
15	A	1120	F6C	C1A-C2A-CAA-CBA
15	G	1120	F6C	C1A-C2A-CAA-CBA
15	a	1120	F6C	C1A-C2A-CAA-CBA
15	b	1230	F6C	C1A-C2A-CAA-CBA
20	A	5005	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
20	B	5002	LMG	C17-C18-C19-C20
20	G	5005	LMG	C35-C36-C37-C38
20	H	5002	LMG	C17-C18-C19-C20
20	L	5007	LMG	C35-C36-C37-C38
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
21	A	6001	LMT	C4B-C5B-C6B-O6B
21	G	6001	LMT	C4B-C5B-C6B-O6B
21	a	6001	LMT	C4B-C5B-C6B-O6B
14	A	1109	CLA	O1D-CGD-O2D-CED
14	A	1116	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	O1D-CGD-O2D-CED
14	G	1116	CLA	O1D-CGD-O2D-CED
14	a	1109	CLA	O1D-CGD-O2D-CED
14	a	1116	CLA	O1D-CGD-O2D-CED
14	A	1111	CLA	C3-C5-C6-C7
14	B	1220	CLA	C3-C5-C6-C7
14	G	1111	CLA	C3-C5-C6-C7
14	H	1220	CLA	C3-C5-C6-C7
14	L	1503	CLA	C3-C5-C6-C7
14	U	1503	CLA	C3-C5-C6-C7
14	a	1111	CLA	C3-C5-C6-C7
14	b	1220	CLA	C3-C5-C6-C7
14	l	1503	CLA	C3-C5-C6-C7
14	A	1127	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	CBD-CGD-O2D-CED
14	B	1204	CLA	CBD-CGD-O2D-CED
14	G	1127	CLA	CBD-CGD-O2D-CED
14	G	1133	CLA	CBD-CGD-O2D-CED
14	H	1204	CLA	CBD-CGD-O2D-CED
14	a	1127	CLA	CBD-CGD-O2D-CED
14	a	1133	CLA	CBD-CGD-O2D-CED
14	b	1204	CLA	CBD-CGD-O2D-CED
14	A	1107	CLA	O1D-CGD-O2D-CED
14	A	1132	CLA	O1D-CGD-O2D-CED
14	B	1227	CLA	O1D-CGD-O2D-CED
14	B	1239	CLA	O1D-CGD-O2D-CED
14	G	1107	CLA	O1D-CGD-O2D-CED
14	G	1132	CLA	O1D-CGD-O2D-CED
14	H	1227	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	H	1239	CLA	O1D-CGD-O2D-CED
14	a	1107	CLA	O1D-CGD-O2D-CED
14	a	1132	CLA	O1D-CGD-O2D-CED
14	b	1227	CLA	O1D-CGD-O2D-CED
14	b	1239	CLA	O1D-CGD-O2D-CED
14	A	1104	CLA	CBA-CGA-O2A-C1
14	A	1117	CLA	CBA-CGA-O2A-C1
14	A	1128	CLA	CBA-CGA-O2A-C1
14	A	1130	CLA	CBA-CGA-O2A-C1
14	B	1021	CLA	CBA-CGA-O2A-C1
14	B	1211	CLA	CBA-CGA-O2A-C1
14	B	1231	CLA	CBA-CGA-O2A-C1
14	G	1104	CLA	CBA-CGA-O2A-C1
14	G	1117	CLA	CBA-CGA-O2A-C1
14	G	1130	CLA	CBA-CGA-O2A-C1
14	H	1021	CLA	CBA-CGA-O2A-C1
14	H	1211	CLA	CBA-CGA-O2A-C1
14	H	1231	CLA	CBA-CGA-O2A-C1
14	a	1104	CLA	CBA-CGA-O2A-C1
14	a	1117	CLA	CBA-CGA-O2A-C1
14	a	1130	CLA	CBA-CGA-O2A-C1
14	b	1021	CLA	CBA-CGA-O2A-C1
14	b	1211	CLA	CBA-CGA-O2A-C1
14	b	1231	CLA	CBA-CGA-O2A-C1
14	A	1102	CLA	O1D-CGD-O2D-CED
14	G	1102	CLA	O1D-CGD-O2D-CED
14	a	1102	CLA	O1D-CGD-O2D-CED
21	A	6001	LMT	O5B-C5B-C6B-O6B
21	G	6001	LMT	O5B-C5B-C6B-O6B
21	a	6001	LMT	O5B-C5B-C6B-O6B
14	A	1130	CLA	CBD-CGD-O2D-CED
14	B	1208	CLA	CBD-CGD-O2D-CED
14	G	1130	CLA	CBD-CGD-O2D-CED
14	H	1208	CLA	CBD-CGD-O2D-CED
14	a	1130	CLA	CBD-CGD-O2D-CED
14	b	1208	CLA	CBD-CGD-O2D-CED
20	B	5002	LMG	C11-C10-O7-C8
20	H	5002	LMG	C11-C10-O7-C8
20	b	5002	LMG	C11-C10-O7-C8
14	A	1104	CLA	O1A-CGA-O2A-C1
14	B	1213	CLA	O1D-CGD-O2D-CED
14	H	1213	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	b	1213	CLA	O1D-CGD-O2D-CED
14	B	1203	CLA	C3-C5-C6-C7
14	H	1203	CLA	C3-C5-C6-C7
14	b	1203	CLA	C3-C5-C6-C7
14	A	1104	CLA	CBD-CGD-O2D-CED
14	A	1113	CLA	CBD-CGD-O2D-CED
14	G	1104	CLA	CBD-CGD-O2D-CED
14	G	1113	CLA	CBD-CGD-O2D-CED
14	a	1104	CLA	CBD-CGD-O2D-CED
14	a	1113	CLA	CBD-CGD-O2D-CED
21	A	6001	LMT	C4'-C5'-C6'-O6'
21	G	6001	LMT	C4'-C5'-C6'-O6'
21	a	6001	LMT	C4'-C5'-C6'-O6'
14	A	1124	CLA	O1D-CGD-O2D-CED
14	A	1137	CLA	O1D-CGD-O2D-CED
14	G	1124	CLA	O1D-CGD-O2D-CED
14	G	1137	CLA	O1D-CGD-O2D-CED
14	L	1501	CLA	O1D-CGD-O2D-CED
14	U	1501	CLA	O1D-CGD-O2D-CED
14	a	1124	CLA	O1D-CGD-O2D-CED
14	a	1137	CLA	O1D-CGD-O2D-CED
14	l	1501	CLA	O1D-CGD-O2D-CED
14	A	1124	CLA	CBA-CGA-O2A-C1
14	G	1124	CLA	CBA-CGA-O2A-C1
14	G	1128	CLA	CBA-CGA-O2A-C1
14	a	1124	CLA	CBA-CGA-O2A-C1
14	a	1128	CLA	CBA-CGA-O2A-C1
13	G	1011	CL0	C4-C3-C5-C6
14	B	1203	CLA	C4-C3-C5-C6
14	H	1203	CLA	C4-C3-C5-C6
14	b	1203	CLA	C4-C3-C5-C6
14	B	1203	CLA	C2-C3-C5-C6
14	H	1203	CLA	C2-C3-C5-C6
14	b	1203	CLA	C2-C3-C5-C6
14	B	1208	CLA	O1A-CGA-O2A-C1
14	B	1211	CLA	O1A-CGA-O2A-C1
14	G	1104	CLA	O1A-CGA-O2A-C1
14	H	1208	CLA	O1A-CGA-O2A-C1
14	H	1211	CLA	O1A-CGA-O2A-C1
14	a	1104	CLA	O1A-CGA-O2A-C1
14	b	1208	CLA	O1A-CGA-O2A-C1
14	b	1211	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1239	CLA	C2C-C3C-CAC-CBC
14	H	1239	CLA	C2C-C3C-CAC-CBC
14	b	1239	CLA	C2C-C3C-CAC-CBC
15	A	1121	F6C	C2A-CAA-CBA-CGA
15	G	1121	F6C	C2A-CAA-CBA-CGA
15	a	1121	F6C	C2A-CAA-CBA-CGA
14	A	1114	CLA	O1D-CGD-O2D-CED
14	A	1118	CLA	O1D-CGD-O2D-CED
14	G	1114	CLA	O1D-CGD-O2D-CED
14	G	1118	CLA	O1D-CGD-O2D-CED
14	a	1114	CLA	O1D-CGD-O2D-CED
14	a	1118	CLA	O1D-CGD-O2D-CED
14	B	1239	CLA	O1A-CGA-O2A-C1
14	H	1239	CLA	O1A-CGA-O2A-C1
14	b	1239	CLA	O1A-CGA-O2A-C1
20	I	5006	LMG	O6-C1-O1-C7
20	R	5006	LMG	O6-C1-O1-C7
20	i	5006	LMG	O6-C1-O1-C7
21	A	6001	LMT	O5'-C1'-O1'-C1
21	G	6001	LMT	O5'-C1'-O1'-C1
21	a	6001	LMT	O5'-C1'-O1'-C1
14	B	1229	CLA	CBA-CGA-O2A-C1
14	B	1239	CLA	CBA-CGA-O2A-C1
14	H	1229	CLA	CBA-CGA-O2A-C1
14	H	1239	CLA	CBA-CGA-O2A-C1
14	b	1229	CLA	CBA-CGA-O2A-C1
14	b	1239	CLA	CBA-CGA-O2A-C1
14	A	1103	CLA	CBD-CGD-O2D-CED
14	B	1225	CLA	CBD-CGD-O2D-CED
14	B	1234	CLA	CBD-CGD-O2D-CED
14	G	1103	CLA	CBD-CGD-O2D-CED
14	H	1225	CLA	CBD-CGD-O2D-CED
14	H	1234	CLA	CBD-CGD-O2D-CED
14	a	1103	CLA	CBD-CGD-O2D-CED
14	b	1225	CLA	CBD-CGD-O2D-CED
14	b	1234	CLA	CBD-CGD-O2D-CED
14	A	1124	CLA	O1A-CGA-O2A-C1
14	B	1021	CLA	O1A-CGA-O2A-C1
14	B	1231	CLA	O1A-CGA-O2A-C1
14	G	1124	CLA	O1A-CGA-O2A-C1
14	H	1021	CLA	O1A-CGA-O2A-C1
14	H	1231	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	a	1124	CLA	O1A-CGA-O2A-C1
14	b	1021	CLA	O1A-CGA-O2A-C1
14	b	1231	CLA	O1A-CGA-O2A-C1
15	B	1237	F6C	O1D-CGD-O2D-CED
15	H	1237	F6C	O1D-CGD-O2D-CED
15	b	1237	F6C	O1D-CGD-O2D-CED
14	B	1215	CLA	C3-C5-C6-C7
14	H	1215	CLA	C3-C5-C6-C7
14	b	1215	CLA	C3-C5-C6-C7
14	A	1117	CLA	O1A-CGA-O2A-C1
14	B	1229	CLA	O1A-CGA-O2A-C1
14	G	1117	CLA	O1A-CGA-O2A-C1
14	H	1229	CLA	O1A-CGA-O2A-C1
14	a	1117	CLA	O1A-CGA-O2A-C1
14	b	1229	CLA	O1A-CGA-O2A-C1
15	B	1230	F6C	C1A-C2A-CAA-CBA
15	H	1230	F6C	C1A-C2A-CAA-CBA
20	B	5002	LMG	O9-C10-O7-C8
20	H	5002	LMG	O9-C10-O7-C8
20	b	5002	LMG	O9-C10-O7-C8
14	A	1115	CLA	CBA-CGA-O2A-C1
14	A	1119	CLA	CBA-CGA-O2A-C1
14	B	1201	CLA	CBA-CGA-O2A-C1
14	B	1215	CLA	CBA-CGA-O2A-C1
14	B	1216	CLA	CBA-CGA-O2A-C1
14	B	1223	CLA	CBA-CGA-O2A-C1
14	B	1234	CLA	CBA-CGA-O2A-C1
14	G	1115	CLA	CBA-CGA-O2A-C1
14	G	1119	CLA	CBA-CGA-O2A-C1
14	H	1201	CLA	CBA-CGA-O2A-C1
14	H	1215	CLA	CBA-CGA-O2A-C1
14	H	1216	CLA	CBA-CGA-O2A-C1
14	H	1223	CLA	CBA-CGA-O2A-C1
14	H	1234	CLA	CBA-CGA-O2A-C1
14	L	1502	CLA	CBA-CGA-O2A-C1
14	U	1502	CLA	CBA-CGA-O2A-C1
14	a	1115	CLA	CBA-CGA-O2A-C1
14	a	1119	CLA	CBA-CGA-O2A-C1
14	b	1201	CLA	CBA-CGA-O2A-C1
14	b	1215	CLA	CBA-CGA-O2A-C1
14	b	1216	CLA	CBA-CGA-O2A-C1
14	b	1223	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	1234	CLA	CBA-CGA-O2A-C1
14	l	1502	CLA	CBA-CGA-O2A-C1
19	A	5001	LHG	C11-C12-C13-C14
19	G	5001	LHG	C11-C12-C13-C14
19	a	5001	LHG	C11-C12-C13-C14
14	B	1218	CLA	O1D-CGD-O2D-CED
14	B	1219	CLA	O1D-CGD-O2D-CED
14	G	1111	CLA	O1D-CGD-O2D-CED
14	H	1218	CLA	O1D-CGD-O2D-CED
14	H	1219	CLA	O1D-CGD-O2D-CED
14	L	1503	CLA	O1D-CGD-O2D-CED
14	U	1503	CLA	O1D-CGD-O2D-CED
14	a	1111	CLA	O1D-CGD-O2D-CED
14	b	1218	CLA	O1D-CGD-O2D-CED
14	b	1219	CLA	O1D-CGD-O2D-CED
14	l	1503	CLA	O1D-CGD-O2D-CED
13	A	1011	CL0	C4-C3-C5-C6
13	a	1011	CL0	C4-C3-C5-C6
14	A	1115	CLA	C4-C3-C5-C6
14	B	1022	CLA	C4-C3-C5-C6
14	G	1115	CLA	C4-C3-C5-C6
14	H	1012	CLA	C4-C3-C5-C6
14	a	1115	CLA	C4-C3-C5-C6
14	b	1022	CLA	C4-C3-C5-C6
16	B	2002	PQN	C14-C13-C15-C16
16	H	2002	PQN	C14-C13-C15-C16
16	b	2002	PQN	C14-C13-C15-C16
14	A	1115	CLA	C2-C3-C5-C6
14	B	1022	CLA	C2-C3-C5-C6
14	G	1115	CLA	C2-C3-C5-C6
14	H	1012	CLA	C2-C3-C5-C6
14	a	1115	CLA	C2-C3-C5-C6
14	b	1022	CLA	C2-C3-C5-C6
16	B	2002	PQN	C12-C13-C15-C16
16	H	2002	PQN	C12-C13-C15-C16
16	b	2002	PQN	C12-C13-C15-C16
14	B	1201	CLA	C3-C5-C6-C7
14	H	1201	CLA	C3-C5-C6-C7
14	b	1201	CLA	C3-C5-C6-C7
14	A	1104	CLA	C6-C7-C8-C9
14	A	1123	CLA	C6-C7-C8-C9
14	A	1126	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	A	1133	CLA	C11-C10-C8-C9
14	A	1140	CLA	C6-C7-C8-C9
14	G	1104	CLA	C6-C7-C8-C9
14	G	1123	CLA	C6-C7-C8-C9
14	G	1126	CLA	C6-C7-C8-C9
14	G	1133	CLA	C11-C10-C8-C9
14	G	1140	CLA	C6-C7-C8-C9
14	a	1104	CLA	C6-C7-C8-C9
14	a	1123	CLA	C6-C7-C8-C9
14	a	1126	CLA	C6-C7-C8-C9
14	a	1133	CLA	C11-C10-C8-C9
14	a	1140	CLA	C6-C7-C8-C9
16	A	2001	PQN	C19-C18-C20-C21
16	G	2001	PQN	C19-C18-C20-C21
16	a	2001	PQN	C19-C18-C20-C21
14	A	1111	CLA	O1D-CGD-O2D-CED
14	B	1212	CLA	O1D-CGD-O2D-CED
14	B	1214	CLA	O1D-CGD-O2D-CED
14	H	1212	CLA	O1D-CGD-O2D-CED
14	H	1214	CLA	O1D-CGD-O2D-CED
14	b	1212	CLA	O1D-CGD-O2D-CED
14	b	1214	CLA	O1D-CGD-O2D-CED
15	A	1120	F6C	O1D-CGD-O2D-CED
15	G	1120	F6C	O1D-CGD-O2D-CED
15	a	1120	F6C	O1D-CGD-O2D-CED
20	I	5006	LMG	C2-C1-O1-C7
20	R	5006	LMG	C2-C1-O1-C7
20	i	5006	LMG	C2-C1-O1-C7
21	A	6001	LMT	C2'-C1'-O1'-C1
21	G	6001	LMT	C2'-C1'-O1'-C1
21	a	6001	LMT	C2'-C1'-O1'-C1
14	A	1106	CLA	O1D-CGD-O2D-CED
14	G	1106	CLA	O1D-CGD-O2D-CED
14	a	1106	CLA	O1D-CGD-O2D-CED
14	H	1223	CLA	O1A-CGA-O2A-C1
14	b	1223	CLA	O1A-CGA-O2A-C1
14	A	1101	CLA	O1D-CGD-O2D-CED
14	A	1112	CLA	O1D-CGD-O2D-CED
14	G	1101	CLA	O1D-CGD-O2D-CED
14	G	1112	CLA	O1D-CGD-O2D-CED
14	a	1101	CLA	O1D-CGD-O2D-CED
14	a	1112	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	4001	BCR	C36-C18-C19-C20
18	A	4002	BCR	C7-C8-C9-C34
18	A	4002	BCR	C37-C22-C23-C24
18	A	4011	BCR	C37-C22-C23-C24
18	B	4004	BCR	C7-C8-C9-C34
18	B	4004	BCR	C37-C22-C23-C24
18	B	4006	BCR	C7-C8-C9-C34
18	B	4006	BCR	C37-C22-C23-C24
18	B	4010	BCR	C36-C18-C19-C20
18	B	4013	BCR	C36-C18-C19-C20
18	B	4013	BCR	C37-C22-C23-C24
18	B	4014	BCR	C36-C18-C19-C20
18	G	4001	BCR	C36-C18-C19-C20
18	G	4002	BCR	C7-C8-C9-C34
18	G	4002	BCR	C37-C22-C23-C24
18	G	4011	BCR	C37-C22-C23-C24
18	H	4004	BCR	C7-C8-C9-C34
18	H	4004	BCR	C37-C22-C23-C24
18	H	4006	BCR	C7-C8-C9-C34
18	H	4006	BCR	C37-C22-C23-C24
18	H	4010	BCR	C36-C18-C19-C20
18	H	4013	BCR	C36-C18-C19-C20
18	H	4013	BCR	C37-C22-C23-C24
18	H	4014	BCR	C36-C18-C19-C20
18	I	4018	BCR	C36-C18-C19-C20
18	L	4022	BCR	C7-C8-C9-C34
18	R	4018	BCR	C36-C18-C19-C20
18	U	4022	BCR	C7-C8-C9-C34
18	a	4001	BCR	C36-C18-C19-C20
18	a	4002	BCR	C7-C8-C9-C34
18	a	4002	BCR	C37-C22-C23-C24
18	a	4011	BCR	C37-C22-C23-C24
18	b	4004	BCR	C7-C8-C9-C34
18	b	4004	BCR	C37-C22-C23-C24
18	b	4006	BCR	C7-C8-C9-C34
18	b	4006	BCR	C37-C22-C23-C24
18	b	4010	BCR	C36-C18-C19-C20
18	b	4013	BCR	C36-C18-C19-C20
18	b	4013	BCR	C37-C22-C23-C24
18	b	4014	BCR	C36-C18-C19-C20
18	i	4018	BCR	C36-C18-C19-C20
18	l	4022	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
18	A	4001	BCR	C7-C8-C9-C10
18	A	4011	BCR	C21-C22-C23-C24
18	B	4004	BCR	C7-C8-C9-C10
18	B	4004	BCR	C21-C22-C23-C24
18	B	4006	BCR	C7-C8-C9-C10
18	B	4006	BCR	C21-C22-C23-C24
18	B	4012	BCR	C7-C8-C9-C10
18	G	4001	BCR	C7-C8-C9-C10
18	G	4011	BCR	C21-C22-C23-C24
18	H	4004	BCR	C7-C8-C9-C10
18	H	4004	BCR	C21-C22-C23-C24
18	H	4006	BCR	C7-C8-C9-C10
18	H	4006	BCR	C21-C22-C23-C24
18	H	4012	BCR	C7-C8-C9-C10
18	L	4022	BCR	C7-C8-C9-C10
18	U	4022	BCR	C7-C8-C9-C10
18	a	4001	BCR	C7-C8-C9-C10
18	a	4011	BCR	C21-C22-C23-C24
18	b	4004	BCR	C7-C8-C9-C10
18	b	4004	BCR	C21-C22-C23-C24
18	b	4006	BCR	C7-C8-C9-C10
18	b	4006	BCR	C21-C22-C23-C24
18	b	4012	BCR	C7-C8-C9-C10
18	l	4022	BCR	C7-C8-C9-C10
14	B	1234	CLA	C2A-CAA-CBA-CGA
14	H	1234	CLA	C2A-CAA-CBA-CGA
14	b	1234	CLA	C2A-CAA-CBA-CGA
14	B	1201	CLA	O1A-CGA-O2A-C1
14	B	1223	CLA	O1A-CGA-O2A-C1
14	H	1201	CLA	O1A-CGA-O2A-C1
14	b	1201	CLA	O1A-CGA-O2A-C1
14	A	1125	CLA	C3-C5-C6-C7
14	G	1125	CLA	C3-C5-C6-C7
14	a	1125	CLA	C3-C5-C6-C7
16	H	2002	PQN	C13-C15-C16-C17
14	B	1220	CLA	CBD-CGD-O2D-CED
14	a	1125	CLA	CBD-CGD-O2D-CED
13	A	1011	CL0	CBA-CGA-O2A-C1
13	G	1011	CL0	CBA-CGA-O2A-C1
13	a	1011	CL0	CBA-CGA-O2A-C1
14	B	1222	CLA	C13-C15-C16-C17
14	B	1222	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	H	1222	CLA	C13-C15-C16-C17
14	H	1222	CLA	C15-C16-C17-C18
14	b	1222	CLA	C13-C15-C16-C17
14	b	1222	CLA	C15-C16-C17-C18
14	A	1111	CLA	C2-C1-O2A-CGA
14	A	1119	CLA	C2-C1-O2A-CGA
14	A	1140	CLA	C2-C1-O2A-CGA
14	G	1111	CLA	C2-C1-O2A-CGA
14	G	1119	CLA	C2-C1-O2A-CGA
14	G	1140	CLA	C2-C1-O2A-CGA
14	L	1502	CLA	C2-C1-O2A-CGA
14	U	1502	CLA	C2-C1-O2A-CGA
14	a	1111	CLA	C2-C1-O2A-CGA
14	a	1119	CLA	C2-C1-O2A-CGA
14	a	1140	CLA	C2-C1-O2A-CGA
14	l	1502	CLA	C2-C1-O2A-CGA
14	A	1013	CLA	O1D-CGD-O2D-CED
14	B	1023	CLA	O1D-CGD-O2D-CED
14	G	1013	CLA	O1D-CGD-O2D-CED
14	H	1023	CLA	O1D-CGD-O2D-CED
14	a	1013	CLA	O1D-CGD-O2D-CED
14	b	1023	CLA	O1D-CGD-O2D-CED
14	A	1125	CLA	CBD-CGD-O2D-CED
14	G	1125	CLA	CBD-CGD-O2D-CED
14	H	1220	CLA	CBD-CGD-O2D-CED
14	b	1220	CLA	CBD-CGD-O2D-CED
14	A	1117	CLA	C15-C16-C17-C18
14	A	1119	CLA	C10-C11-C12-C13
14	A	1125	CLA	C10-C11-C12-C13
14	G	1117	CLA	C15-C16-C17-C18
14	G	1119	CLA	C10-C11-C12-C13
14	G	1125	CLA	C10-C11-C12-C13
14	a	1117	CLA	C15-C16-C17-C18
14	a	1119	CLA	C10-C11-C12-C13
14	a	1125	CLA	C10-C11-C12-C13
14	B	1217	CLA	C3-C5-C6-C7
14	H	1217	CLA	C3-C5-C6-C7
14	b	1217	CLA	C3-C5-C6-C7
16	B	2002	PQN	C13-C15-C16-C17
16	b	2002	PQN	C13-C15-C16-C17
14	B	1239	CLA	C4C-C3C-CAC-CBC
14	A	1105	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	1128	CLA	O1D-CGD-O2D-CED
14	B	1238	CLA	O1D-CGD-O2D-CED
14	G	1012	CLA	O1D-CGD-O2D-CED
14	G	1105	CLA	O1D-CGD-O2D-CED
14	G	1128	CLA	O1D-CGD-O2D-CED
14	H	1238	CLA	O1D-CGD-O2D-CED
14	a	1105	CLA	O1D-CGD-O2D-CED
14	a	1128	CLA	O1D-CGD-O2D-CED
14	b	1238	CLA	O1D-CGD-O2D-CED
14	H	1239	CLA	C4C-C3C-CAC-CBC
14	b	1239	CLA	C4C-C3C-CAC-CBC
14	A	1125	CLA	C11-C12-C13-C15
14	G	1125	CLA	C11-C12-C13-C15
14	L	1502	CLA	C6-C7-C8-C10
14	U	1502	CLA	C6-C7-C8-C10
14	a	1125	CLA	C11-C12-C13-C15
14	l	1502	CLA	C6-C7-C8-C10
14	A	1012	CLA	O1D-CGD-O2D-CED
14	a	1012	CLA	O1D-CGD-O2D-CED
18	A	4003	BCR	C19-C20-C21-C22
18	A	4007	BCR	C19-C20-C21-C22
18	B	4013	BCR	C19-C20-C21-C22
18	B	4014	BCR	C9-C10-C11-C12
18	G	4003	BCR	C19-C20-C21-C22
18	G	4007	BCR	C19-C20-C21-C22
18	H	4013	BCR	C19-C20-C21-C22
18	H	4014	BCR	C9-C10-C11-C12
18	I	4020	BCR	C15-C16-C17-C18
18	R	4020	BCR	C15-C16-C17-C18
18	a	4003	BCR	C19-C20-C21-C22
18	a	4007	BCR	C19-C20-C21-C22
18	b	4013	BCR	C19-C20-C21-C22
18	b	4014	BCR	C9-C10-C11-C12
18	i	4020	BCR	C15-C16-C17-C18
14	B	1221	CLA	C3-C5-C6-C7
14	H	1221	CLA	C3-C5-C6-C7
14	b	1221	CLA	C3-C5-C6-C7
14	A	1138	CLA	C10-C11-C12-C13
14	G	1138	CLA	C10-C11-C12-C13
14	a	1138	CLA	C10-C11-C12-C13
19	H	5004	LHG	C28-C29-C30-C31
19	b	5004	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
19	A	5001	LHG	C23-C24-C25-C26
19	G	5001	LHG	C23-C24-C25-C26
19	a	5001	LHG	C23-C24-C25-C26
20	B	5002	LMG	C10-C11-C12-C13
20	H	5002	LMG	C10-C11-C12-C13
20	b	5002	LMG	C10-C11-C12-C13
14	B	1234	CLA	O1A-CGA-O2A-C1
14	G	1115	CLA	O1A-CGA-O2A-C1
14	H	1216	CLA	O1A-CGA-O2A-C1
14	H	1234	CLA	O1A-CGA-O2A-C1
14	b	1216	CLA	O1A-CGA-O2A-C1
14	b	1234	CLA	O1A-CGA-O2A-C1
14	B	1222	CLA	O1D-CGD-O2D-CED
14	B	1236	CLA	O1D-CGD-O2D-CED
14	H	1222	CLA	O1D-CGD-O2D-CED
14	H	1236	CLA	O1D-CGD-O2D-CED
14	b	1222	CLA	O1D-CGD-O2D-CED
14	b	1236	CLA	O1D-CGD-O2D-CED
14	A	1119	CLA	C15-C16-C17-C18
14	A	1125	CLA	C8-C10-C11-C12
14	B	1023	CLA	C13-C15-C16-C17
14	B	1210	CLA	C10-C11-C12-C13
14	B	1214	CLA	C8-C10-C11-C12
14	B	1215	CLA	C10-C11-C12-C13
14	G	1119	CLA	C15-C16-C17-C18
14	H	1023	CLA	C13-C15-C16-C17
14	H	1210	CLA	C10-C11-C12-C13
14	H	1214	CLA	C8-C10-C11-C12
14	H	1215	CLA	C10-C11-C12-C13
14	a	1119	CLA	C15-C16-C17-C18
14	b	1023	CLA	C13-C15-C16-C17
14	b	1210	CLA	C10-C11-C12-C13
14	b	1214	CLA	C8-C10-C11-C12
14	b	1215	CLA	C10-C11-C12-C13
15	B	1237	F6C	C5-C6-C7-C8
15	H	1237	F6C	C5-C6-C7-C8
15	b	1237	F6C	C5-C6-C7-C8
16	B	2002	PQN	C18-C20-C21-C22
16	H	2002	PQN	C18-C20-C21-C22
16	b	2002	PQN	C18-C20-C21-C22
14	A	1111	CLA	C2A-CAA-CBA-CGA
14	A	1123	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	A	1132	CLA	C2A-CAA-CBA-CGA
14	A	1135	CLA	C2A-CAA-CBA-CGA
14	B	1022	CLA	C2A-CAA-CBA-CGA
14	B	1206	CLA	C2A-CAA-CBA-CGA
14	B	1210	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	1238	CLA	C2A-CAA-CBA-CGA
14	G	1111	CLA	C2A-CAA-CBA-CGA
14	G	1123	CLA	C2A-CAA-CBA-CGA
14	G	1132	CLA	C2A-CAA-CBA-CGA
14	G	1135	CLA	C2A-CAA-CBA-CGA
14	H	1012	CLA	C2A-CAA-CBA-CGA
14	H	1206	CLA	C2A-CAA-CBA-CGA
14	H	1210	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	1238	CLA	C2A-CAA-CBA-CGA
14	a	1111	CLA	C2A-CAA-CBA-CGA
14	a	1123	CLA	C2A-CAA-CBA-CGA
14	a	1132	CLA	C2A-CAA-CBA-CGA
14	a	1135	CLA	C2A-CAA-CBA-CGA
14	b	1022	CLA	C2A-CAA-CBA-CGA
14	b	1206	CLA	C2A-CAA-CBA-CGA
14	b	1210	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	1238	CLA	C2A-CAA-CBA-CGA
18	B	4006	BCR	C10-C11-C12-C13
18	L	4022	BCR	C10-C11-C12-C13
18	U	4022	BCR	C10-C11-C12-C13
18	l	4022	BCR	C10-C11-C12-C13
14	A	1013	CLA	C5-C6-C7-C8
14	A	1104	CLA	C15-C16-C17-C18
14	A	1125	CLA	C15-C16-C17-C18
14	A	1140	CLA	C5-C6-C7-C8
14	B	1204	CLA	C5-C6-C7-C8
14	B	1204	CLA	C10-C11-C12-C13
14	B	1211	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	B	1211	CLA	C15-C16-C17-C18
14	B	1226	CLA	C13-C15-C16-C17
14	G	1013	CLA	C5-C6-C7-C8
14	G	1125	CLA	C8-C10-C11-C12
14	G	1125	CLA	C15-C16-C17-C18
14	G	1140	CLA	C5-C6-C7-C8
14	H	1204	CLA	C5-C6-C7-C8
14	H	1204	CLA	C10-C11-C12-C13
14	H	1211	CLA	C5-C6-C7-C8
14	H	1226	CLA	C13-C15-C16-C17
14	L	1501	CLA	C10-C11-C12-C13
14	U	1501	CLA	C10-C11-C12-C13
14	a	1013	CLA	C5-C6-C7-C8
14	a	1125	CLA	C8-C10-C11-C12
14	a	1125	CLA	C15-C16-C17-C18
14	a	1140	CLA	C5-C6-C7-C8
14	b	1204	CLA	C5-C6-C7-C8
14	b	1204	CLA	C10-C11-C12-C13
14	b	1211	CLA	C5-C6-C7-C8
14	b	1211	CLA	C15-C16-C17-C18
14	b	1226	CLA	C13-C15-C16-C17
14	l	1501	CLA	C10-C11-C12-C13
14	A	1115	CLA	O1A-CGA-O2A-C1
14	A	1119	CLA	O1A-CGA-O2A-C1
14	B	1216	CLA	O1A-CGA-O2A-C1
14	G	1119	CLA	O1A-CGA-O2A-C1
14	a	1115	CLA	O1A-CGA-O2A-C1
14	a	1119	CLA	O1A-CGA-O2A-C1
14	A	1136	CLA	C3-C5-C6-C7
14	G	1136	CLA	C3-C5-C6-C7
14	a	1136	CLA	C3-C5-C6-C7
19	B	5004	LHG	C28-C29-C30-C31
14	A	1102	CLA	C10-C11-C12-C13
14	A	1117	CLA	C10-C11-C12-C13
14	A	1122	CLA	C5-C6-C7-C8
14	A	1132	CLA	C5-C6-C7-C8
14	B	1204	CLA	C13-C15-C16-C17
14	B	1213	CLA	C5-C6-C7-C8
14	B	1214	CLA	C5-C6-C7-C8
14	B	1221	CLA	C10-C11-C12-C13
14	B	1225	CLA	C5-C6-C7-C8
14	B	1239	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	G	1102	CLA	C10-C11-C12-C13
14	G	1104	CLA	C15-C16-C17-C18
14	G	1117	CLA	C10-C11-C12-C13
14	G	1122	CLA	C5-C6-C7-C8
14	G	1132	CLA	C5-C6-C7-C8
14	H	1204	CLA	C13-C15-C16-C17
14	H	1211	CLA	C15-C16-C17-C18
14	H	1213	CLA	C5-C6-C7-C8
14	H	1214	CLA	C5-C6-C7-C8
14	H	1221	CLA	C10-C11-C12-C13
14	H	1225	CLA	C5-C6-C7-C8
14	H	1239	CLA	C10-C11-C12-C13
14	a	1102	CLA	C10-C11-C12-C13
14	a	1104	CLA	C15-C16-C17-C18
14	a	1117	CLA	C10-C11-C12-C13
14	a	1122	CLA	C5-C6-C7-C8
14	a	1132	CLA	C5-C6-C7-C8
14	b	1204	CLA	C13-C15-C16-C17
14	b	1213	CLA	C5-C6-C7-C8
14	b	1214	CLA	C5-C6-C7-C8
14	b	1221	CLA	C10-C11-C12-C13
14	b	1225	CLA	C5-C6-C7-C8
14	b	1239	CLA	C10-C11-C12-C13
16	B	2002	PQN	C20-C21-C22-C23
16	H	2002	PQN	C20-C21-C22-C23
16	b	2002	PQN	C20-C21-C22-C23
14	L	1502	CLA	O1A-CGA-O2A-C1
14	U	1502	CLA	O1A-CGA-O2A-C1
14	l	1502	CLA	O1A-CGA-O2A-C1
14	H	1229	CLA	C8-C10-C11-C12
14	b	1229	CLA	C8-C10-C11-C12
14	B	1208	CLA	O1D-CGD-O2D-CED
14	H	1208	CLA	O1D-CGD-O2D-CED
14	b	1208	CLA	O1D-CGD-O2D-CED
20	L	5007	LMG	C20-C21-C22-C23
20	U	5007	LMG	C20-C21-C22-C23
20	l	5007	LMG	C20-C21-C22-C23
14	B	1223	CLA	O1D-CGD-O2D-CED
14	B	1235	CLA	O1D-CGD-O2D-CED
14	H	1223	CLA	O1D-CGD-O2D-CED
14	H	1235	CLA	O1D-CGD-O2D-CED
14	b	1204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	b	1223	CLA	O1D-CGD-O2D-CED
14	b	1235	CLA	O1D-CGD-O2D-CED
14	A	1128	CLA	C10-C11-C12-C13
14	A	1133	CLA	C10-C11-C12-C13
14	B	1223	CLA	C8-C10-C11-C12
14	B	1229	CLA	C8-C10-C11-C12
14	G	1128	CLA	C10-C11-C12-C13
14	G	1133	CLA	C10-C11-C12-C13
14	H	1223	CLA	C8-C10-C11-C12
14	a	1128	CLA	C10-C11-C12-C13
14	a	1133	CLA	C10-C11-C12-C13
14	b	1223	CLA	C8-C10-C11-C12
15	B	1237	F6C	C8-C10-C11-C12
15	H	1237	F6C	C8-C10-C11-C12
15	b	1237	F6C	C8-C10-C11-C12
16	B	2002	PQN	C25-C26-C27-C28
16	H	2002	PQN	C25-C26-C27-C28
16	b	2002	PQN	C25-C26-C27-C28
14	A	1127	CLA	O1D-CGD-O2D-CED
14	B	1201	CLA	O1D-CGD-O2D-CED
14	B	1204	CLA	O1D-CGD-O2D-CED
14	G	1127	CLA	O1D-CGD-O2D-CED
14	H	1201	CLA	O1D-CGD-O2D-CED
14	H	1204	CLA	O1D-CGD-O2D-CED
14	a	1127	CLA	O1D-CGD-O2D-CED
14	b	1201	CLA	O1D-CGD-O2D-CED
14	B	1021	CLA	C8-C10-C11-C12
14	H	1021	CLA	C8-C10-C11-C12
14	L	1503	CLA	C8-C10-C11-C12
14	U	1503	CLA	C8-C10-C11-C12
14	b	1021	CLA	C8-C10-C11-C12
14	l	1503	CLA	C8-C10-C11-C12
16	G	2001	PQN	C23-C25-C26-C27
16	a	2001	PQN	C23-C25-C26-C27
14	B	1215	CLA	O1A-CGA-O2A-C1
14	H	1215	CLA	O1A-CGA-O2A-C1
14	b	1215	CLA	O1A-CGA-O2A-C1
16	A	2001	PQN	C23-C25-C26-C27
18	A	4008	BCR	C9-C10-C11-C12
14	B	1203	CLA	C15-C16-C17-C18
14	b	1203	CLA	C15-C16-C17-C18
14	A	1140	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	B	1023	CLA	C2A-CAA-CBA-CGA
14	G	1140	CLA	C2A-CAA-CBA-CGA
14	H	1023	CLA	C2A-CAA-CBA-CGA
14	H	1213	CLA	C2A-CAA-CBA-CGA
14	a	1140	CLA	C2A-CAA-CBA-CGA
14	b	1023	CLA	C2A-CAA-CBA-CGA
14	b	1213	CLA	C2A-CAA-CBA-CGA
14	A	1130	CLA	O1D-CGD-O2D-CED
14	a	1130	CLA	O1D-CGD-O2D-CED
14	B	1238	CLA	CBA-CGA-O2A-C1
14	H	1238	CLA	CBA-CGA-O2A-C1
14	b	1238	CLA	CBA-CGA-O2A-C1
20	L	5007	LMG	C29-C28-O8-C9
20	U	5007	LMG	C29-C28-O8-C9
20	l	5007	LMG	C29-C28-O8-C9
14	A	1104	CLA	C10-C11-C12-C13
14	A	1119	CLA	C5-C6-C7-C8
14	B	1021	CLA	C15-C16-C17-C18
14	B	1221	CLA	C5-C6-C7-C8
14	G	1104	CLA	C10-C11-C12-C13
14	G	1119	CLA	C5-C6-C7-C8
14	H	1021	CLA	C15-C16-C17-C18
14	H	1203	CLA	C15-C16-C17-C18
14	a	1104	CLA	C10-C11-C12-C13
14	a	1119	CLA	C5-C6-C7-C8
14	b	1021	CLA	C15-C16-C17-C18
14	G	1130	CLA	O1D-CGD-O2D-CED
14	A	1126	CLA	C3-C5-C6-C7
14	B	1205	CLA	C3-C5-C6-C7
14	G	1126	CLA	C3-C5-C6-C7
14	H	1205	CLA	C3-C5-C6-C7
14	a	1126	CLA	C3-C5-C6-C7
14	b	1205	CLA	C3-C5-C6-C7
14	G	1133	CLA	O1D-CGD-O2D-CED
14	a	1133	CLA	O1D-CGD-O2D-CED
14	B	1203	CLA	C8-C10-C11-C12
14	B	1205	CLA	C10-C11-C12-C13
14	B	1234	CLA	C5-C6-C7-C8
14	H	1203	CLA	C8-C10-C11-C12
14	H	1205	CLA	C10-C11-C12-C13
14	H	1221	CLA	C5-C6-C7-C8
14	H	1234	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	a	1126	CLA	C10-C11-C12-C13
14	b	1203	CLA	C8-C10-C11-C12
14	b	1221	CLA	C5-C6-C7-C8
14	b	1234	CLA	C5-C6-C7-C8
14	A	1133	CLA	O1D-CGD-O2D-CED
14	A	1012	CLA	C15-C16-C17-C18
14	A	1119	CLA	C8-C10-C11-C12
14	A	1126	CLA	C10-C11-C12-C13
14	A	1127	CLA	C10-C11-C12-C13
14	A	1127	CLA	C13-C15-C16-C17
14	B	1022	CLA	C8-C10-C11-C12
14	B	1022	CLA	C13-C15-C16-C17
14	B	1211	CLA	C8-C10-C11-C12
14	G	1012	CLA	C15-C16-C17-C18
14	G	1119	CLA	C8-C10-C11-C12
14	G	1126	CLA	C10-C11-C12-C13
14	G	1127	CLA	C10-C11-C12-C13
14	G	1127	CLA	C13-C15-C16-C17
14	H	1012	CLA	C8-C10-C11-C12
14	H	1012	CLA	C13-C15-C16-C17
14	H	1211	CLA	C8-C10-C11-C12
14	H	1222	CLA	C5-C6-C7-C8
14	L	1503	CLA	C13-C15-C16-C17
14	U	1503	CLA	C13-C15-C16-C17
14	a	1012	CLA	C15-C16-C17-C18
14	a	1119	CLA	C8-C10-C11-C12
14	a	1127	CLA	C10-C11-C12-C13
14	a	1127	CLA	C13-C15-C16-C17
14	b	1022	CLA	C8-C10-C11-C12
14	b	1022	CLA	C13-C15-C16-C17
14	b	1205	CLA	C10-C11-C12-C13
14	b	1211	CLA	C8-C10-C11-C12
14	l	1503	CLA	C13-C15-C16-C17
14	A	1113	CLA	O1D-CGD-O2D-CED
14	G	1113	CLA	O1D-CGD-O2D-CED
14	a	1113	CLA	O1D-CGD-O2D-CED
14	B	1238	CLA	C4-C3-C5-C6
14	H	1238	CLA	C4-C3-C5-C6
14	b	1238	CLA	C4-C3-C5-C6
13	G	1011	CL0	C2-C3-C5-C6
13	a	1011	CL0	C2-C3-C5-C6
14	B	1238	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	G	1104	CLA	O1D-CGD-O2D-CED
14	a	1104	CLA	O1D-CGD-O2D-CED
14	B	1021	CLA	C13-C15-C16-C17
14	B	1222	CLA	C5-C6-C7-C8
14	H	1021	CLA	C13-C15-C16-C17
14	b	1021	CLA	C13-C15-C16-C17
14	b	1222	CLA	C5-C6-C7-C8
19	A	5001	LHG	C8-C7-O7-C5
19	G	5001	LHG	C8-C7-O7-C5
19	a	5001	LHG	C8-C7-O7-C5
14	A	1104	CLA	O1D-CGD-O2D-CED
19	A	5001	LHG	O9-C7-O7-C5
19	G	5001	LHG	O9-C7-O7-C5
19	a	5001	LHG	O9-C7-O7-C5
14	B	1225	CLA	C15-C16-C17-C18
14	H	1225	CLA	C15-C16-C17-C18
14	b	1225	CLA	C15-C16-C17-C18
14	A	1103	CLA	C11-C12-C13-C15
14	B	1215	CLA	C11-C12-C13-C15
14	G	1103	CLA	C11-C12-C13-C15
14	H	1215	CLA	C11-C12-C13-C15
14	a	1103	CLA	C11-C12-C13-C15
14	b	1215	CLA	C11-C12-C13-C15
13	A	1011	CL0	O1A-CGA-O2A-C1
13	a	1011	CL0	O1A-CGA-O2A-C1
18	L	4019	BCR	C11-C10-C9-C34
18	U	4019	BCR	C11-C10-C9-C34
18	l	4019	BCR	C11-C10-C9-C34
18	A	4001	BCR	C7-C8-C9-C34
18	A	4007	BCR	C36-C18-C19-C20
18	B	4005	BCR	C36-C18-C19-C20
18	G	4001	BCR	C7-C8-C9-C34
18	G	4007	BCR	C36-C18-C19-C20
18	H	4005	BCR	C36-C18-C19-C20
18	L	4022	BCR	C11-C12-C13-C35
18	U	4022	BCR	C11-C12-C13-C35
18	a	4001	BCR	C7-C8-C9-C34
18	a	4007	BCR	C36-C18-C19-C20
18	b	4005	BCR	C36-C18-C19-C20
18	l	4022	BCR	C11-C12-C13-C35
18	A	4002	BCR	C7-C8-C9-C10
18	A	4002	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	G	4002	BCR	C7-C8-C9-C10
18	G	4002	BCR	C21-C22-C23-C24
18	a	4002	BCR	C7-C8-C9-C10
18	a	4002	BCR	C21-C22-C23-C24
15	B	1237	F6C	C2A-CAA-CBA-CGA
15	H	1237	F6C	C2A-CAA-CBA-CGA
15	b	1237	F6C	C2A-CAA-CBA-CGA
13	G	1011	CL0	O1A-CGA-O2A-C1
14	A	1113	CLA	C2A-CAA-CBA-CGA
14	B	1213	CLA	C2A-CAA-CBA-CGA
14	B	1214	CLA	C2A-CAA-CBA-CGA
14	G	1113	CLA	C2A-CAA-CBA-CGA
14	H	1214	CLA	C2A-CAA-CBA-CGA
14	K	1401	CLA	C2A-CAA-CBA-CGA
14	T	1401	CLA	C2A-CAA-CBA-CGA
14	a	1113	CLA	C2A-CAA-CBA-CGA
14	b	1214	CLA	C2A-CAA-CBA-CGA
14	k	1401	CLA	C2A-CAA-CBA-CGA
13	A	1011	CL0	C16-C17-C18-C20
13	G	1011	CL0	C16-C17-C18-C20
13	a	1011	CL0	C16-C17-C18-C20
14	A	1133	CLA	C11-C12-C13-C14
14	B	1022	CLA	C16-C17-C18-C20
14	B	1225	CLA	C16-C17-C18-C19
14	G	1133	CLA	C11-C12-C13-C14
14	H	1012	CLA	C16-C17-C18-C20
14	H	1225	CLA	C16-C17-C18-C19
14	H	1238	CLA	C16-C17-C18-C20
14	a	1133	CLA	C11-C12-C13-C14
14	b	1022	CLA	C16-C17-C18-C20
14	b	1225	CLA	C16-C17-C18-C19
14	A	1122	CLA	C3-C5-C6-C7
14	G	1122	CLA	C3-C5-C6-C7
14	a	1122	CLA	C3-C5-C6-C7
18	B	4016	BCR	C11-C10-C9-C8
18	H	4016	BCR	C11-C10-C9-C8
18	I	4020	BCR	C11-C10-C9-C8
18	L	4019	BCR	C11-C10-C9-C8
18	R	4020	BCR	C11-C10-C9-C8
18	U	4019	BCR	C11-C10-C9-C8
18	b	4016	BCR	C11-C10-C9-C8
18	i	4020	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	l	4019	BCR	C11-C10-C9-C8
13	A	1011	CL0	C2-C3-C5-C6
14	H	1238	CLA	C2-C3-C5-C6
14	b	1238	CLA	C2-C3-C5-C6
14	A	1117	CLA	C13-C15-C16-C17
14	G	1117	CLA	C13-C15-C16-C17
14	a	1117	CLA	C13-C15-C16-C17
14	A	1012	CLA	C2-C1-O2A-CGA
14	A	1102	CLA	C2-C1-O2A-CGA
14	A	1128	CLA	C2-C1-O2A-CGA
14	A	1133	CLA	C2-C1-O2A-CGA
14	A	1136	CLA	C2-C1-O2A-CGA
14	B	1213	CLA	C2-C1-O2A-CGA
14	G	1012	CLA	C2-C1-O2A-CGA
14	G	1102	CLA	C2-C1-O2A-CGA
14	G	1103	CLA	C2-C1-O2A-CGA
14	G	1128	CLA	C2-C1-O2A-CGA
14	G	1133	CLA	C2-C1-O2A-CGA
14	G	1136	CLA	C2-C1-O2A-CGA
14	H	1213	CLA	C2-C1-O2A-CGA
14	L	1503	CLA	C2-C1-O2A-CGA
14	U	1503	CLA	C2-C1-O2A-CGA
14	a	1012	CLA	C2-C1-O2A-CGA
14	a	1102	CLA	C2-C1-O2A-CGA
14	a	1128	CLA	C2-C1-O2A-CGA
14	a	1133	CLA	C2-C1-O2A-CGA
14	a	1136	CLA	C2-C1-O2A-CGA
14	b	1213	CLA	C2-C1-O2A-CGA
14	l	1503	CLA	C2-C1-O2A-CGA
14	A	1136	CLA	C6-C7-C8-C10
14	B	1211	CLA	C16-C17-C18-C19
14	B	1215	CLA	C11-C12-C13-C14
14	B	1238	CLA	C16-C17-C18-C20
14	G	1136	CLA	C6-C7-C8-C10
14	H	1211	CLA	C16-C17-C18-C19
14	H	1215	CLA	C11-C12-C13-C14
14	a	1136	CLA	C6-C7-C8-C10
14	b	1211	CLA	C16-C17-C18-C19
14	b	1215	CLA	C11-C12-C13-C14
14	b	1238	CLA	C16-C17-C18-C20
19	A	5001	LHG	C29-C30-C31-C32
19	B	5004	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	G	5001	LHG	C29-C30-C31-C32
19	H	5004	LHG	C11-C12-C13-C14
19	a	5001	LHG	C29-C30-C31-C32
19	b	5004	LHG	C11-C12-C13-C14
20	A	5005	LMG	C13-C14-C15-C16
20	G	5005	LMG	C13-C14-C15-C16
20	a	5005	LMG	C13-C14-C15-C16
19	B	5004	LHG	C25-C26-C27-C28
19	H	5004	LHG	C25-C26-C27-C28
21	G	6001	LMT	O5'-C5'-C6'-O6'
21	a	6001	LMT	O5'-C5'-C6'-O6'
19	A	5001	LHG	O1-C1-C2-O2
19	G	5001	LHG	O1-C1-C2-O2
19	a	5001	LHG	O1-C1-C2-O2
19	b	5004	LHG	C25-C26-C27-C28
14	B	1225	CLA	O1D-CGD-O2D-CED
14	H	1225	CLA	O1D-CGD-O2D-CED
14	b	1225	CLA	O1D-CGD-O2D-CED
14	A	1116	CLA	C4B-C3B-CAB-CBB
14	B	1022	CLA	C4B-C3B-CAB-CBB
14	B	1023	CLA	C4B-C3B-CAB-CBB
14	B	1203	CLA	C4B-C3B-CAB-CBB
14	B	1227	CLA	C4B-C3B-CAB-CBB
14	G	1116	CLA	C4B-C3B-CAB-CBB
14	H	1012	CLA	C4B-C3B-CAB-CBB
14	H	1023	CLA	C4B-C3B-CAB-CBB
14	H	1203	CLA	C4B-C3B-CAB-CBB
14	H	1227	CLA	C4B-C3B-CAB-CBB
14	a	1116	CLA	C4B-C3B-CAB-CBB
14	b	1022	CLA	C4B-C3B-CAB-CBB
14	b	1023	CLA	C4B-C3B-CAB-CBB
14	b	1203	CLA	C4B-C3B-CAB-CBB
14	b	1227	CLA	C4B-C3B-CAB-CBB
21	A	6001	LMT	O5'-C5'-C6'-O6'
14	A	1103	CLA	C11-C12-C13-C14
14	A	1133	CLA	C11-C12-C13-C15
14	B	1022	CLA	C16-C17-C18-C19
14	B	1225	CLA	C16-C17-C18-C20
14	G	1103	CLA	C11-C12-C13-C14
14	G	1133	CLA	C11-C12-C13-C15
14	H	1012	CLA	C16-C17-C18-C19
14	H	1225	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	a	1103	CLA	C11-C12-C13-C14
14	a	1133	CLA	C11-C12-C13-C15
14	b	1022	CLA	C16-C17-C18-C19
14	b	1225	CLA	C16-C17-C18-C20
19	B	5004	LHG	C8-C7-O7-C5
19	H	5004	LHG	C8-C7-O7-C5
19	b	5004	LHG	C8-C7-O7-C5
20	A	5005	LMG	C11-C10-O7-C8
20	G	5005	LMG	C11-C10-O7-C8
20	a	5005	LMG	C11-C10-O7-C8
14	H	1223	CLA	C13-C15-C16-C17
19	A	5001	LHG	C30-C31-C32-C33
19	G	5001	LHG	C30-C31-C32-C33
19	a	5001	LHG	C30-C31-C32-C33
20	L	5007	LMG	O10-C28-O8-C9
20	U	5007	LMG	O10-C28-O8-C9
20	l	5007	LMG	O10-C28-O8-C9
14	B	1223	CLA	C3-C5-C6-C7
14	H	1223	CLA	C3-C5-C6-C7
14	b	1223	CLA	C3-C5-C6-C7
14	A	1013	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	1135	CLA	C3A-C2A-CAA-CBA
14	A	1138	CLA	C3A-C2A-CAA-CBA
14	A	1139	CLA	C3A-C2A-CAA-CBA
14	B	1022	CLA	C3A-C2A-CAA-CBA
14	B	1209	CLA	C3A-C2A-CAA-CBA
14	B	1210	CLA	C3A-C2A-CAA-CBA
14	B	1212	CLA	C3A-C2A-CAA-CBA
14	B	1213	CLA	C3A-C2A-CAA-CBA
14	B	1220	CLA	C3A-C2A-CAA-CBA
14	B	1227	CLA	C3A-C2A-CAA-CBA
14	B	1233	CLA	C3A-C2A-CAA-CBA
14	G	1013	CLA	C3A-C2A-CAA-CBA
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	1135	CLA	C3A-C2A-CAA-CBA
14	G	1138	CLA	C3A-C2A-CAA-CBA
14	G	1139	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	1012	CLA	C3A-C2A-CAA-CBA
14	H	1209	CLA	C3A-C2A-CAA-CBA
14	H	1210	CLA	C3A-C2A-CAA-CBA
14	H	1212	CLA	C3A-C2A-CAA-CBA
14	H	1213	CLA	C3A-C2A-CAA-CBA
14	H	1220	CLA	C3A-C2A-CAA-CBA
14	H	1227	CLA	C3A-C2A-CAA-CBA
14	H	1233	CLA	C3A-C2A-CAA-CBA
14	L	1501	CLA	C3A-C2A-CAA-CBA
14	U	1501	CLA	C3A-C2A-CAA-CBA
14	a	1013	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	1135	CLA	C3A-C2A-CAA-CBA
14	a	1138	CLA	C3A-C2A-CAA-CBA
14	a	1139	CLA	C3A-C2A-CAA-CBA
14	b	1022	CLA	C3A-C2A-CAA-CBA
14	b	1209	CLA	C3A-C2A-CAA-CBA
14	b	1210	CLA	C3A-C2A-CAA-CBA
14	b	1212	CLA	C3A-C2A-CAA-CBA
14	b	1213	CLA	C3A-C2A-CAA-CBA
14	b	1220	CLA	C3A-C2A-CAA-CBA
14	b	1227	CLA	C3A-C2A-CAA-CBA
14	b	1233	CLA	C3A-C2A-CAA-CBA
14	l	1501	CLA	C3A-C2A-CAA-CBA
14	B	1223	CLA	C13-C15-C16-C17
14	B	1224	CLA	C10-C11-C12-C13
14	b	1223	CLA	C13-C15-C16-C17
19	B	5004	LHG	C23-C24-C25-C26
19	H	5004	LHG	C23-C24-C25-C26
19	b	5004	LHG	C23-C24-C25-C26
18	G	4008	BCR	C9-C10-C11-C12
18	a	4008	BCR	C9-C10-C11-C12
13	A	1011	CL0	C16-C17-C18-C19
13	G	1011	CL0	C16-C17-C18-C19
13	a	1011	CL0	C16-C17-C18-C19
14	A	1136	CLA	C6-C7-C8-C9
14	B	1211	CLA	C16-C17-C18-C20
14	B	1238	CLA	C16-C17-C18-C19
14	G	1136	CLA	C6-C7-C8-C9
14	H	1211	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	H	1238	CLA	C16-C17-C18-C19
14	a	1136	CLA	C6-C7-C8-C9
14	b	1211	CLA	C16-C17-C18-C20
14	b	1238	CLA	C16-C17-C18-C19
20	B	5002	LMG	C34-C35-C36-C37
20	H	5002	LMG	C34-C35-C36-C37
19	B	5004	LHG	C32-C33-C34-C35
19	H	5004	LHG	C32-C33-C34-C35
19	b	5004	LHG	C32-C33-C34-C35
14	A	1125	CLA	CBA-CGA-O2A-C1
14	G	1125	CLA	CBA-CGA-O2A-C1
14	a	1125	CLA	CBA-CGA-O2A-C1
20	b	5002	LMG	C34-C35-C36-C37
14	H	1224	CLA	C10-C11-C12-C13
14	b	1224	CLA	C10-C11-C12-C13
21	G	6001	LMT	C2-C3-C4-C5
21	A	6001	LMT	C2-C3-C4-C5
21	a	6001	LMT	C2-C3-C4-C5
20	I	5006	LMG	C32-C33-C34-C35
20	R	5006	LMG	C32-C33-C34-C35
20	i	5006	LMG	C32-C33-C34-C35
14	A	1140	CLA	C8-C10-C11-C12
14	G	1140	CLA	C8-C10-C11-C12
14	G	1103	CLA	O1D-CGD-O2D-CED
14	a	1103	CLA	O1D-CGD-O2D-CED
14	B	1238	CLA	O1A-CGA-O2A-C1
14	H	1238	CLA	O1A-CGA-O2A-C1
14	b	1238	CLA	O1A-CGA-O2A-C1
14	A	1108	CLA	C2B-C3B-CAB-CBB
14	B	1216	CLA	C2B-C3B-CAB-CBB
14	G	1108	CLA	C2B-C3B-CAB-CBB
14	H	1216	CLA	C2B-C3B-CAB-CBB
14	a	1108	CLA	C2B-C3B-CAB-CBB
14	b	1216	CLA	C2B-C3B-CAB-CBB
18	A	4001	BCR	C1-C6-C7-C8
18	A	4001	BCR	C5-C6-C7-C8
18	A	4002	BCR	C1-C6-C7-C8
18	A	4003	BCR	C1-C6-C7-C8
18	A	4003	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	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	B	4006	BCR	C23-C24-C25-C30
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	G	4001	BCR	C1-C6-C7-C8
18	G	4001	BCR	C5-C6-C7-C8
18	G	4002	BCR	C1-C6-C7-C8
18	G	4003	BCR	C1-C6-C7-C8
18	G	4003	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	C23-C24-C25-C26
18	H	4006	BCR	C23-C24-C25-C30
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	a	4001	BCR	C1-C6-C7-C8
18	a	4001	BCR	C5-C6-C7-C8
18	a	4002	BCR	C1-C6-C7-C8
18	a	4003	BCR	C1-C6-C7-C8
18	a	4003	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	C23-C24-C25-C26
18	b	4006	BCR	C23-C24-C25-C30
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
14	A	1126	CLA	CBA-CGA-O2A-C1
14	G	1126	CLA	CBA-CGA-O2A-C1
14	a	1126	CLA	CBA-CGA-O2A-C1
14	B	1225	CLA	C13-C15-C16-C17
14	H	1225	CLA	C13-C15-C16-C17
14	a	1140	CLA	C8-C10-C11-C12
14	b	1225	CLA	C13-C15-C16-C17
14	A	1103	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	1012	CLA	C2A-CAA-CBA-CGA
14	A	1106	CLA	C2A-CAA-CBA-CGA
14	B	1224	CLA	C2A-CAA-CBA-CGA
14	G	1012	CLA	C2A-CAA-CBA-CGA
14	G	1106	CLA	C2A-CAA-CBA-CGA
14	H	1224	CLA	C2A-CAA-CBA-CGA
14	a	1012	CLA	C2A-CAA-CBA-CGA
14	a	1106	CLA	C2A-CAA-CBA-CGA
14	b	1224	CLA	C2A-CAA-CBA-CGA
14	A	1138	CLA	C5-C6-C7-C8
14	G	1138	CLA	C5-C6-C7-C8
14	a	1138	CLA	C5-C6-C7-C8
20	A	5005	LMG	O9-C10-O7-C8
20	G	5005	LMG	O9-C10-O7-C8
20	a	5005	LMG	O9-C10-O7-C8
14	A	1138	CLA	C4-C3-C5-C6
14	G	1138	CLA	C4-C3-C5-C6
14	a	1138	CLA	C4-C3-C5-C6
18	A	4002	BCR	C10-C11-C12-C13
18	B	4004	BCR	C10-C11-C12-C13
18	B	4017	BCR	C18-C19-C20-C21
18	G	4002	BCR	C10-C11-C12-C13
18	H	4004	BCR	C10-C11-C12-C13
18	H	4006	BCR	C10-C11-C12-C13
18	H	4017	BCR	C18-C19-C20-C21
18	M	4021	BCR	C10-C11-C12-C13
18	V	4021	BCR	C10-C11-C12-C13
18	a	4002	BCR	C10-C11-C12-C13
18	b	4004	BCR	C10-C11-C12-C13
18	b	4006	BCR	C10-C11-C12-C13
18	b	4017	BCR	C18-C19-C20-C21
18	m	4021	BCR	C10-C11-C12-C13
14	A	1140	CLA	C10-C11-C12-C13
14	G	1140	CLA	C10-C11-C12-C13
14	a	1140	CLA	C10-C11-C12-C13
14	B	1210	CLA	C11-C12-C13-C14
14	H	1210	CLA	C11-C12-C13-C14
14	b	1210	CLA	C11-C12-C13-C14
14	A	1012	CLA	C13-C15-C16-C17
14	B	1239	CLA	C5-C6-C7-C8
14	H	1239	CLA	C5-C6-C7-C8
14	b	1239	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	5004	LHG	C33-C34-C35-C36
19	H	5004	LHG	C33-C34-C35-C36
19	b	5004	LHG	C33-C34-C35-C36
18	I	4018	BCR	C14-C15-C16-C17
18	R	4018	BCR	C14-C15-C16-C17
18	i	4018	BCR	C14-C15-C16-C17
20	B	5002	LMG	C2-C1-O1-C7
20	H	5002	LMG	C2-C1-O1-C7
20	b	5002	LMG	C2-C1-O1-C7
14	A	1126	CLA	C5-C6-C7-C8
14	G	1012	CLA	C13-C15-C16-C17
14	G	1126	CLA	C5-C6-C7-C8
14	a	1012	CLA	C13-C15-C16-C17
14	a	1126	CLA	C5-C6-C7-C8
14	a	1126	CLA	C2C-C3C-CAC-CBC
14	G	1126	CLA	C2C-C3C-CAC-CBC
18	B	4016	BCR	C15-C16-C17-C18
18	H	4016	BCR	C15-C16-C17-C18
18	b	4016	BCR	C15-C16-C17-C18
20	A	5005	LMG	C36-C37-C38-C39
14	B	1204	CLA	C15-C16-C17-C18
14	H	1204	CLA	C15-C16-C17-C18
14	b	1204	CLA	C15-C16-C17-C18
19	B	5004	LHG	O9-C7-O7-C5
19	H	5004	LHG	O9-C7-O7-C5
19	b	5004	LHG	O9-C7-O7-C5
14	A	1126	CLA	C2C-C3C-CAC-CBC
20	G	5005	LMG	C36-C37-C38-C39
20	a	5005	LMG	C36-C37-C38-C39
14	A	1110	CLA	C2A-CAA-CBA-CGA
14	a	1110	CLA	C2A-CAA-CBA-CGA
14	A	1125	CLA	O1A-CGA-O2A-C1
14	G	1125	CLA	O1A-CGA-O2A-C1
14	a	1125	CLA	O1A-CGA-O2A-C1
14	A	1132	CLA	C10-C11-C12-C13
14	B	1204	CLA	C8-C10-C11-C12
14	G	1132	CLA	C10-C11-C12-C13
14	H	1204	CLA	C8-C10-C11-C12
14	a	1132	CLA	C10-C11-C12-C13
14	b	1204	CLA	C8-C10-C11-C12
19	A	5001	LHG	C28-C29-C30-C31
19	G	5001	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
19	a	5001	LHG	C28-C29-C30-C31
14	b	1238	CLA	C10-C11-C12-C13
16	A	2001	PQN	C18-C20-C21-C22
16	G	2001	PQN	C18-C20-C21-C22
14	b	1234	CLA	O1D-CGD-O2D-CED
14	B	1234	CLA	O1D-CGD-O2D-CED
14	H	1234	CLA	O1D-CGD-O2D-CED
14	B	1238	CLA	C10-C11-C12-C13
14	H	1238	CLA	C10-C11-C12-C13
16	a	2001	PQN	C18-C20-C21-C22
14	B	1214	CLA	C2C-C3C-CAC-CBC
14	H	1214	CLA	C2C-C3C-CAC-CBC
14	A	1103	CLA	C2-C1-O2A-CGA
14	B	1202	CLA	C2-C1-O2A-CGA
14	H	1202	CLA	C2-C1-O2A-CGA
14	a	1103	CLA	C2-C1-O2A-CGA
14	b	1202	CLA	C2-C1-O2A-CGA
15	B	1237	F6C	C1A-C2A-CAA-CBA
15	H	1237	F6C	C1A-C2A-CAA-CBA
15	b	1237	F6C	C1A-C2A-CAA-CBA
14	b	1214	CLA	C2C-C3C-CAC-CBC
14	B	1204	CLA	C2A-CAA-CBA-CGA
14	B	1217	CLA	C2A-CAA-CBA-CGA
14	B	1227	CLA	C2A-CAA-CBA-CGA
14	G	1110	CLA	C2A-CAA-CBA-CGA
14	H	1204	CLA	C2A-CAA-CBA-CGA
14	H	1217	CLA	C2A-CAA-CBA-CGA
14	H	1227	CLA	C2A-CAA-CBA-CGA
14	b	1204	CLA	C2A-CAA-CBA-CGA
14	b	1217	CLA	C2A-CAA-CBA-CGA
14	b	1227	CLA	C2A-CAA-CBA-CGA
14	B	1220	CLA	O1D-CGD-O2D-CED
14	H	1220	CLA	O1D-CGD-O2D-CED
14	b	1220	CLA	O1D-CGD-O2D-CED
14	B	1208	CLA	C15-C16-C17-C18
14	H	1208	CLA	C15-C16-C17-C18
14	b	1208	CLA	C15-C16-C17-C18
21	G	6002	LMT	O5B-C5B-C6B-O6B
21	a	6002	LMT	O5B-C5B-C6B-O6B
21	A	6002	LMT	O5B-C5B-C6B-O6B
19	B	5004	LHG	O1-C1-C2-O2
19	H	5004	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	b	5004	LHG	O1-C1-C2-O2
14	A	1126	CLA	O1A-CGA-O2A-C1
14	G	1126	CLA	O1A-CGA-O2A-C1
14	a	1126	CLA	O1A-CGA-O2A-C1
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	1109	CLA	C1A-C2A-CAA-CBA
14	A	1110	CLA	C1A-C2A-CAA-CBA
14	A	1113	CLA	C1A-C2A-CAA-CBA
14	A	1118	CLA	C1A-C2A-CAA-CBA
14	A	1122	CLA	C1A-C2A-CAA-CBA
14	A	1125	CLA	C1A-C2A-CAA-CBA
14	A	1127	CLA	C1A-C2A-CAA-CBA
14	A	1129	CLA	C1A-C2A-CAA-CBA
14	A	1130	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	A	1139	CLA	C1A-C2A-CAA-CBA
14	B	1204	CLA	C1A-C2A-CAA-CBA
14	B	1209	CLA	C1A-C2A-CAA-CBA
14	B	1212	CLA	C1A-C2A-CAA-CBA
14	B	1215	CLA	C1A-C2A-CAA-CBA
14	B	1217	CLA	C1A-C2A-CAA-CBA
14	B	1219	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	1233	CLA	C1A-C2A-CAA-CBA
14	B	1236	CLA	C1A-C2A-CAA-CBA
14	B	1239	CLA	C1A-C2A-CAA-CBA
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	1109	CLA	C1A-C2A-CAA-CBA
14	G	1110	CLA	C1A-C2A-CAA-CBA
14	G	1113	CLA	C1A-C2A-CAA-CBA
14	G	1118	CLA	C1A-C2A-CAA-CBA
14	G	1122	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	G	1125	CLA	C1A-C2A-CAA-CBA
14	G	1127	CLA	C1A-C2A-CAA-CBA
14	G	1129	CLA	C1A-C2A-CAA-CBA
14	G	1130	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	G	1139	CLA	C1A-C2A-CAA-CBA
14	H	1204	CLA	C1A-C2A-CAA-CBA
14	H	1209	CLA	C1A-C2A-CAA-CBA
14	H	1212	CLA	C1A-C2A-CAA-CBA
14	H	1215	CLA	C1A-C2A-CAA-CBA
14	H	1217	CLA	C1A-C2A-CAA-CBA
14	H	1219	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	1233	CLA	C1A-C2A-CAA-CBA
14	H	1236	CLA	C1A-C2A-CAA-CBA
14	H	1239	CLA	C1A-C2A-CAA-CBA
14	L	1502	CLA	C1A-C2A-CAA-CBA
14	U	1502	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	1109	CLA	C1A-C2A-CAA-CBA
14	a	1110	CLA	C1A-C2A-CAA-CBA
14	a	1113	CLA	C1A-C2A-CAA-CBA
14	a	1118	CLA	C1A-C2A-CAA-CBA
14	a	1122	CLA	C1A-C2A-CAA-CBA
14	a	1125	CLA	C1A-C2A-CAA-CBA
14	a	1127	CLA	C1A-C2A-CAA-CBA
14	a	1129	CLA	C1A-C2A-CAA-CBA
14	a	1130	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	a	1139	CLA	C1A-C2A-CAA-CBA
14	b	1204	CLA	C1A-C2A-CAA-CBA
14	b	1209	CLA	C1A-C2A-CAA-CBA
14	b	1212	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	1215	CLA	C1A-C2A-CAA-CBA
14	b	1217	CLA	C1A-C2A-CAA-CBA
14	b	1219	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	1233	CLA	C1A-C2A-CAA-CBA
14	b	1236	CLA	C1A-C2A-CAA-CBA
14	b	1239	CLA	C1A-C2A-CAA-CBA
14	l	1502	CLA	C1A-C2A-CAA-CBA
20	L	5007	LMG	O6-C5-C6-O5
20	U	5007	LMG	O6-C5-C6-O5
20	l	5007	LMG	O6-C5-C6-O5
14	L	1502	CLA	C3-C5-C6-C7
14	U	1502	CLA	C3-C5-C6-C7
14	l	1502	CLA	C3-C5-C6-C7
14	A	1117	CLA	C6-C7-C8-C10
14	A	1131	CLA	C6-C7-C8-C10
14	A	1140	CLA	C6-C7-C8-C10
14	B	1023	CLA	C11-C10-C8-C7
14	B	1210	CLA	C11-C10-C8-C7
14	B	1211	CLA	C12-C13-C15-C16
14	B	1221	CLA	C11-C10-C8-C7
14	G	1117	CLA	C6-C7-C8-C10
14	G	1131	CLA	C6-C7-C8-C10
14	G	1140	CLA	C6-C7-C8-C10
14	H	1023	CLA	C11-C10-C8-C7
14	H	1210	CLA	C11-C10-C8-C7
14	H	1211	CLA	C12-C13-C15-C16
14	H	1221	CLA	C11-C10-C8-C7
14	a	1117	CLA	C6-C7-C8-C10
14	a	1131	CLA	C6-C7-C8-C10
14	a	1140	CLA	C6-C7-C8-C10
14	b	1023	CLA	C11-C10-C8-C7
14	b	1210	CLA	C11-C10-C8-C7
14	b	1211	CLA	C12-C13-C15-C16
14	b	1221	CLA	C11-C10-C8-C7
14	A	1102	CLA	C8-C10-C11-C12
14	G	1102	CLA	C8-C10-C11-C12
14	a	1102	CLA	C8-C10-C11-C12
16	A	2001	PQN	C25-C26-C27-C28
16	a	2001	PQN	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
16	G	2001	PQN	C25-C26-C27-C28
14	B	1205	CLA	C4-C3-C5-C6
14	H	1205	CLA	C4-C3-C5-C6
14	b	1205	CLA	C4-C3-C5-C6
14	A	1138	CLA	C2-C3-C5-C6
14	G	1138	CLA	C2-C3-C5-C6
14	a	1138	CLA	C2-C3-C5-C6
20	A	5005	LMG	O6-C5-C6-O5
20	G	5005	LMG	O6-C5-C6-O5
20	a	5005	LMG	O6-C5-C6-O5
16	A	2001	PQN	C15-C16-C17-C18
16	G	2001	PQN	C15-C16-C17-C18
16	a	2001	PQN	C15-C16-C17-C18
14	L	1503	CLA	C2A-CAA-CBA-CGA
14	U	1503	CLA	C2A-CAA-CBA-CGA
14	l	1503	CLA	C2A-CAA-CBA-CGA
14	A	1127	CLA	C14-C13-C15-C16
14	A	1131	CLA	C6-C7-C8-C9
14	B	1023	CLA	C11-C10-C8-C9
14	B	1210	CLA	C11-C10-C8-C9
14	G	1127	CLA	C14-C13-C15-C16
14	G	1131	CLA	C6-C7-C8-C9
14	H	1023	CLA	C11-C10-C8-C9
14	H	1210	CLA	C11-C10-C8-C9
14	a	1127	CLA	C14-C13-C15-C16
14	a	1131	CLA	C6-C7-C8-C9
14	b	1023	CLA	C11-C10-C8-C9
14	b	1210	CLA	C11-C10-C8-C9
16	B	2002	PQN	C21-C22-C23-C24
16	H	2002	PQN	C21-C22-C23-C24
16	b	2002	PQN	C21-C22-C23-C24
14	A	1140	CLA	CBA-CGA-O2A-C1
14	G	1140	CLA	CBA-CGA-O2A-C1
14	a	1140	CLA	CBA-CGA-O2A-C1
20	B	5002	LMG	O6-C5-C6-O5
20	H	5002	LMG	O6-C5-C6-O5
20	b	5002	LMG	O6-C5-C6-O5
14	a	1140	CLA	C15-C16-C17-C18
20	B	5002	LMG	C7-C8-C9-O8
20	H	5002	LMG	C7-C8-C9-O8
20	b	5002	LMG	C7-C8-C9-O8
20	I	5006	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
20	R	5006	LMG	O6-C5-C6-O5
20	i	5006	LMG	O6-C5-C6-O5
14	A	1125	CLA	C5-C6-C7-C8
14	A	1140	CLA	C15-C16-C17-C18
14	G	1125	CLA	C5-C6-C7-C8
14	G	1140	CLA	C15-C16-C17-C18
14	B	1220	CLA	CBA-CGA-O2A-C1
14	H	1220	CLA	CBA-CGA-O2A-C1
14	b	1220	CLA	CBA-CGA-O2A-C1
14	a	1125	CLA	C5-C6-C7-C8
19	G	5001	LHG	C25-C26-C27-C28
19	a	5001	LHG	C25-C26-C27-C28
14	A	1125	CLA	O1D-CGD-O2D-CED
14	a	1125	CLA	O1D-CGD-O2D-CED
13	A	1011	CL0	CHA-CBD-CGD-O2D
13	G	1011	CL0	CHA-CBD-CGD-O2D
13	a	1011	CL0	CHA-CBD-CGD-O2D
19	A	5001	LHG	C25-C26-C27-C28
19	B	5004	LHG	C13-C14-C15-C16
19	b	5004	LHG	C13-C14-C15-C16
19	H	5004	LHG	C13-C14-C15-C16
14	B	1205	CLA	C2-C3-C5-C6
14	H	1205	CLA	C2-C3-C5-C6
14	b	1205	CLA	C2-C3-C5-C6
14	G	1125	CLA	O1D-CGD-O2D-CED
18	R	4018	BCR	C10-C11-C12-C13
15	A	1120	F6C	C3B-C2B-CMB-OMB
15	A	1121	F6C	C3B-C2B-CMB-OMB
15	G	1120	F6C	C3B-C2B-CMB-OMB
15	G	1121	F6C	C3B-C2B-CMB-OMB
15	H	1230	F6C	C3B-C2B-CMB-OMB
15	a	1120	F6C	C3B-C2B-CMB-OMB
15	a	1121	F6C	C3B-C2B-CMB-OMB
14	A	1126	CLA	C11-C12-C13-C15
14	G	1126	CLA	C11-C12-C13-C15
14	a	1126	CLA	C11-C12-C13-C15
14	G	1140	CLA	O1A-CGA-O2A-C1
14	a	1140	CLA	O1A-CGA-O2A-C1
14	A	1140	CLA	O1A-CGA-O2A-C1
14	a	1131	CLA	C5-C6-C7-C8
20	B	5002	LMG	O7-C8-C9-O8
20	H	5002	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
20	b	5002	LMG	O7-C8-C9-O8
14	G	1131	CLA	C5-C6-C7-C8
14	A	1119	CLA	C2A-CAA-CBA-CGA
14	G	1119	CLA	C2A-CAA-CBA-CGA
14	a	1119	CLA	C2A-CAA-CBA-CGA
14	A	1131	CLA	C5-C6-C7-C8
14	L	1502	CLA	C8-C10-C11-C12
14	U	1502	CLA	C8-C10-C11-C12
14	l	1502	CLA	C8-C10-C11-C12
16	b	2002	PQN	C15-C16-C17-C18
20	G	5005	LMG	C30-C31-C32-C33
20	a	5005	LMG	C30-C31-C32-C33
14	A	1013	CLA	CBA-CGA-O2A-C1
14	G	1013	CLA	CBA-CGA-O2A-C1
14	G	1103	CLA	CBA-CGA-O2A-C1
14	a	1013	CLA	CBA-CGA-O2A-C1
14	a	1103	CLA	CBA-CGA-O2A-C1
20	A	5005	LMG	C30-C31-C32-C33
16	B	2002	PQN	C15-C16-C17-C18
16	H	2002	PQN	C15-C16-C17-C18
14	B	1211	CLA	C13-C15-C16-C17
14	H	1211	CLA	C13-C15-C16-C17
14	b	1211	CLA	C13-C15-C16-C17
14	A	1126	CLA	C11-C12-C13-C14
14	G	1126	CLA	C11-C12-C13-C14
14	a	1126	CLA	C11-C12-C13-C14
14	G	1119	CLA	C4-C3-C5-C6
14	a	1119	CLA	C4-C3-C5-C6
14	A	1103	CLA	CBA-CGA-O2A-C1
14	B	1023	CLA	CBA-CGA-O2A-C1
14	H	1023	CLA	CBA-CGA-O2A-C1
14	b	1023	CLA	CBA-CGA-O2A-C1
14	A	1117	CLA	C6-C7-C8-C9
14	A	1117	CLA	C14-C13-C15-C16
14	A	1126	CLA	C11-C10-C8-C9
14	B	1022	CLA	C14-C13-C15-C16
14	B	1211	CLA	C14-C13-C15-C16
14	B	1221	CLA	C11-C10-C8-C9
14	B	1239	CLA	C11-C10-C8-C9
14	G	1117	CLA	C6-C7-C8-C9
14	G	1117	CLA	C14-C13-C15-C16
14	G	1126	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	H	1012	CLA	C14-C13-C15-C16
14	H	1211	CLA	C14-C13-C15-C16
14	H	1221	CLA	C11-C10-C8-C9
14	H	1239	CLA	C11-C10-C8-C9
14	a	1117	CLA	C6-C7-C8-C9
14	a	1117	CLA	C14-C13-C15-C16
14	a	1126	CLA	C11-C10-C8-C9
14	b	1022	CLA	C14-C13-C15-C16
14	b	1211	CLA	C14-C13-C15-C16
14	b	1221	CLA	C11-C10-C8-C9
14	b	1239	CLA	C11-C10-C8-C9
14	G	1133	CLA	C8-C10-C11-C12
14	a	1133	CLA	C8-C10-C11-C12
14	A	1106	CLA	C4B-C3B-CAB-CBB
14	A	1109	CLA	C4B-C3B-CAB-CBB
14	A	1112	CLA	C4B-C3B-CAB-CBB
14	A	1124	CLA	C4B-C3B-CAB-CBB
14	A	1129	CLA	C4B-C3B-CAB-CBB
14	A	1133	CLA	C4B-C3B-CAB-CBB
14	A	1136	CLA	C4B-C3B-CAB-CBB
14	B	1202	CLA	C4B-C3B-CAB-CBB
14	B	1213	CLA	C4B-C3B-CAB-CBB
14	B	1219	CLA	C4B-C3B-CAB-CBB
14	B	1224	CLA	C4B-C3B-CAB-CBB
14	B	1238	CLA	C4B-C3B-CAB-CBB
14	G	1106	CLA	C4B-C3B-CAB-CBB
14	G	1109	CLA	C4B-C3B-CAB-CBB
14	G	1112	CLA	C4B-C3B-CAB-CBB
14	G	1124	CLA	C4B-C3B-CAB-CBB
14	G	1129	CLA	C4B-C3B-CAB-CBB
14	G	1133	CLA	C4B-C3B-CAB-CBB
14	G	1136	CLA	C4B-C3B-CAB-CBB
14	H	1202	CLA	C4B-C3B-CAB-CBB
14	H	1213	CLA	C4B-C3B-CAB-CBB
14	H	1219	CLA	C4B-C3B-CAB-CBB
14	H	1224	CLA	C4B-C3B-CAB-CBB
14	H	1238	CLA	C4B-C3B-CAB-CBB
14	a	1106	CLA	C4B-C3B-CAB-CBB
14	a	1109	CLA	C4B-C3B-CAB-CBB
14	a	1112	CLA	C4B-C3B-CAB-CBB
14	a	1124	CLA	C4B-C3B-CAB-CBB
14	a	1129	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	a	1133	CLA	C4B-C3B-CAB-CBB
14	a	1136	CLA	C4B-C3B-CAB-CBB
14	b	1202	CLA	C4B-C3B-CAB-CBB
14	b	1213	CLA	C4B-C3B-CAB-CBB
14	b	1219	CLA	C4B-C3B-CAB-CBB
14	b	1224	CLA	C4B-C3B-CAB-CBB
14	b	1238	CLA	C4B-C3B-CAB-CBB
14	B	1220	CLA	CAA-CBA-CGA-O2A
14	H	1220	CLA	CAA-CBA-CGA-O2A
14	b	1220	CLA	CAA-CBA-CGA-O2A
14	A	1133	CLA	C8-C10-C11-C12
14	B	1201	CLA	C2A-CAA-CBA-CGA
14	H	1201	CLA	C2A-CAA-CBA-CGA
14	b	1201	CLA	C2A-CAA-CBA-CGA
14	A	1117	CLA	C12-C13-C15-C16
14	A	1126	CLA	C11-C10-C8-C7
14	A	1127	CLA	C12-C13-C15-C16
14	B	1021	CLA	C12-C13-C15-C16
14	B	1022	CLA	C12-C13-C15-C16
14	B	1214	CLA	C11-C10-C8-C7
14	B	1239	CLA	C11-C10-C8-C7
14	G	1117	CLA	C12-C13-C15-C16
14	G	1126	CLA	C11-C10-C8-C7
14	G	1127	CLA	C12-C13-C15-C16
14	H	1012	CLA	C12-C13-C15-C16
14	H	1021	CLA	C12-C13-C15-C16
14	H	1214	CLA	C11-C10-C8-C7
14	H	1239	CLA	C11-C10-C8-C7
14	L	1503	CLA	C11-C10-C8-C7
14	U	1503	CLA	C11-C10-C8-C7
14	a	1117	CLA	C12-C13-C15-C16
14	a	1126	CLA	C11-C10-C8-C7
14	a	1127	CLA	C12-C13-C15-C16
14	b	1021	CLA	C12-C13-C15-C16
14	b	1022	CLA	C12-C13-C15-C16
14	b	1214	CLA	C11-C10-C8-C7
14	b	1239	CLA	C11-C10-C8-C7
14	l	1503	CLA	C11-C10-C8-C7
16	B	2002	PQN	C21-C22-C23-C25
16	H	2002	PQN	C21-C22-C23-C25
16	b	2002	PQN	C21-C22-C23-C25
14	l	1503	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	L	1503	CLA	C10-C11-C12-C13
14	U	1503	CLA	C10-C11-C12-C13
14	B	1220	CLA	O1A-CGA-O2A-C1
14	H	1220	CLA	O1A-CGA-O2A-C1
14	b	1220	CLA	O1A-CGA-O2A-C1
14	B	1238	CLA	C3-C5-C6-C7
14	A	1119	CLA	C4-C3-C5-C6
14	A	1140	CLA	C3A-C2A-CAA-CBA
14	B	1203	CLA	C3A-C2A-CAA-CBA
14	B	1205	CLA	C3A-C2A-CAA-CBA
14	G	1140	CLA	C3A-C2A-CAA-CBA
14	H	1203	CLA	C3A-C2A-CAA-CBA
14	H	1205	CLA	C3A-C2A-CAA-CBA
14	a	1140	CLA	C3A-C2A-CAA-CBA
14	b	1203	CLA	C3A-C2A-CAA-CBA
14	b	1205	CLA	C3A-C2A-CAA-CBA
14	A	1132	CLA	C13-C15-C16-C17
14	G	1132	CLA	C13-C15-C16-C17
14	a	1132	CLA	C13-C15-C16-C17
18	B	4014	BCR	C19-C20-C21-C22
18	H	4014	BCR	C19-C20-C21-C22
18	b	4014	BCR	C19-C20-C21-C22
14	H	1238	CLA	C3-C5-C6-C7
14	b	1238	CLA	C3-C5-C6-C7
18	I	4018	BCR	C17-C18-C19-C20
18	R	4018	BCR	C17-C18-C19-C20
18	i	4018	BCR	C17-C18-C19-C20
21	G	6001	LMT	C3-C4-C5-C6
21	a	6001	LMT	C3-C4-C5-C6
21	A	6001	LMT	C3-C4-C5-C6
14	G	1126	CLA	C4C-C3C-CAC-CBC
14	a	1126	CLA	C4C-C3C-CAC-CBC
14	B	1023	CLA	C8-C10-C11-C12
14	H	1023	CLA	C8-C10-C11-C12
14	b	1023	CLA	C8-C10-C11-C12
14	A	1126	CLA	C4C-C3C-CAC-CBC
14	B	1225	CLA	C4-C3-C5-C6
14	H	1225	CLA	C4-C3-C5-C6
14	L	1501	CLA	C4-C3-C5-C6
14	U	1501	CLA	C4-C3-C5-C6
14	b	1225	CLA	C4-C3-C5-C6
14	l	1501	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	1119	CLA	C2-C3-C5-C6
14	G	1119	CLA	C2-C3-C5-C6
14	a	1119	CLA	C2-C3-C5-C6
14	A	1116	CLA	C3-C5-C6-C7
14	G	1116	CLA	C3-C5-C6-C7
14	a	1116	CLA	C3-C5-C6-C7
14	A	1136	CLA	C2B-C3B-CAB-CBB
14	B	1202	CLA	C2B-C3B-CAB-CBB
14	G	1136	CLA	C2B-C3B-CAB-CBB
14	H	1202	CLA	C2B-C3B-CAB-CBB
14	a	1136	CLA	C2B-C3B-CAB-CBB
14	b	1202	CLA	C2B-C3B-CAB-CBB
18	A	4003	BCR	C23-C24-C25-C30
18	A	4007	BCR	C23-C24-C25-C30
18	A	4008	BCR	C1-C6-C7-C8
18	G	4003	BCR	C23-C24-C25-C30
18	G	4007	BCR	C23-C24-C25-C30
18	G	4008	BCR	C1-C6-C7-C8
18	H	4012	BCR	C5-C6-C7-C8
18	I	4020	BCR	C23-C24-C25-C30
18	M	4021	BCR	C23-C24-C25-C30
18	R	4020	BCR	C23-C24-C25-C30
18	V	4021	BCR	C23-C24-C25-C30
18	a	4003	BCR	C23-C24-C25-C30
18	a	4007	BCR	C23-C24-C25-C30
18	a	4008	BCR	C1-C6-C7-C8
18	b	4012	BCR	C5-C6-C7-C8
18	i	4020	BCR	C23-C24-C25-C30
18	m	4021	BCR	C23-C24-C25-C30
13	A	1011	CL0	C5-C6-C7-C8
13	G	1011	CL0	C5-C6-C7-C8
13	a	1011	CL0	C5-C6-C7-C8
14	A	1126	CLA	C8-C10-C11-C12
14	G	1126	CLA	C8-C10-C11-C12
14	a	1126	CLA	C8-C10-C11-C12
14	B	1211	CLA	C10-C11-C12-C13
14	H	1211	CLA	C10-C11-C12-C13
14	b	1211	CLA	C10-C11-C12-C13
20	A	5005	LMG	O7-C8-C9-O8
20	G	5005	LMG	O7-C8-C9-O8
20	a	5005	LMG	O7-C8-C9-O8
14	G	1111	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	b	1222	CLA	C10-C11-C12-C13
14	G	1111	CLA	C10-C11-C12-C13
14	H	1222	CLA	C10-C11-C12-C13
14	A	1125	CLA	C6-C7-C8-C9
14	B	1208	CLA	C14-C13-C15-C16
14	B	1221	CLA	C6-C7-C8-C9
14	G	1125	CLA	C6-C7-C8-C9
14	H	1208	CLA	C14-C13-C15-C16
14	H	1221	CLA	C6-C7-C8-C9
14	a	1125	CLA	C6-C7-C8-C9
14	b	1208	CLA	C14-C13-C15-C16
14	b	1221	CLA	C6-C7-C8-C9
14	A	1111	CLA	C10-C11-C12-C13
14	B	1222	CLA	C10-C11-C12-C13
14	a	1111	CLA	C10-C11-C12-C13
14	A	1111	CLA	C8-C10-C11-C12
14	a	1111	CLA	C8-C10-C11-C12
14	B	1207	CLA	C2A-CAA-CBA-CGA
14	H	1207	CLA	C2A-CAA-CBA-CGA
14	b	1207	CLA	C2A-CAA-CBA-CGA
14	H	1229	CLA	C10-C11-C12-C13
14	b	1229	CLA	C10-C11-C12-C13
14	B	1229	CLA	C10-C11-C12-C13
14	L	1501	CLA	C2-C3-C5-C6
14	U	1501	CLA	C2-C3-C5-C6
14	l	1501	CLA	C2-C3-C5-C6
14	B	1208	CLA	C16-C17-C18-C20
14	b	1208	CLA	C16-C17-C18-C20
19	A	5001	LHG	O6-C4-C5-C6
19	G	5001	LHG	O6-C4-C5-C6
19	a	5001	LHG	O6-C4-C5-C6
14	A	1118	CLA	C6-C7-C8-C9
14	G	1118	CLA	C6-C7-C8-C9
14	H	1208	CLA	C16-C17-C18-C20
14	a	1118	CLA	C6-C7-C8-C9
14	b	1214	CLA	C4C-C3C-CAC-CBC
14	A	1104	CLA	C6-C7-C8-C10
14	A	1123	CLA	C6-C7-C8-C10
14	A	1125	CLA	C6-C7-C8-C10
14	B	1203	CLA	C6-C7-C8-C10
14	B	1204	CLA	C6-C7-C8-C10
14	B	1226	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	G	1104	CLA	C6-C7-C8-C10
14	G	1123	CLA	C6-C7-C8-C10
14	G	1125	CLA	C6-C7-C8-C10
14	G	1126	CLA	C6-C7-C8-C10
14	H	1203	CLA	C6-C7-C8-C10
14	H	1204	CLA	C6-C7-C8-C10
14	H	1226	CLA	C6-C7-C8-C10
14	a	1104	CLA	C6-C7-C8-C10
14	a	1123	CLA	C6-C7-C8-C10
14	a	1125	CLA	C6-C7-C8-C10
14	b	1203	CLA	C6-C7-C8-C10
14	b	1204	CLA	C6-C7-C8-C10
14	b	1226	CLA	C6-C7-C8-C10
16	A	2001	PQN	C17-C18-C20-C21
16	G	2001	PQN	C17-C18-C20-C21
16	a	2001	PQN	C17-C18-C20-C21
14	B	1214	CLA	C4C-C3C-CAC-CBC
14	H	1214	CLA	C4C-C3C-CAC-CBC
18	A	4007	BCR	C17-C18-C19-C20
18	B	4005	BCR	C17-C18-C19-C20
18	G	4007	BCR	C17-C18-C19-C20
18	H	4005	BCR	C17-C18-C19-C20
18	L	4022	BCR	C11-C12-C13-C14
18	U	4022	BCR	C11-C12-C13-C14
18	a	4007	BCR	C17-C18-C19-C20
18	b	4005	BCR	C17-C18-C19-C20
18	l	4022	BCR	C11-C12-C13-C14
19	A	5001	LHG	O8-C23-C24-C25
19	G	5001	LHG	O8-C23-C24-C25
19	a	5001	LHG	O8-C23-C24-C25
14	A	1103	CLA	O1A-CGA-O2A-C1
14	B	1023	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	O1A-CGA-O2A-C1
14	H	1023	CLA	O1A-CGA-O2A-C1
14	a	1103	CLA	O1A-CGA-O2A-C1
14	b	1023	CLA	O1A-CGA-O2A-C1
14	B	1225	CLA	C2-C3-C5-C6
14	H	1225	CLA	C2-C3-C5-C6
14	b	1225	CLA	C2-C3-C5-C6
15	A	1121	F6C	C2B-C3B-CAB-CBB
15	G	1121	F6C	C2B-C3B-CAB-CBB
15	a	1121	F6C	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	B	1223	CLA	C5-C6-C7-C8
14	H	1223	CLA	C5-C6-C7-C8
14	b	1223	CLA	C5-C6-C7-C8
19	A	5001	LHG	O6-C4-C5-O7
19	G	5001	LHG	O6-C4-C5-O7
19	a	5001	LHG	O6-C4-C5-O7
14	B	1216	CLA	C5-C6-C7-C8
14	H	1216	CLA	C5-C6-C7-C8
15	B	1237	F6C	C4B-C3B-CAB-CBB
15	H	1237	F6C	C4B-C3B-CAB-CBB
15	b	1237	F6C	C4B-C3B-CAB-CBB
14	b	1216	CLA	C5-C6-C7-C8
20	A	5005	LMG	C12-C13-C14-C15
20	G	5005	LMG	C12-C13-C14-C15
14	B	1203	CLA	C11-C10-C8-C9
14	B	1204	CLA	C6-C7-C8-C9
14	B	1214	CLA	C11-C10-C8-C9
14	H	1203	CLA	C11-C10-C8-C9
14	H	1204	CLA	C6-C7-C8-C9
14	H	1214	CLA	C11-C10-C8-C9
14	b	1203	CLA	C11-C10-C8-C9
14	b	1204	CLA	C6-C7-C8-C9
14	b	1214	CLA	C11-C10-C8-C9
20	a	5005	LMG	C12-C13-C14-C15
20	B	5002	LMG	C19-C20-C21-C22
20	H	5002	LMG	C19-C20-C21-C22
20	b	5002	LMG	C19-C20-C21-C22
14	B	1235	CLA	C8-C10-C11-C12
14	b	1235	CLA	C8-C10-C11-C12
14	B	1205	CLA	C2-C1-O2A-CGA
14	H	1205	CLA	C2-C1-O2A-CGA
14	b	1205	CLA	C2-C1-O2A-CGA
14	A	1118	CLA	C6-C7-C8-C10
14	G	1118	CLA	C6-C7-C8-C10
14	a	1118	CLA	C6-C7-C8-C10
13	A	1011	CL0	C10-C11-C12-C13
13	G	1011	CL0	C10-C11-C12-C13
13	a	1011	CL0	C10-C11-C12-C13
14	A	1117	CLA	C5-C6-C7-C8
14	G	1117	CLA	C5-C6-C7-C8
14	H	1235	CLA	C8-C10-C11-C12
14	a	1117	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	A	1126	CLA	C4-C3-C5-C6
14	G	1126	CLA	C4-C3-C5-C6
14	a	1126	CLA	C4-C3-C5-C6
14	B	1222	CLA	C3-C5-C6-C7
14	H	1222	CLA	C3-C5-C6-C7
14	b	1222	CLA	C3-C5-C6-C7
14	A	1124	CLA	C1A-C2A-CAA-CBA
14	B	1022	CLA	C1A-C2A-CAA-CBA
14	G	1124	CLA	C1A-C2A-CAA-CBA
14	H	1012	CLA	C1A-C2A-CAA-CBA
14	a	1124	CLA	C1A-C2A-CAA-CBA
14	b	1022	CLA	C1A-C2A-CAA-CBA
14	A	1136	CLA	CBA-CGA-O2A-C1
14	G	1136	CLA	CBA-CGA-O2A-C1
14	a	1136	CLA	CBA-CGA-O2A-C1
20	I	5006	LMG	O7-C10-C11-C12
20	R	5006	LMG	O7-C10-C11-C12
20	i	5006	LMG	O7-C10-C11-C12
18	B	4012	BCR	C13-C14-C15-C16
18	H	4012	BCR	C13-C14-C15-C16
18	b	4012	BCR	C13-C14-C15-C16
14	B	1211	CLA	C2A-CAA-CBA-CGA
14	H	1211	CLA	C2A-CAA-CBA-CGA
14	b	1211	CLA	C2A-CAA-CBA-CGA
19	B	5004	LHG	C11-C10-C9-C8
19	H	5004	LHG	C11-C10-C9-C8
19	b	5004	LHG	C11-C10-C9-C8
14	A	1104	CLA	C12-C13-C15-C16
14	A	1117	CLA	C11-C12-C13-C15
14	A	1126	CLA	C6-C7-C8-C10
14	A	1132	CLA	C11-C10-C8-C7
14	A	1133	CLA	C11-C10-C8-C7
14	B	1205	CLA	C11-C10-C8-C7
14	B	1239	CLA	C11-C12-C13-C15
14	G	1104	CLA	C12-C13-C15-C16
14	G	1117	CLA	C11-C12-C13-C15
14	G	1132	CLA	C11-C10-C8-C7
14	G	1133	CLA	C11-C10-C8-C7
14	H	1205	CLA	C11-C10-C8-C7
14	H	1239	CLA	C11-C12-C13-C15
14	a	1104	CLA	C12-C13-C15-C16
14	a	1117	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	a	1126	CLA	C6-C7-C8-C10
14	a	1132	CLA	C11-C10-C8-C7
14	a	1133	CLA	C11-C10-C8-C7
14	b	1205	CLA	C11-C10-C8-C7
14	b	1239	CLA	C11-C12-C13-C15
16	A	2001	PQN	C21-C22-C23-C25
16	G	2001	PQN	C21-C22-C23-C25
16	a	2001	PQN	C21-C22-C23-C25
14	A	1123	CLA	C11-C12-C13-C15
14	G	1123	CLA	C11-C12-C13-C15
14	a	1123	CLA	C11-C12-C13-C15
20	B	5002	LMG	C12-C13-C14-C15
20	H	5002	LMG	C12-C13-C14-C15
20	b	5002	LMG	C12-C13-C14-C15
14	A	1013	CLA	O1A-CGA-O2A-C1
14	G	1013	CLA	O1A-CGA-O2A-C1
14	a	1013	CLA	O1A-CGA-O2A-C1
14	A	1131	CLA	C4-C3-C5-C6
14	G	1131	CLA	C4-C3-C5-C6
14	a	1131	CLA	C4-C3-C5-C6
14	B	1021	CLA	C14-C13-C15-C16
14	B	1203	CLA	C6-C7-C8-C9
14	H	1021	CLA	C14-C13-C15-C16
14	H	1203	CLA	C6-C7-C8-C9
14	L	1502	CLA	C6-C7-C8-C9
14	U	1502	CLA	C6-C7-C8-C9
14	b	1021	CLA	C14-C13-C15-C16
14	b	1203	CLA	C6-C7-C8-C9
14	l	1502	CLA	C6-C7-C8-C9
18	L	4019	BCR	C13-C14-C15-C16
18	U	4019	BCR	C13-C14-C15-C16
18	l	4019	BCR	C13-C14-C15-C16
14	G	1122	CLA	CBD-CGD-O2D-CED
14	a	1122	CLA	CBD-CGD-O2D-CED
14	A	1012	CLA	C10-C11-C12-C13
14	G	1012	CLA	C10-C11-C12-C13
14	a	1012	CLA	C10-C11-C12-C13
15	B	1230	F6C	C1B-C2B-CMB-OMB
15	B	1237	F6C	C1B-C2B-CMB-OMB
15	H	1230	F6C	C1B-C2B-CMB-OMB
15	H	1237	F6C	C1B-C2B-CMB-OMB
15	b	1237	F6C	C1B-C2B-CMB-OMB

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Mol	Chain	Res	Type	Atoms
20	l	5007	LMG	O9-C10-O7-C8
20	A	5005	LMG	C7-C8-C9-O8
20	G	5005	LMG	C7-C8-C9-O8
20	a	5005	LMG	C7-C8-C9-O8
14	A	1122	CLA	CBD-CGD-O2D-CED
14	B	1226	CLA	CBD-CGD-O2D-CED
14	H	1226	CLA	CBD-CGD-O2D-CED
14	b	1226	CLA	CBD-CGD-O2D-CED
14	A	1103	CLA	CAD-CBD-CGD-O2D
14	A	1111	CLA	CAD-CBD-CGD-O2D
14	A	1136	CLA	CAD-CBD-CGD-O2D
14	B	1022	CLA	CAD-CBD-CGD-O2D
14	G	1103	CLA	CAD-CBD-CGD-O2D
14	G	1111	CLA	CAD-CBD-CGD-O2D
14	G	1136	CLA	CAD-CBD-CGD-O2D
14	H	1012	CLA	CAD-CBD-CGD-O2D
14	a	1103	CLA	CAD-CBD-CGD-O2D
14	a	1111	CLA	CAD-CBD-CGD-O2D
14	a	1136	CLA	CAD-CBD-CGD-O2D
14	b	1022	CLA	CAD-CBD-CGD-O2D
15	A	1120	F6C	CAD-CBD-CGD-O2D
15	G	1120	F6C	CAD-CBD-CGD-O2D
15	a	1120	F6C	CAD-CBD-CGD-O2D
14	G	1136	CLA	O1A-CGA-O2A-C1
14	a	1136	CLA	O1A-CGA-O2A-C1
14	B	1021	CLA	C16-C17-C18-C20
14	B	1226	CLA	C16-C17-C18-C20
14	H	1021	CLA	C16-C17-C18-C20
14	H	1222	CLA	C16-C17-C18-C20
14	b	1021	CLA	C16-C17-C18-C20
14	b	1222	CLA	C16-C17-C18-C20
14	A	1136	CLA	O1A-CGA-O2A-C1
20	L	5007	LMG	O9-C10-O7-C8
20	U	5007	LMG	O9-C10-O7-C8
14	A	1103	CLA	CAD-CBD-CGD-O1D
14	A	1111	CLA	CAD-CBD-CGD-O1D
14	A	1112	CLA	CHA-CBD-CGD-O1D
14	A	1112	CLA	CHA-CBD-CGD-O2D
14	A	1114	CLA	CHA-CBD-CGD-O1D
14	A	1114	CLA	CHA-CBD-CGD-O2D
14	A	1135	CLA	CHA-CBD-CGD-O1D
14	A	1135	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	A	1136	CLA	CAD-CBD-CGD-O1D
14	B	1022	CLA	CAD-CBD-CGD-O1D
14	G	1103	CLA	CAD-CBD-CGD-O1D
14	G	1111	CLA	CAD-CBD-CGD-O1D
14	G	1112	CLA	CHA-CBD-CGD-O1D
14	G	1112	CLA	CHA-CBD-CGD-O2D
14	G	1114	CLA	CHA-CBD-CGD-O1D
14	G	1114	CLA	CHA-CBD-CGD-O2D
14	G	1135	CLA	CHA-CBD-CGD-O1D
14	G	1135	CLA	CHA-CBD-CGD-O2D
14	G	1136	CLA	CAD-CBD-CGD-O1D
14	H	1012	CLA	CAD-CBD-CGD-O1D
14	a	1103	CLA	CAD-CBD-CGD-O1D
14	a	1111	CLA	CAD-CBD-CGD-O1D
14	a	1112	CLA	CHA-CBD-CGD-O1D
14	a	1112	CLA	CHA-CBD-CGD-O2D
14	a	1114	CLA	CHA-CBD-CGD-O1D
14	a	1114	CLA	CHA-CBD-CGD-O2D
14	a	1135	CLA	CHA-CBD-CGD-O1D
14	a	1135	CLA	CHA-CBD-CGD-O2D
14	a	1136	CLA	CAD-CBD-CGD-O1D
14	b	1022	CLA	CAD-CBD-CGD-O1D
15	A	1120	F6C	CAD-CBD-CGD-O1D
15	G	1120	F6C	CAD-CBD-CGD-O1D
15	a	1120	F6C	CAD-CBD-CGD-O1D
18	A	4011	BCR	C19-C20-C21-C22
18	B	4012	BCR	C15-C16-C17-C18
18	G	4011	BCR	C19-C20-C21-C22
18	a	4011	BCR	C19-C20-C21-C22
19	A	5001	LHG	C3-O3-P-O5
19	G	5001	LHG	C3-O3-P-O5
19	a	5001	LHG	C3-O3-P-O5
14	H	1229	CLA	C3-C5-C6-C7
14	B	1222	CLA	C16-C17-C18-C20
14	b	1226	CLA	C16-C17-C18-C20
14	B	1235	CLA	C10-C11-C12-C13
14	b	1214	CLA	C10-C11-C12-C13
14	b	1235	CLA	C10-C11-C12-C13
14	A	1116	CLA	C2B-C3B-CAB-CBB
14	B	1022	CLA	C2B-C3B-CAB-CBB
14	B	1023	CLA	C2B-C3B-CAB-CBB
14	B	1203	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	B	1227	CLA	C2B-C3B-CAB-CBB
14	G	1116	CLA	C2B-C3B-CAB-CBB
14	H	1012	CLA	C2B-C3B-CAB-CBB
14	H	1023	CLA	C2B-C3B-CAB-CBB
14	H	1203	CLA	C2B-C3B-CAB-CBB
14	H	1227	CLA	C2B-C3B-CAB-CBB
14	a	1116	CLA	C2B-C3B-CAB-CBB
14	b	1022	CLA	C2B-C3B-CAB-CBB
14	b	1023	CLA	C2B-C3B-CAB-CBB
14	b	1203	CLA	C2B-C3B-CAB-CBB
14	b	1227	CLA	C2B-C3B-CAB-CBB
18	B	4012	BCR	C1-C6-C7-C8
18	B	4012	BCR	C5-C6-C7-C8
18	B	4013	BCR	C1-C6-C7-C8
18	H	4012	BCR	C1-C6-C7-C8
18	H	4013	BCR	C1-C6-C7-C8
18	b	4012	BCR	C1-C6-C7-C8
18	b	4013	BCR	C1-C6-C7-C8
14	B	1226	CLA	C10-C11-C12-C13
14	B	1226	CLA	C15-C16-C17-C18
14	H	1226	CLA	C10-C11-C12-C13
14	H	1235	CLA	C10-C11-C12-C13
18	B	4014	BCR	C7-C8-C9-C34
18	H	4014	BCR	C7-C8-C9-C34
18	I	4020	BCR	C37-C22-C23-C24
18	R	4020	BCR	C37-C22-C23-C24
18	b	4014	BCR	C7-C8-C9-C34
18	i	4020	BCR	C37-C22-C23-C24
19	B	5004	LHG	C2-C3-O3-P
19	H	5004	LHG	C2-C3-O3-P
19	b	5004	LHG	C2-C3-O3-P
14	B	1229	CLA	C3-C5-C6-C7
14	b	1229	CLA	C3-C5-C6-C7
14	B	1214	CLA	C10-C11-C12-C13
14	b	1226	CLA	C10-C11-C12-C13
14	B	1226	CLA	C16-C17-C18-C19
14	H	1226	CLA	C16-C17-C18-C19
14	H	1226	CLA	C16-C17-C18-C20
14	b	1226	CLA	C16-C17-C18-C19
14	B	1226	CLA	O1D-CGD-O2D-CED
14	H	1214	CLA	C10-C11-C12-C13
14	b	1226	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	b	1226	CLA	O1D-CGD-O2D-CED
14	H	1226	CLA	C15-C16-C17-C18
18	A	4003	BCR	C18-C19-C20-C21
18	B	4006	BCR	C18-C19-C20-C21
18	B	4012	BCR	C18-C19-C20-C21
18	B	4013	BCR	C18-C19-C20-C21
18	G	4003	BCR	C18-C19-C20-C21
18	H	4006	BCR	C18-C19-C20-C21
18	H	4012	BCR	C18-C19-C20-C21
18	H	4013	BCR	C18-C19-C20-C21
18	I	4020	BCR	C18-C19-C20-C21
18	M	4021	BCR	C18-C19-C20-C21
18	R	4020	BCR	C18-C19-C20-C21
18	V	4021	BCR	C18-C19-C20-C21
18	a	4003	BCR	C18-C19-C20-C21
18	b	4006	BCR	C18-C19-C20-C21
18	b	4012	BCR	C18-C19-C20-C21
18	b	4013	BCR	C18-C19-C20-C21
18	i	4020	BCR	C18-C19-C20-C21
18	m	4021	BCR	C18-C19-C20-C21
14	H	1226	CLA	O1D-CGD-O2D-CED
18	B	4013	BCR	C13-C14-C15-C16
18	H	4012	BCR	C15-C16-C17-C18
18	H	4013	BCR	C13-C14-C15-C16
18	b	4012	BCR	C15-C16-C17-C18
18	b	4013	BCR	C13-C14-C15-C16
14	B	1221	CLA	C11-C12-C13-C14
14	H	1221	CLA	C11-C12-C13-C14
14	b	1221	CLA	C11-C12-C13-C14
14	A	1013	CLA	C8-C10-C11-C12
14	G	1013	CLA	C8-C10-C11-C12
14	a	1013	CLA	C8-C10-C11-C12
14	G	1140	CLA	CAA-CBA-CGA-O2A
14	a	1140	CLA	CAA-CBA-CGA-O2A
14	A	1013	CLA	C11-C10-C8-C9
14	B	1205	CLA	C11-C10-C8-C9
14	B	1226	CLA	C6-C7-C8-C9
14	G	1013	CLA	C11-C10-C8-C9
14	H	1205	CLA	C11-C10-C8-C9
14	H	1226	CLA	C6-C7-C8-C9
14	L	1503	CLA	C11-C10-C8-C9
14	U	1503	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	a	1013	CLA	C11-C10-C8-C9
14	b	1205	CLA	C11-C10-C8-C9
14	b	1226	CLA	C6-C7-C8-C9
14	l	1503	CLA	C11-C10-C8-C9
14	A	1140	CLA	CAA-CBA-CGA-O2A
14	B	1217	CLA	CAA-CBA-CGA-O2A
14	B	1204	CLA	C4-C3-C5-C6
14	H	1204	CLA	C4-C3-C5-C6
14	b	1204	CLA	C4-C3-C5-C6
14	H	1217	CLA	CAA-CBA-CGA-O2A
14	a	1116	CLA	CAA-CBA-CGA-O2A
14	b	1217	CLA	CAA-CBA-CGA-O2A
20	i	5006	LMG	O9-C10-O7-C8
14	A	1116	CLA	CAA-CBA-CGA-O2A
19	B	5004	LHG	C7-C8-C9-C10
18	B	4009	BCR	C9-C10-C11-C12
18	H	4016	BCR	C19-C20-C21-C22
14	G	1116	CLA	CAA-CBA-CGA-O2A
19	H	5004	LHG	C7-C8-C9-C10
19	b	5004	LHG	C7-C8-C9-C10
14	B	1211	CLA	C3-C5-C6-C7
20	I	5006	LMG	O9-C10-O7-C8
20	R	5006	LMG	O9-C10-O7-C8
14	A	1124	CLA	C2-C1-O2A-CGA
14	B	1215	CLA	C2-C1-O2A-CGA
14	G	1124	CLA	C2-C1-O2A-CGA
14	H	1215	CLA	C2-C1-O2A-CGA
14	a	1124	CLA	C2-C1-O2A-CGA
14	a	1131	CLA	C2-C1-O2A-CGA
14	b	1215	CLA	C2-C1-O2A-CGA
14	A	1125	CLA	C16-C17-C18-C20
14	G	1125	CLA	C16-C17-C18-C20
14	a	1125	CLA	C16-C17-C18-C20
14	B	1202	CLA	CAA-CBA-CGA-O2A
14	H	1202	CLA	CAA-CBA-CGA-O2A
14	b	1202	CLA	CAA-CBA-CGA-O2A
18	A	4001	BCR	C37-C22-C23-C24
18	G	4001	BCR	C37-C22-C23-C24
18	H	4016	BCR	C7-C8-C9-C34
18	a	4001	BCR	C37-C22-C23-C24
20	i	5006	LMG	C30-C31-C32-C33
14	H	1211	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	b	1211	CLA	C3-C5-C6-C7
15	B	1237	F6C	C3A-C2A-CAA-CBA
15	H	1237	F6C	C3A-C2A-CAA-CBA
15	b	1237	F6C	C3A-C2A-CAA-CBA
14	b	1022	CLA	C15-C16-C17-C18
20	I	5006	LMG	C30-C31-C32-C33
14	A	1140	CLA	O1D-CGD-O2D-CED
18	B	4016	BCR	C19-C20-C21-C22
18	H	4009	BCR	C9-C10-C11-C12
18	H	4016	BCR	C9-C10-C11-C12
18	b	4009	BCR	C9-C10-C11-C12
18	b	4016	BCR	C19-C20-C21-C22
20	R	5006	LMG	C30-C31-C32-C33
14	B	1022	CLA	C15-C16-C17-C18
14	H	1012	CLA	C15-C16-C17-C18
14	B	1204	CLA	C2-C3-C5-C6
14	H	1204	CLA	C2-C3-C5-C6
14	b	1204	CLA	C2-C3-C5-C6
14	a	1140	CLA	O1D-CGD-O2D-CED
21	A	6001	LMT	C2-C1-O1'-C1'
21	G	6001	LMT	C2-C1-O1'-C1'
21	a	6001	LMT	C2-C1-O1'-C1'
14	B	1208	CLA	C16-C17-C18-C19
14	H	1208	CLA	C16-C17-C18-C19
14	b	1208	CLA	C16-C17-C18-C19
14	A	1104	CLA	C14-C13-C15-C16
14	B	1224	CLA	C14-C13-C15-C16
14	G	1104	CLA	C14-C13-C15-C16
14	H	1224	CLA	C14-C13-C15-C16
14	a	1104	CLA	C14-C13-C15-C16
14	b	1224	CLA	C14-C13-C15-C16
14	G	1140	CLA	O1D-CGD-O2D-CED
14	A	1104	CLA	C4B-C3B-CAB-CBB
14	A	1126	CLA	C4B-C3B-CAB-CBB
14	B	1212	CLA	C4B-C3B-CAB-CBB
14	G	1104	CLA	C4B-C3B-CAB-CBB
14	G	1126	CLA	C4B-C3B-CAB-CBB
14	H	1212	CLA	C4B-C3B-CAB-CBB
14	a	1104	CLA	C4B-C3B-CAB-CBB
14	a	1126	CLA	C4B-C3B-CAB-CBB
14	b	1212	CLA	C4B-C3B-CAB-CBB
14	B	1214	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	H	1214	CLA	C11-C12-C13-C15
14	b	1214	CLA	C11-C12-C13-C15
14	A	1012	CLA	C4-C3-C5-C6
14	G	1012	CLA	C4-C3-C5-C6
14	a	1012	CLA	C4-C3-C5-C6
18	b	4016	BCR	C9-C10-C11-C12
20	I	5006	LMG	C11-C10-O7-C8
20	L	5007	LMG	C11-C10-O7-C8
20	i	5006	LMG	C11-C10-O7-C8
14	B	1205	CLA	C5-C6-C7-C8
14	H	1205	CLA	C5-C6-C7-C8
14	H	1229	CLA	C5-C6-C7-C8
14	b	1205	CLA	C5-C6-C7-C8
14	b	1229	CLA	C5-C6-C7-C8
14	B	1221	CLA	C11-C12-C13-C15
14	H	1221	CLA	C11-C12-C13-C15
14	b	1221	CLA	C11-C12-C13-C15
14	A	1125	CLA	C12-C13-C15-C16
14	A	1127	CLA	C6-C7-C8-C10
14	B	1205	CLA	C11-C12-C13-C15
14	B	1222	CLA	C6-C7-C8-C10
14	G	1125	CLA	C12-C13-C15-C16
14	G	1127	CLA	C6-C7-C8-C10
14	H	1205	CLA	C11-C12-C13-C15
14	H	1222	CLA	C6-C7-C8-C10
14	a	1125	CLA	C12-C13-C15-C16
14	a	1127	CLA	C6-C7-C8-C10
14	b	1205	CLA	C11-C12-C13-C15
14	b	1222	CLA	C6-C7-C8-C10
14	B	1229	CLA	C5-C6-C7-C8
14	A	1123	CLA	O1D-CGD-O2D-CED
14	b	1226	CLA	C3-C5-C6-C7
14	G	1123	CLA	O1D-CGD-O2D-CED
14	K	1401	CLA	C3A-C2A-CAA-CBA
14	T	1401	CLA	C3A-C2A-CAA-CBA
14	W	1701	CLA	C3A-C2A-CAA-CBA
14	X	1701	CLA	C3A-C2A-CAA-CBA
14	k	1401	CLA	C3A-C2A-CAA-CBA
14	x	1701	CLA	C3A-C2A-CAA-CBA
14	A	1131	CLA	C2-C3-C5-C6
14	a	1131	CLA	C2-C3-C5-C6
14	B	1233	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	H	1233	CLA	C2A-CAA-CBA-CGA
14	b	1233	CLA	C2A-CAA-CBA-CGA
20	R	5006	LMG	C11-C10-O7-C8
18	A	4007	BCR	C16-C17-C18-C36
18	A	4011	BCR	C11-C10-C9-C34
18	A	4011	BCR	C16-C17-C18-C36
18	B	4010	BCR	C16-C17-C18-C36
18	B	4016	BCR	C35-C13-C14-C15
18	G	4007	BCR	C16-C17-C18-C36
18	G	4011	BCR	C11-C10-C9-C34
18	G	4011	BCR	C16-C17-C18-C36
18	H	4010	BCR	C16-C17-C18-C36
18	H	4016	BCR	C35-C13-C14-C15
18	I	4020	BCR	C20-C21-C22-C37
18	R	4020	BCR	C20-C21-C22-C37
18	a	4007	BCR	C16-C17-C18-C36
18	a	4011	BCR	C11-C10-C9-C34
18	a	4011	BCR	C16-C17-C18-C36
18	b	4010	BCR	C16-C17-C18-C36
18	b	4016	BCR	C35-C13-C14-C15
18	i	4020	BCR	C20-C21-C22-C37
14	B	1226	CLA	C3-C5-C6-C7
14	H	1226	CLA	C3-C5-C6-C7
20	I	5006	LMG	C28-C29-C30-C31
14	A	1131	CLA	C2-C1-O2A-CGA
14	G	1131	CLA	C2-C1-O2A-CGA
18	A	4011	BCR	C9-C10-C11-C12
18	B	4016	BCR	C9-C10-C11-C12
18	G	4011	BCR	C9-C10-C11-C12
18	B	4016	BCR	C7-C8-C9-C34
18	M	4021	BCR	C37-C22-C23-C24
18	V	4021	BCR	C37-C22-C23-C24
18	b	4016	BCR	C7-C8-C9-C34
18	m	4021	BCR	C37-C22-C23-C24
14	W	1701	CLA	CAA-CBA-CGA-O1A
20	R	5006	LMG	C28-C29-C30-C31
20	i	5006	LMG	C28-C29-C30-C31
14	B	1023	CLA	C10-C11-C12-C13
14	G	1123	CLA	C10-C11-C12-C13
20	I	5006	LMG	C33-C34-C35-C36
20	R	5006	LMG	C33-C34-C35-C36
20	i	5006	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
14	a	1123	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	CAA-CBA-CGA-O1A
14	x	1701	CLA	CAA-CBA-CGA-O1A
14	A	1123	CLA	C10-C11-C12-C13
14	H	1023	CLA	C10-C11-C12-C13
14	a	1123	CLA	C10-C11-C12-C13
14	b	1023	CLA	C10-C11-C12-C13
20	l	5007	LMG	C11-C10-O7-C8
14	A	1132	CLA	C4-C3-C5-C6
14	G	1132	CLA	C4-C3-C5-C6
14	a	1132	CLA	C4-C3-C5-C6
14	G	1131	CLA	C2-C3-C5-C6
14	A	1128	CLA	C11-C12-C13-C15
14	G	1128	CLA	C11-C12-C13-C15
14	a	1128	CLA	C11-C12-C13-C15
14	A	1131	CLA	C10-C11-C12-C13
14	a	1131	CLA	C10-C11-C12-C13
14	G	1131	CLA	C10-C11-C12-C13
21	A	6002	LMT	C5'-C4'-O1B-C1B
21	a	6002	LMT	C5'-C4'-O1B-C1B
14	H	1218	CLA	CAA-CBA-CGA-O1A
14	b	1218	CLA	CAA-CBA-CGA-O1A
14	A	1012	CLA	C11-C10-C8-C9
14	A	1117	CLA	C11-C12-C13-C14
14	A	1127	CLA	C6-C7-C8-C9
14	B	1021	CLA	C6-C7-C8-C9
14	B	1229	CLA	C6-C7-C8-C9
14	G	1012	CLA	C11-C10-C8-C9
14	G	1117	CLA	C11-C12-C13-C14
14	G	1127	CLA	C6-C7-C8-C9
14	H	1021	CLA	C6-C7-C8-C9
14	H	1229	CLA	C6-C7-C8-C9
14	a	1012	CLA	C11-C10-C8-C9
14	a	1117	CLA	C11-C12-C13-C14
14	a	1127	CLA	C6-C7-C8-C9
14	b	1021	CLA	C6-C7-C8-C9
14	b	1229	CLA	C6-C7-C8-C9
21	G	6002	LMT	C5'-C4'-O1B-C1B
14	H	1216	CLA	C3-C5-C6-C7
14	b	1216	CLA	C3-C5-C6-C7
20	U	5007	LMG	C11-C10-O7-C8
18	a	4011	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	B	1218	CLA	CAA-CBA-CGA-O1A
14	G	1137	CLA	CAA-CBA-CGA-O1A
14	H	1210	CLA	CAA-CBA-CGA-O2A
14	b	1210	CLA	CAA-CBA-CGA-O2A
14	A	1012	CLA	C2-C3-C5-C6
14	G	1012	CLA	C2-C3-C5-C6
14	a	1012	CLA	C2-C3-C5-C6
14	B	1216	CLA	C3-C5-C6-C7
14	A	1101	CLA	CAA-CBA-CGA-O1A
14	A	1137	CLA	CAA-CBA-CGA-O1A
14	B	1233	CLA	CAA-CBA-CGA-O1A
14	B	1233	CLA	CAA-CBA-CGA-O2A
14	H	1233	CLA	CAA-CBA-CGA-O1A
14	H	1233	CLA	CAA-CBA-CGA-O2A
14	a	1137	CLA	CAA-CBA-CGA-O1A
14	b	1233	CLA	CAA-CBA-CGA-O1A
14	b	1233	CLA	CAA-CBA-CGA-O2A
14	G	1140	CLA	CBD-CGD-O2D-CED
14	a	1140	CLA	CBD-CGD-O2D-CED
15	B	1230	F6C	CBD-CGD-O2D-CED
14	B	1210	CLA	CAA-CBA-CGA-O2A
14	A	1140	CLA	C1A-C2A-CAA-CBA
14	B	1228	CLA	C1A-C2A-CAA-CBA
14	B	1238	CLA	C1A-C2A-CAA-CBA
14	G	1140	CLA	C1A-C2A-CAA-CBA
14	H	1228	CLA	C1A-C2A-CAA-CBA
14	H	1238	CLA	C1A-C2A-CAA-CBA
14	a	1140	CLA	C1A-C2A-CAA-CBA
14	b	1228	CLA	C1A-C2A-CAA-CBA
14	b	1238	CLA	C1A-C2A-CAA-CBA
18	A	4007	BCR	C16-C17-C18-C19
18	A	4011	BCR	C11-C10-C9-C8
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	G	4007	BCR	C16-C17-C18-C19
18	G	4011	BCR	C11-C10-C9-C8
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	I	4020	BCR	C20-C21-C22-C23
18	R	4020	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	a	4007	BCR	C16-C17-C18-C19
18	a	4011	BCR	C11-C10-C9-C8
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	i	4020	BCR	C20-C21-C22-C23
14	G	1101	CLA	CAA-CBA-CGA-O1A
14	B	1201	CLA	C5-C6-C7-C8
14	b	1201	CLA	C5-C6-C7-C8
14	A	1104	CLA	C2B-C3B-CAB-CBB
14	A	1109	CLA	C2B-C3B-CAB-CBB
14	A	1124	CLA	C2B-C3B-CAB-CBB
14	A	1126	CLA	C2B-C3B-CAB-CBB
14	A	1133	CLA	C2B-C3B-CAB-CBB
14	B	1212	CLA	C2B-C3B-CAB-CBB
14	B	1219	CLA	C2B-C3B-CAB-CBB
14	G	1104	CLA	C2B-C3B-CAB-CBB
14	G	1109	CLA	C2B-C3B-CAB-CBB
14	G	1124	CLA	C2B-C3B-CAB-CBB
14	G	1126	CLA	C2B-C3B-CAB-CBB
14	G	1133	CLA	C2B-C3B-CAB-CBB
14	H	1212	CLA	C2B-C3B-CAB-CBB
14	H	1219	CLA	C2B-C3B-CAB-CBB
14	a	1104	CLA	C2B-C3B-CAB-CBB
14	a	1109	CLA	C2B-C3B-CAB-CBB
14	a	1124	CLA	C2B-C3B-CAB-CBB
14	a	1126	CLA	C2B-C3B-CAB-CBB
14	a	1133	CLA	C2B-C3B-CAB-CBB
14	b	1212	CLA	C2B-C3B-CAB-CBB
14	b	1219	CLA	C2B-C3B-CAB-CBB
18	A	4001	BCR	C23-C24-C25-C26
18	A	4001	BCR	C23-C24-C25-C30
18	A	4003	BCR	C23-C24-C25-C26
18	A	4007	BCR	C23-C24-C25-C26
18	A	4008	BCR	C5-C6-C7-C8
18	B	4010	BCR	C23-C24-C25-C26
18	B	4010	BCR	C23-C24-C25-C30
18	B	4013	BCR	C5-C6-C7-C8
18	B	4016	BCR	C23-C24-C25-C26
18	B	4016	BCR	C23-C24-C25-C30
18	B	4017	BCR	C1-C6-C7-C8
18	G	4001	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	G	4001	BCR	C23-C24-C25-C30
18	G	4003	BCR	C23-C24-C25-C26
18	G	4007	BCR	C23-C24-C25-C26
18	G	4008	BCR	C5-C6-C7-C8
18	H	4010	BCR	C23-C24-C25-C26
18	H	4010	BCR	C23-C24-C25-C30
18	H	4013	BCR	C5-C6-C7-C8
18	H	4016	BCR	C23-C24-C25-C26
18	H	4016	BCR	C23-C24-C25-C30
18	H	4017	BCR	C1-C6-C7-C8
18	I	4020	BCR	C23-C24-C25-C26
18	M	4021	BCR	C23-C24-C25-C26
18	R	4020	BCR	C23-C24-C25-C26
18	V	4021	BCR	C23-C24-C25-C26
18	a	4001	BCR	C23-C24-C25-C26
18	a	4001	BCR	C23-C24-C25-C30
18	a	4003	BCR	C23-C24-C25-C26
18	a	4007	BCR	C23-C24-C25-C26
18	a	4008	BCR	C5-C6-C7-C8
18	b	4010	BCR	C23-C24-C25-C26
18	b	4010	BCR	C23-C24-C25-C30
18	b	4013	BCR	C5-C6-C7-C8
18	b	4016	BCR	C23-C24-C25-C26
18	b	4016	BCR	C23-C24-C25-C30
18	b	4017	BCR	C1-C6-C7-C8
18	i	4020	BCR	C23-C24-C25-C26
18	m	4021	BCR	C23-C24-C25-C26
14	B	1218	CLA	CAA-CBA-CGA-O2A
14	H	1218	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O2A
14	a	1101	CLA	CAA-CBA-CGA-O1A
14	b	1218	CLA	CAA-CBA-CGA-O2A
14	x	1701	CLA	CAA-CBA-CGA-O2A
14	A	1140	CLA	CBD-CGD-O2D-CED
14	H	1201	CLA	C5-C6-C7-C8
14	W	1701	CLA	CAA-CBA-CGA-O2A
14	A	1125	CLA	C4-C3-C5-C6
14	B	1202	CLA	C4-C3-C5-C6
14	G	1125	CLA	C4-C3-C5-C6
14	H	1202	CLA	C4-C3-C5-C6
14	a	1125	CLA	C4-C3-C5-C6
14	b	1202	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
15	B	1230	F6C	O1D-CGD-O2D-CED
14	A	1012	CLA	C11-C10-C8-C7
14	A	1103	CLA	C11-C10-C8-C7
14	A	1132	CLA	C11-C12-C13-C15
14	B	1224	CLA	C12-C13-C15-C16
14	B	1226	CLA	C12-C13-C15-C16
14	G	1012	CLA	C11-C10-C8-C7
14	G	1103	CLA	C11-C10-C8-C7
14	G	1132	CLA	C11-C12-C13-C15
14	H	1224	CLA	C12-C13-C15-C16
14	H	1226	CLA	C12-C13-C15-C16
14	a	1012	CLA	C11-C10-C8-C7
14	a	1103	CLA	C11-C10-C8-C7
14	a	1132	CLA	C11-C12-C13-C15
14	b	1224	CLA	C12-C13-C15-C16
14	b	1226	CLA	C12-C13-C15-C16
14	a	1129	CLA	C2A-CAA-CBA-CGA
19	A	5001	LHG	O7-C5-C6-O8
19	G	5001	LHG	O7-C5-C6-O8
19	a	5001	LHG	O7-C5-C6-O8
14	B	1205	CLA	CAA-CBA-CGA-O2A
14	H	1205	CLA	CAA-CBA-CGA-O2A
14	B	1222	CLA	C16-C17-C18-C19
14	H	1222	CLA	C16-C17-C18-C19
14	b	1222	CLA	C16-C17-C18-C19
14	A	1101	CLA	CAA-CBA-CGA-O2A
14	a	1101	CLA	CAA-CBA-CGA-O2A
14	b	1205	CLA	CAA-CBA-CGA-O2A
14	A	1129	CLA	C2A-CAA-CBA-CGA
14	G	1129	CLA	C2A-CAA-CBA-CGA
14	G	1101	CLA	CAA-CBA-CGA-O2A
14	G	1137	CLA	CAA-CBA-CGA-O2A
14	a	1137	CLA	CAA-CBA-CGA-O2A
14	B	1203	CLA	C14-C13-C15-C16
14	B	1205	CLA	C11-C12-C13-C14
14	H	1203	CLA	C14-C13-C15-C16
14	H	1205	CLA	C11-C12-C13-C14
14	b	1203	CLA	C14-C13-C15-C16
14	b	1205	CLA	C11-C12-C13-C14
14	A	1119	CLA	C13-C15-C16-C17
14	G	1119	CLA	C13-C15-C16-C17
14	a	1119	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	1137	CLA	CAA-CBA-CGA-O2A
14	A	1116	CLA	C5-C6-C7-C8
14	A	1127	CLA	C4-C3-C5-C6
14	G	1104	CLA	C4-C3-C5-C6
14	G	1127	CLA	C4-C3-C5-C6
14	L	1502	CLA	C4-C3-C5-C6
14	U	1502	CLA	C4-C3-C5-C6
14	a	1127	CLA	C4-C3-C5-C6
14	l	1502	CLA	C4-C3-C5-C6
14	G	1116	CLA	C5-C6-C7-C8
14	a	1116	CLA	C5-C6-C7-C8
14	A	1126	CLA	C2-C3-C5-C6
14	A	1132	CLA	C2-C3-C5-C6
14	G	1126	CLA	C2-C3-C5-C6
14	G	1132	CLA	C2-C3-C5-C6
14	a	1126	CLA	C2-C3-C5-C6
14	a	1132	CLA	C2-C3-C5-C6
20	l	5007	LMG	C28-C29-C30-C31
20	U	5007	LMG	C28-C29-C30-C31
14	B	1220	CLA	CAA-CBA-CGA-O1A
14	H	1220	CLA	CAA-CBA-CGA-O1A
14	b	1220	CLA	CAA-CBA-CGA-O1A
20	L	5007	LMG	C28-C29-C30-C31
14	A	1116	CLA	C2A-CAA-CBA-CGA
14	A	1125	CLA	C2A-CAA-CBA-CGA
14	A	1126	CLA	C2A-CAA-CBA-CGA
14	G	1116	CLA	C2A-CAA-CBA-CGA
14	G	1125	CLA	C2A-CAA-CBA-CGA
14	G	1126	CLA	C2A-CAA-CBA-CGA
14	a	1116	CLA	C2A-CAA-CBA-CGA
14	a	1125	CLA	C2A-CAA-CBA-CGA
14	a	1126	CLA	C2A-CAA-CBA-CGA
14	A	1104	CLA	C4-C3-C5-C6
14	a	1104	CLA	C4-C3-C5-C6
14	B	1219	CLA	CAA-CBA-CGA-O2A
14	H	1219	CLA	CAA-CBA-CGA-O2A
14	b	1219	CLA	CAA-CBA-CGA-O2A
14	A	1136	CLA	CAA-CBA-CGA-O2A
14	G	1136	CLA	CAA-CBA-CGA-O2A
14	a	1136	CLA	CAA-CBA-CGA-O2A
14	A	1111	CLA	C4B-C3B-CAB-CBB
14	A	1130	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	A	1138	CLA	C4B-C3B-CAB-CBB
14	B	1221	CLA	C4B-C3B-CAB-CBB
14	B	1228	CLA	C4B-C3B-CAB-CBB
14	B	1232	CLA	C4B-C3B-CAB-CBB
14	G	1111	CLA	C4B-C3B-CAB-CBB
14	G	1130	CLA	C4B-C3B-CAB-CBB
14	G	1138	CLA	C4B-C3B-CAB-CBB
14	H	1221	CLA	C4B-C3B-CAB-CBB
14	H	1228	CLA	C4B-C3B-CAB-CBB
14	H	1232	CLA	C4B-C3B-CAB-CBB
14	a	1111	CLA	C4B-C3B-CAB-CBB
14	a	1130	CLA	C4B-C3B-CAB-CBB
14	a	1138	CLA	C4B-C3B-CAB-CBB
14	b	1221	CLA	C4B-C3B-CAB-CBB
14	b	1228	CLA	C4B-C3B-CAB-CBB
14	b	1232	CLA	C4B-C3B-CAB-CBB
14	B	1207	CLA	CAA-CBA-CGA-O2A
14	H	1207	CLA	CAA-CBA-CGA-O2A
14	b	1207	CLA	CAA-CBA-CGA-O2A
20	A	5005	LMG	C28-C29-C30-C31
20	G	5005	LMG	C28-C29-C30-C31
20	a	5005	LMG	C28-C29-C30-C31
18	B	4006	BCR	C11-C10-C9-C34
18	H	4006	BCR	C11-C10-C9-C34
18	b	4006	BCR	C11-C10-C9-C34
14	A	1114	CLA	CAA-CBA-CGA-O2A
14	B	1236	CLA	CAA-CBA-CGA-O1A
14	B	1236	CLA	CAA-CBA-CGA-O2A
14	H	1236	CLA	CAA-CBA-CGA-O1A
14	a	1114	CLA	CAA-CBA-CGA-O2A
14	b	1236	CLA	CAA-CBA-CGA-O1A
14	A	1125	CLA	C16-C17-C18-C19
14	G	1114	CLA	CAA-CBA-CGA-O2A
14	H	1236	CLA	CAA-CBA-CGA-O2A
14	b	1236	CLA	CAA-CBA-CGA-O2A
14	B	1225	CLA	C10-C11-C12-C13
14	H	1225	CLA	C10-C11-C12-C13
14	L	1501	CLA	C8-C10-C11-C12
14	U	1501	CLA	C8-C10-C11-C12
14	b	1225	CLA	C10-C11-C12-C13
14	l	1501	CLA	C8-C10-C11-C12
20	l	5007	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
14	B	1021	CLA	C6-C7-C8-C10
14	B	1203	CLA	C12-C13-C15-C16
14	B	1229	CLA	C6-C7-C8-C10
14	H	1021	CLA	C6-C7-C8-C10
14	H	1203	CLA	C12-C13-C15-C16
14	H	1229	CLA	C6-C7-C8-C10
14	b	1021	CLA	C6-C7-C8-C10
14	b	1203	CLA	C12-C13-C15-C16
14	b	1229	CLA	C6-C7-C8-C10
20	L	5007	LMG	C33-C34-C35-C36
20	U	5007	LMG	C33-C34-C35-C36
18	H	4012	BCR	C9-C10-C11-C12
20	B	5002	LMG	C29-C30-C31-C32
14	a	1125	CLA	C16-C17-C18-C19
20	H	5002	LMG	C29-C30-C31-C32
20	b	5002	LMG	C29-C30-C31-C32
14	A	1125	CLA	C11-C12-C13-C14
14	B	1211	CLA	C11-C12-C13-C14
14	B	1215	CLA	C6-C7-C8-C9
14	B	1239	CLA	C11-C12-C13-C14
14	B	1239	CLA	C14-C13-C15-C16
14	G	1125	CLA	C11-C12-C13-C14
14	H	1211	CLA	C11-C12-C13-C14
14	H	1215	CLA	C6-C7-C8-C9
14	H	1239	CLA	C11-C12-C13-C14
14	H	1239	CLA	C14-C13-C15-C16
14	a	1125	CLA	C11-C12-C13-C14
14	b	1211	CLA	C11-C12-C13-C14
14	b	1215	CLA	C6-C7-C8-C9
14	b	1239	CLA	C11-C12-C13-C14
14	b	1239	CLA	C14-C13-C15-C16
14	B	1220	CLA	C2A-CAA-CBA-CGA
14	H	1220	CLA	C2A-CAA-CBA-CGA
14	b	1220	CLA	C2A-CAA-CBA-CGA
14	B	1217	CLA	C2-C1-O2A-CGA
14	B	1221	CLA	C2-C1-O2A-CGA
14	B	1231	CLA	C2-C1-O2A-CGA
14	H	1217	CLA	C2-C1-O2A-CGA
14	H	1221	CLA	C2-C1-O2A-CGA
14	H	1231	CLA	C2-C1-O2A-CGA
14	b	1217	CLA	C2-C1-O2A-CGA
14	b	1221	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	b	1231	CLA	C2-C1-O2A-CGA
14	A	1128	CLA	C11-C12-C13-C14
14	G	1125	CLA	C16-C17-C18-C19
14	G	1128	CLA	C11-C12-C13-C14
14	a	1128	CLA	C11-C12-C13-C14
14	A	1012	CLA	C3A-C2A-CAA-CBA
14	A	1112	CLA	C3A-C2A-CAA-CBA
14	A	1124	CLA	C3A-C2A-CAA-CBA
14	A	1136	CLA	C3A-C2A-CAA-CBA
14	G	1012	CLA	C3A-C2A-CAA-CBA
14	G	1112	CLA	C3A-C2A-CAA-CBA
14	G	1124	CLA	C3A-C2A-CAA-CBA
14	G	1136	CLA	C3A-C2A-CAA-CBA
14	a	1012	CLA	C3A-C2A-CAA-CBA
14	a	1112	CLA	C3A-C2A-CAA-CBA
14	a	1124	CLA	C3A-C2A-CAA-CBA
14	a	1136	CLA	C3A-C2A-CAA-CBA
14	G	1108	CLA	CAA-CBA-CGA-O2A
20	G	5005	LMG	C34-C35-C36-C37
14	A	1108	CLA	CAA-CBA-CGA-O2A
14	a	1108	CLA	CAA-CBA-CGA-O2A
14	A	1117	CLA	C16-C17-C18-C20
14	G	1117	CLA	C16-C17-C18-C20
14	a	1117	CLA	C16-C17-C18-C20
14	a	1119	CLA	C16-C17-C18-C19
20	A	5005	LMG	C34-C35-C36-C37
20	a	5005	LMG	C34-C35-C36-C37
18	i	4018	BCR	C10-C11-C12-C13
14	B	1207	CLA	CAA-CBA-CGA-O1A
14	H	1207	CLA	CAA-CBA-CGA-O1A
14	b	1207	CLA	CAA-CBA-CGA-O1A
14	A	1125	CLA	CAA-CBA-CGA-O2A
14	G	1125	CLA	CAA-CBA-CGA-O2A
14	a	1125	CLA	CAA-CBA-CGA-O2A
14	A	1119	CLA	C16-C17-C18-C19
14	G	1119	CLA	C16-C17-C18-C19
14	a	1110	CLA	CAA-CBA-CGA-O2A
14	A	1110	CLA	CAA-CBA-CGA-O2A
14	G	1110	CLA	CAA-CBA-CGA-O2A
14	H	1219	CLA	CAA-CBA-CGA-O1A
14	b	1219	CLA	CAA-CBA-CGA-O1A
18	B	4010	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	H	4010	BCR	C16-C17-C18-C19
18	b	4010	BCR	C16-C17-C18-C19
14	B	1219	CLA	CAA-CBA-CGA-O1A
14	a	1105	CLA	CAA-CBA-CGA-O2A
14	A	1122	CLA	O1D-CGD-O2D-CED
14	G	1105	CLA	CAA-CBA-CGA-O2A
20	L	5007	LMG	O1-C7-C8-C9
20	U	5007	LMG	O1-C7-C8-C9
20	l	5007	LMG	O1-C7-C8-C9
14	L	1502	CLA	C5-C6-C7-C8
15	A	1121	F6C	C4B-C3B-CAB-CBB
15	G	1121	F6C	C4B-C3B-CAB-CBB
15	a	1121	F6C	C4B-C3B-CAB-CBB
14	a	1122	CLA	O1D-CGD-O2D-CED
14	l	1502	CLA	C5-C6-C7-C8
14	A	1105	CLA	CAA-CBA-CGA-O2A
14	A	1013	CLA	C4-C3-C5-C6
14	G	1013	CLA	C4-C3-C5-C6
14	a	1013	CLA	C4-C3-C5-C6
14	a	1105	CLA	CAA-CBA-CGA-O1A
18	B	4012	BCR	C9-C10-C11-C12
14	U	1502	CLA	C5-C6-C7-C8
14	A	1105	CLA	CAA-CBA-CGA-O1A
14	G	1105	CLA	CAA-CBA-CGA-O1A
14	G	1110	CLA	CAA-CBA-CGA-O1A
14	A	1125	CLA	C14-C13-C15-C16
14	A	1132	CLA	C6-C7-C8-C9
14	G	1125	CLA	C14-C13-C15-C16
14	G	1132	CLA	C6-C7-C8-C9
14	a	1125	CLA	C14-C13-C15-C16
14	a	1132	CLA	C6-C7-C8-C9
14	G	1138	CLA	CAA-CBA-CGA-O2A
14	a	1138	CLA	CAA-CBA-CGA-O2A
14	A	1110	CLA	CAA-CBA-CGA-O1A
14	a	1110	CLA	CAA-CBA-CGA-O1A
18	B	4016	BCR	C7-C8-C9-C10
18	H	4016	BCR	C7-C8-C9-C10
18	b	4016	BCR	C7-C8-C9-C10
14	G	1122	CLA	O1D-CGD-O2D-CED
14	A	1138	CLA	CAA-CBA-CGA-O2A
14	A	1114	CLA	CAA-CBA-CGA-O1A
14	G	1114	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	a	1114	CLA	CAA-CBA-CGA-O1A
14	B	1215	CLA	C2A-CAA-CBA-CGA
14	H	1215	CLA	C2A-CAA-CBA-CGA
14	b	1215	CLA	C2A-CAA-CBA-CGA
14	B	1215	CLA	C6-C7-C8-C10
14	B	1223	CLA	C11-C10-C8-C7
14	H	1215	CLA	C6-C7-C8-C10
14	H	1223	CLA	C11-C10-C8-C7
14	b	1215	CLA	C6-C7-C8-C10
14	b	1223	CLA	C11-C10-C8-C7
14	A	1108	CLA	CAA-CBA-CGA-O1A
14	a	1108	CLA	CAA-CBA-CGA-O1A
14	A	1105	CLA	C2B-C3B-CAB-CBB
14	A	1106	CLA	C2B-C3B-CAB-CBB
14	A	1111	CLA	C2B-C3B-CAB-CBB
14	A	1112	CLA	C2B-C3B-CAB-CBB
14	A	1129	CLA	C2B-C3B-CAB-CBB
14	A	1130	CLA	C2B-C3B-CAB-CBB
14	B	1213	CLA	C2B-C3B-CAB-CBB
14	B	1221	CLA	C2B-C3B-CAB-CBB
14	B	1224	CLA	C2B-C3B-CAB-CBB
14	B	1228	CLA	C2B-C3B-CAB-CBB
14	B	1232	CLA	C2B-C3B-CAB-CBB
14	B	1238	CLA	C2B-C3B-CAB-CBB
14	G	1105	CLA	C2B-C3B-CAB-CBB
14	G	1106	CLA	C2B-C3B-CAB-CBB
14	G	1111	CLA	C2B-C3B-CAB-CBB
14	G	1112	CLA	C2B-C3B-CAB-CBB
14	G	1129	CLA	C2B-C3B-CAB-CBB
14	G	1130	CLA	C2B-C3B-CAB-CBB
14	H	1213	CLA	C2B-C3B-CAB-CBB
14	H	1221	CLA	C2B-C3B-CAB-CBB
14	H	1224	CLA	C2B-C3B-CAB-CBB
14	H	1228	CLA	C2B-C3B-CAB-CBB
14	H	1232	CLA	C2B-C3B-CAB-CBB
14	H	1238	CLA	C2B-C3B-CAB-CBB
14	a	1105	CLA	C2B-C3B-CAB-CBB
14	a	1106	CLA	C2B-C3B-CAB-CBB
14	a	1111	CLA	C2B-C3B-CAB-CBB
14	a	1112	CLA	C2B-C3B-CAB-CBB
14	a	1129	CLA	C2B-C3B-CAB-CBB
14	a	1130	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	1213	CLA	C2B-C3B-CAB-CBB
14	b	1221	CLA	C2B-C3B-CAB-CBB
14	b	1224	CLA	C2B-C3B-CAB-CBB
14	b	1228	CLA	C2B-C3B-CAB-CBB
14	b	1232	CLA	C2B-C3B-CAB-CBB
14	b	1238	CLA	C2B-C3B-CAB-CBB
14	A	1126	CLA	C2-C1-O2A-CGA
14	G	1126	CLA	C2-C1-O2A-CGA
14	a	1126	CLA	C2-C1-O2A-CGA
15	B	1237	F6C	CAA-CBA-CGA-O2A
15	H	1237	F6C	CAA-CBA-CGA-O2A
15	b	1237	F6C	CAA-CBA-CGA-O2A
14	G	1108	CLA	CAA-CBA-CGA-O1A
14	b	1235	CLA	CAA-CBA-CGA-O2A
20	R	5006	LMG	C31-C32-C33-C34
14	A	1136	CLA	C2A-CAA-CBA-CGA
14	G	1136	CLA	C2A-CAA-CBA-CGA
14	a	1136	CLA	C2A-CAA-CBA-CGA
14	G	1127	CLA	C8-C10-C11-C12
14	H	1226	CLA	C5-C6-C7-C8
14	a	1127	CLA	C8-C10-C11-C12
14	A	1131	CLA	CAA-CBA-CGA-O2A
14	B	1235	CLA	CAA-CBA-CGA-O2A
14	G	1131	CLA	CAA-CBA-CGA-O2A
14	H	1235	CLA	CAA-CBA-CGA-O2A
14	a	1131	CLA	CAA-CBA-CGA-O2A
20	i	5006	LMG	C31-C32-C33-C34
14	A	1127	CLA	C8-C10-C11-C12
14	B	1226	CLA	C5-C6-C7-C8
20	I	5006	LMG	C31-C32-C33-C34
14	a	1132	CLA	C2C-C3C-CAC-CBC
14	B	1231	CLA	CAA-CBA-CGA-O2A
14	H	1231	CLA	CAA-CBA-CGA-O2A
14	L	1503	CLA	CAA-CBA-CGA-O2A
14	U	1503	CLA	CAA-CBA-CGA-O2A
14	b	1231	CLA	CAA-CBA-CGA-O2A
14	l	1503	CLA	CAA-CBA-CGA-O2A
18	b	4013	BCR	C9-C10-C11-C12
14	b	1226	CLA	C5-C6-C7-C8
14	A	1132	CLA	C2C-C3C-CAC-CBC
14	G	1132	CLA	C2C-C3C-CAC-CBC
14	B	1239	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	G	1126	CLA	CAA-CBA-CGA-O2A
14	H	1239	CLA	CAA-CBA-CGA-O2A
14	a	1126	CLA	CAA-CBA-CGA-O2A
14	b	1239	CLA	CAA-CBA-CGA-O2A
14	A	1126	CLA	CAA-CBA-CGA-O2A
14	A	1103	CLA	C11-C10-C8-C9
14	A	1132	CLA	C11-C10-C8-C9
14	A	1132	CLA	C11-C12-C13-C14
14	B	1226	CLA	C14-C13-C15-C16
14	G	1103	CLA	C11-C10-C8-C9
14	G	1132	CLA	C11-C10-C8-C9
14	G	1132	CLA	C11-C12-C13-C14
14	H	1226	CLA	C14-C13-C15-C16
14	a	1103	CLA	C11-C10-C8-C9
14	a	1132	CLA	C11-C10-C8-C9
14	a	1132	CLA	C11-C12-C13-C14
14	b	1226	CLA	C14-C13-C15-C16
20	b	5002	LMG	C11-C12-C13-C14
14	A	1133	CLA	CAA-CBA-CGA-O2A
14	G	1133	CLA	CAA-CBA-CGA-O2A
14	a	1133	CLA	CAA-CBA-CGA-O2A
14	A	1123	CLA	CBD-CGD-O2D-CED
14	B	1222	CLA	C8-C10-C11-C12
14	H	1222	CLA	C8-C10-C11-C12
14	b	1222	CLA	C8-C10-C11-C12
14	A	1013	CLA	C1A-C2A-CAA-CBA
14	A	1105	CLA	C4B-C3B-CAB-CBB
14	A	1114	CLA	C1A-C2A-CAA-CBA
14	B	1223	CLA	C1A-C2A-CAA-CBA
14	G	1013	CLA	C1A-C2A-CAA-CBA
14	G	1105	CLA	C4B-C3B-CAB-CBB
14	G	1114	CLA	C1A-C2A-CAA-CBA
14	H	1223	CLA	C1A-C2A-CAA-CBA
14	W	1701	CLA	C1A-C2A-CAA-CBA
14	X	1701	CLA	C1A-C2A-CAA-CBA
14	a	1013	CLA	C1A-C2A-CAA-CBA
14	a	1105	CLA	C4B-C3B-CAB-CBB
14	a	1114	CLA	C1A-C2A-CAA-CBA
14	b	1223	CLA	C1A-C2A-CAA-CBA
14	x	1701	CLA	C1A-C2A-CAA-CBA
20	B	5002	LMG	C30-C31-C32-C33
14	G	1123	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	H	5002	LMG	C11-C12-C13-C14
19	B	5004	LHG	O7-C5-C6-O8
19	H	5004	LHG	O7-C5-C6-O8
19	b	5004	LHG	O7-C5-C6-O8
20	B	5002	LMG	C11-C12-C13-C14
18	B	4013	BCR	C7-C8-C9-C10
18	B	4014	BCR	C7-C8-C9-C10
18	H	4013	BCR	C7-C8-C9-C10
18	H	4014	BCR	C7-C8-C9-C10
18	I	4020	BCR	C21-C22-C23-C24
18	R	4020	BCR	C21-C22-C23-C24
18	b	4013	BCR	C7-C8-C9-C10
18	b	4014	BCR	C7-C8-C9-C10
18	i	4020	BCR	C21-C22-C23-C24
18	B	4004	BCR	C15-C16-C17-C18
18	B	4013	BCR	C9-C10-C11-C12
18	G	4007	BCR	C9-C10-C11-C12
18	H	4004	BCR	C15-C16-C17-C18
18	H	4010	BCR	C19-C20-C21-C22
18	H	4013	BCR	C9-C10-C11-C12
18	L	4019	BCR	C19-C20-C21-C22
18	U	4019	BCR	C19-C20-C21-C22
18	a	4007	BCR	C9-C10-C11-C12
18	b	4004	BCR	C15-C16-C17-C18
18	b	4012	BCR	C9-C10-C11-C12
18	l	4019	BCR	C19-C20-C21-C22
14	a	1123	CLA	CBD-CGD-O2D-CED
20	H	5002	LMG	C30-C31-C32-C33
14	A	1140	CLA	C16-C17-C18-C19
14	G	1140	CLA	C16-C17-C18-C19
20	b	5002	LMG	C30-C31-C32-C33
14	L	1501	CLA	CAA-CBA-CGA-O2A
14	U	1501	CLA	CAA-CBA-CGA-O2A
14	l	1501	CLA	CAA-CBA-CGA-O2A
20	A	5005	LMG	O8-C28-C29-C30
20	G	5005	LMG	O8-C28-C29-C30
20	a	5005	LMG	O8-C28-C29-C30
14	a	1132	CLA	C4C-C3C-CAC-CBC
14	a	1140	CLA	C16-C17-C18-C19
14	b	1224	CLA	C16-C17-C18-C19
14	B	1213	CLA	CAA-CBA-CGA-O2A
14	H	1213	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	b	1213	CLA	CAA-CBA-CGA-O2A
14	B	1201	CLA	C2-C1-O2A-CGA
14	H	1201	CLA	C2-C1-O2A-CGA
14	b	1201	CLA	C2-C1-O2A-CGA
14	B	1202	CLA	C6-C7-C8-C10
14	H	1202	CLA	C6-C7-C8-C10
14	b	1202	CLA	C6-C7-C8-C10
14	A	1125	CLA	C2-C3-C5-C6
14	G	1125	CLA	C2-C3-C5-C6
14	a	1125	CLA	C2-C3-C5-C6
16	b	2002	PQN	C23-C25-C26-C27
14	G	1132	CLA	C4C-C3C-CAC-CBC
14	B	1224	CLA	C16-C17-C18-C19
14	G	1119	CLA	C16-C17-C18-C20
14	H	1224	CLA	C16-C17-C18-C19
14	A	1132	CLA	C4C-C3C-CAC-CBC
16	H	2002	PQN	C23-C25-C26-C27
16	B	2002	PQN	C23-C25-C26-C27
14	A	1119	CLA	C16-C17-C18-C20
14	a	1119	CLA	C16-C17-C18-C20
14	A	1013	CLA	CAA-CBA-CGA-O2A
14	a	1013	CLA	CAA-CBA-CGA-O2A
14	b	1023	CLA	C5-C6-C7-C8
14	B	1238	CLA	C3A-C2A-CAA-CBA
14	H	1238	CLA	C3A-C2A-CAA-CBA
14	b	1238	CLA	C3A-C2A-CAA-CBA
14	A	1138	CLA	CAA-CBA-CGA-O1A
14	G	1138	CLA	CAA-CBA-CGA-O1A
14	a	1138	CLA	CAA-CBA-CGA-O1A
19	A	5001	LHG	O10-C23-C24-C25
19	G	5001	LHG	O10-C23-C24-C25
19	a	5001	LHG	O10-C23-C24-C25
14	B	1225	CLA	CBA-CGA-O2A-C1
14	H	1023	CLA	C5-C6-C7-C8
14	G	1013	CLA	CAA-CBA-CGA-O2A
14	B	1231	CLA	CAA-CBA-CGA-O1A
14	b	1231	CLA	CAA-CBA-CGA-O1A
14	B	1023	CLA	C5-C6-C7-C8
14	H	1225	CLA	CBA-CGA-O2A-C1
14	b	1225	CLA	CBA-CGA-O2A-C1
14	B	1202	CLA	C6-C7-C8-C9
14	H	1202	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	b	1202	CLA	C6-C7-C8-C9
16	A	2001	PQN	C21-C22-C23-C24
16	B	2002	PQN	C19-C18-C20-C21
16	G	2001	PQN	C21-C22-C23-C24
16	H	2002	PQN	C19-C18-C20-C21
16	a	2001	PQN	C21-C22-C23-C24
16	b	2002	PQN	C19-C18-C20-C21
20	L	5007	LMG	O8-C28-C29-C30
20	U	5007	LMG	O8-C28-C29-C30
20	l	5007	LMG	O8-C28-C29-C30
14	H	1235	CLA	CAA-CBA-CGA-O1A
14	U	1501	CLA	CAA-CBA-CGA-O1A
15	B	1237	F6C	CAA-CBA-CGA-O1A
15	H	1237	F6C	CAA-CBA-CGA-O1A
15	b	1237	F6C	CAA-CBA-CGA-O1A
14	a	1103	CLA	C5-C6-C7-C8
18	B	4010	BCR	C19-C20-C21-C22
18	b	4010	BCR	C19-C20-C21-C22
14	A	1103	CLA	C5-C6-C7-C8
14	G	1103	CLA	C5-C6-C7-C8
14	A	1131	CLA	CAA-CBA-CGA-O1A
14	B	1213	CLA	CAA-CBA-CGA-O1A
14	G	1131	CLA	CAA-CBA-CGA-O1A
14	H	1231	CLA	CAA-CBA-CGA-O1A
14	L	1501	CLA	CAA-CBA-CGA-O1A
14	a	1131	CLA	CAA-CBA-CGA-O1A
14	l	1501	CLA	CAA-CBA-CGA-O1A
14	A	1133	CLA	CAA-CBA-CGA-O1A
14	B	1235	CLA	CAA-CBA-CGA-O1A
14	G	1133	CLA	CAA-CBA-CGA-O1A
14	H	1213	CLA	CAA-CBA-CGA-O1A
14	a	1133	CLA	CAA-CBA-CGA-O1A
14	b	1213	CLA	CAA-CBA-CGA-O1A
14	b	1235	CLA	CAA-CBA-CGA-O1A
18	A	4001	BCR	C21-C22-C23-C24
18	G	4001	BCR	C21-C22-C23-C24
18	a	4001	BCR	C21-C22-C23-C24
14	A	1115	CLA	C5-C6-C7-C8
14	G	1115	CLA	C5-C6-C7-C8
14	a	1115	CLA	C5-C6-C7-C8
20	L	5007	LMG	O1-C7-C8-O7
20	U	5007	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
20	l	5007	LMG	O1-C7-C8-O7
14	B	1228	CLA	CAA-CBA-CGA-O2A
20	G	5005	LMG	C29-C30-C31-C32
20	A	5005	LMG	C29-C30-C31-C32
20	L	5007	LMG	C19-C20-C21-C22
20	U	5007	LMG	C19-C20-C21-C22
20	a	5005	LMG	C29-C30-C31-C32
20	l	5007	LMG	C19-C20-C21-C22
14	A	1109	CLA	CAA-CBA-CGA-O2A
14	H	1228	CLA	CAA-CBA-CGA-O2A
15	A	1120	F6C	CAA-CBA-CGA-O2A
15	G	1120	F6C	CAA-CBA-CGA-O2A
15	a	1120	F6C	CAA-CBA-CGA-O2A
14	B	1239	CLA	CAA-CBA-CGA-O1A
14	b	1239	CLA	CAA-CBA-CGA-O1A
14	B	1202	CLA	C2-C3-C5-C6
14	H	1202	CLA	C2-C3-C5-C6
14	b	1202	CLA	C2-C3-C5-C6
14	B	1212	CLA	CAA-CBA-CGA-O2A
14	H	1212	CLA	CAA-CBA-CGA-O2A
14	b	1212	CLA	CAA-CBA-CGA-O2A
14	b	1228	CLA	CAA-CBA-CGA-O2A
14	A	1103	CLA	C10-C11-C12-C13
14	A	1126	CLA	CAA-CBA-CGA-O1A
14	H	1239	CLA	CAA-CBA-CGA-O1A
14	L	1503	CLA	CAA-CBA-CGA-O1A
14	U	1503	CLA	CAA-CBA-CGA-O1A
14	l	1503	CLA	CAA-CBA-CGA-O1A
19	a	5001	LHG	C31-C32-C33-C34
14	B	1224	CLA	C16-C17-C18-C20
14	A	1118	CLA	CAD-CBD-CGD-O2D
14	A	1135	CLA	CAD-CBD-CGD-O2D
14	G	1118	CLA	CAD-CBD-CGD-O2D
14	G	1135	CLA	CAD-CBD-CGD-O2D
14	a	1118	CLA	CAD-CBD-CGD-O2D
14	a	1135	CLA	CAD-CBD-CGD-O2D
19	H	5004	LHG	O7-C7-C8-C9
14	A	1109	CLA	CAA-CBA-CGA-O1A
14	G	1109	CLA	CAA-CBA-CGA-O1A
14	a	1109	CLA	CAA-CBA-CGA-O1A
14	a	1109	CLA	CAA-CBA-CGA-O2A
14	G	1126	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
14	a	1126	CLA	CAA-CBA-CGA-O1A
20	G	5005	LMG	O10-C28-C29-C30
14	b	1208	CLA	C13-C15-C16-C17
19	A	5001	LHG	C31-C32-C33-C34
14	G	1103	CLA	C10-C11-C12-C13
14	a	1103	CLA	C10-C11-C12-C13
14	G	1109	CLA	CAA-CBA-CGA-O2A
15	B	1230	F6C	CAA-CBA-CGA-O2A
19	B	5004	LHG	O7-C7-C8-C9
19	b	5004	LHG	O7-C7-C8-C9
14	H	1224	CLA	C16-C17-C18-C20
14	b	1224	CLA	C16-C17-C18-C20
19	G	5001	LHG	C31-C32-C33-C34
14	B	1208	CLA	C13-C15-C16-C17
16	A	2001	PQN	C13-C15-C16-C17
16	G	2001	PQN	C13-C15-C16-C17
16	a	2001	PQN	C13-C15-C16-C17
14	B	1021	CLA	C2A-CAA-CBA-CGA
20	A	5005	LMG	O10-C28-C29-C30
20	a	5005	LMG	O10-C28-C29-C30
14	H	1208	CLA	C13-C15-C16-C17
14	A	1127	CLA	CAA-CBA-CGA-O2A
14	B	1204	CLA	CAA-CBA-CGA-O2A
14	G	1127	CLA	CAA-CBA-CGA-O2A
14	H	1204	CLA	CAA-CBA-CGA-O2A
14	a	1127	CLA	CAA-CBA-CGA-O2A
14	b	1204	CLA	CAA-CBA-CGA-O2A
14	B	1212	CLA	CAA-CBA-CGA-O1A
14	H	1212	CLA	CAA-CBA-CGA-O1A
14	b	1212	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

292 monomers are involved in 651 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	R	5006	LMG	5	0
18	G	4007	BCR	2	0
18	B	4017	BCR	1	0
14	H	1224	CLA	6	0
14	G	1118	CLA	1	0
14	B	1021	CLA	3	0
14	B	1231	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	1119	CLA	6	0
14	b	1206	CLA	1	0
14	G	1104	CLA	2	0
14	B	1211	CLA	4	0
14	B	1209	CLA	1	0
14	H	1234	CLA	2	0
13	A	1011	CL0	1	0
14	G	1131	CLA	1	0
18	B	4010	BCR	6	0
14	A	1138	CLA	1	0
14	B	1221	CLA	2	0
14	A	1126	CLA	4	0
18	U	4019	BCR	1	0
20	L	5007	LMG	2	0
18	b	4012	BCR	5	0
14	G	1138	CLA	2	0
14	b	1211	CLA	3	0
14	b	1210	CLA	6	0
16	b	2002	PQN	4	0
18	B	4006	BCR	4	0
15	B	1230	F6C	4	0
18	b	4005	BCR	3	0
18	B	4004	BCR	1	0
14	H	1209	CLA	1	0
18	b	4010	BCR	6	0
14	G	1122	CLA	1	0
14	H	1221	CLA	1	0
14	B	1023	CLA	5	0
14	a	1125	CLA	2	0
14	A	1110	CLA	1	0
18	b	4014	BCR	1	0
14	B	1215	CLA	6	0
14	H	1206	CLA	1	0
14	A	1119	CLA	4	0
18	I	4018	BCR	5	0
14	G	1125	CLA	2	0
14	B	1203	CLA	5	0
14	a	1112	CLA	1	0
14	l	1503	CLA	3	0
14	b	1204	CLA	5	0
20	l	5007	LMG	2	0
18	a	4007	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1124	CLA	4	0
14	b	1222	CLA	4	0
14	a	1138	CLA	1	0
14	G	1012	CLA	4	0
14	G	1106	CLA	2	0
18	H	4004	BCR	1	0
14	a	1123	CLA	4	0
14	b	1223	CLA	3	0
14	A	1136	CLA	2	0
14	G	1132	CLA	2	0
14	a	1118	CLA	1	0
18	R	4020	BCR	4	0
14	G	1112	CLA	1	0
14	A	1125	CLA	2	0
14	b	1232	CLA	1	0
14	G	1140	CLA	3	0
14	H	1023	CLA	5	0
14	H	1232	CLA	1	0
20	i	5006	LMG	2	0
14	A	1123	CLA	3	0
19	A	5001	LHG	1	0
14	H	1236	CLA	1	0
20	I	5006	LMG	2	0
14	B	1223	CLA	3	0
14	a	1131	CLA	3	0
14	A	1111	CLA	2	0
14	B	1208	CLA	3	0
14	H	1231	CLA	1	0
14	b	1224	CLA	6	0
18	a	4003	BCR	5	0
14	B	1238	CLA	7	0
14	G	1102	CLA	1	0
14	H	1212	CLA	1	0
18	a	4011	BCR	5	0
19	H	5004	LHG	1	0
14	b	1214	CLA	4	0
14	b	1203	CLA	3	0
18	m	4021	BCR	2	0
14	B	1235	CLA	2	0
14	a	1012	CLA	4	0
14	A	1013	CLA	5	0
14	H	1220	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1205	CLA	7	0
18	a	4001	BCR	3	0
14	H	1012	CLA	5	0
14	b	1208	CLA	2	0
14	B	1210	CLA	6	0
18	b	4009	BCR	6	0
14	B	1234	CLA	2	0
14	x	1701	CLA	1	0
14	a	1109	CLA	2	0
14	b	1202	CLA	6	0
14	a	1013	CLA	3	0
14	a	1117	CLA	2	0
14	b	1239	CLA	4	0
14	B	1227	CLA	1	0
18	B	4005	BCR	4	0
19	a	5001	LHG	1	0
14	a	1124	CLA	5	0
14	A	1109	CLA	2	0
14	A	1104	CLA	2	0
14	B	1214	CLA	3	0
14	A	1128	CLA	1	0
18	B	4012	BCR	5	0
14	H	1021	CLA	3	0
14	b	1226	CLA	3	0
14	H	1238	CLA	7	0
14	U	1503	CLA	3	0
14	b	1229	CLA	2	0
14	H	1203	CLA	3	0
20	U	5007	LMG	3	0
18	G	4003	BCR	6	0
14	a	1116	CLA	3	0
14	b	1217	CLA	3	0
14	b	1238	CLA	7	0
18	l	4022	BCR	5	0
14	G	1110	CLA	1	0
14	B	1236	CLA	1	0
18	U	4022	BCR	5	0
14	A	1012	CLA	3	0
14	W	1701	CLA	2	0
18	b	4006	BCR	5	0
14	b	1220	CLA	1	0
18	L	4019	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	4011	BCR	6	0
14	a	1132	CLA	2	0
14	G	1103	CLA	5	0
14	A	1122	CLA	1	0
18	i	4018	BCR	4	0
18	B	4014	BCR	2	0
14	B	1212	CLA	1	0
14	A	1127	CLA	3	0
18	A	4003	BCR	6	0
14	B	1213	CLA	1	0
14	b	1201	CLA	1	0
18	A	4008	BCR	2	0
14	L	1501	CLA	4	0
14	L	1502	CLA	1	0
14	H	1227	CLA	1	0
14	a	1106	CLA	2	0
20	G	5005	LMG	1	0
18	H	4016	BCR	1	0
18	b	4004	BCR	1	0
14	H	1226	CLA	4	0
14	H	1215	CLA	5	0
14	H	1229	CLA	2	0
14	a	1136	CLA	2	0
18	b	4017	BCR	1	0
18	V	4021	BCR	4	0
21	G	6001	LMT	1	0
14	G	1117	CLA	3	0
14	B	1216	CLA	2	0
14	b	1021	CLA	4	0
14	H	1222	CLA	3	0
14	H	1239	CLA	3	0
14	b	1022	CLA	5	0
14	A	1112	CLA	1	0
14	B	1217	CLA	3	0
14	H	1210	CLA	3	0
13	a	1011	CL0	1	0
14	A	1140	CLA	3	0
18	l	4019	BCR	1	0
18	H	4012	BCR	4	0
14	H	1214	CLA	3	0
14	B	1224	CLA	5	0
16	B	2002	PQN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	b	5002	LMG	3	0
14	U	1502	CLA	1	0
14	b	1207	CLA	1	0
14	b	1209	CLA	1	0
14	b	1205	CLA	7	0
14	H	1211	CLA	4	0
14	G	1116	CLA	3	0
14	b	1221	CLA	1	0
18	I	4020	BCR	3	0
14	l	1501	CLA	3	0
18	G	4002	BCR	1	0
14	a	1110	CLA	1	0
14	A	1131	CLA	1	0
14	G	1130	CLA	2	0
14	H	1223	CLA	4	0
15	b	1230	F6C	6	0
14	b	1219	CLA	4	0
18	H	4006	BCR	4	0
14	b	1215	CLA	6	0
14	B	1202	CLA	4	0
14	B	1204	CLA	4	0
14	G	1109	CLA	1	0
14	G	1013	CLA	3	0
14	b	1216	CLA	2	0
14	H	1204	CLA	5	0
14	l	1502	CLA	1	0
14	B	1225	CLA	3	0
18	H	4010	BCR	6	0
16	G	2001	PQN	6	0
14	X	1701	CLA	1	0
20	a	5005	LMG	1	0
20	H	5002	LMG	3	0
14	B	1220	CLA	1	0
14	a	1103	CLA	3	0
14	A	1116	CLA	3	0
14	B	1229	CLA	2	0
14	L	1503	CLA	3	0
14	b	1225	CLA	3	0
14	A	1118	CLA	1	0
14	a	1107	CLA	1	0
14	B	1222	CLA	4	0
14	H	1219	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	1132	CLA	3	0
19	G	5001	LHG	1	0
18	A	4001	BCR	1	0
14	H	1208	CLA	3	0
14	H	1225	CLA	3	0
14	A	1107	CLA	1	0
14	B	1232	CLA	1	0
18	G	4008	BCR	1	0
18	H	4009	BCR	7	0
14	H	1216	CLA	2	0
14	G	1126	CLA	3	0
16	H	2002	PQN	4	0
14	B	1226	CLA	3	0
14	G	1127	CLA	3	0
14	G	1137	CLA	1	0
14	G	1107	CLA	1	0
16	a	2001	PQN	6	0
14	G	1124	CLA	5	0
18	a	4002	BCR	1	0
14	a	1133	CLA	4	0
14	A	1102	CLA	1	0
14	B	1207	CLA	1	0
14	B	1022	CLA	5	0
14	a	1130	CLA	2	0
14	a	1122	CLA	1	0
14	H	1235	CLA	3	0
14	U	1501	CLA	5	0
14	B	1205	CLA	7	0
14	b	1234	CLA	2	0
14	A	1103	CLA	4	0
18	R	4018	BCR	5	0
18	A	4011	BCR	6	0
14	A	1133	CLA	3	0
14	A	1106	CLA	1	0
18	H	4017	BCR	1	0
14	B	1219	CLA	4	0
14	G	1133	CLA	4	0
14	H	1201	CLA	1	0
18	i	4020	BCR	1	0
18	H	4005	BCR	4	0
14	G	1119	CLA	4	0
14	a	1111	CLA	2	0

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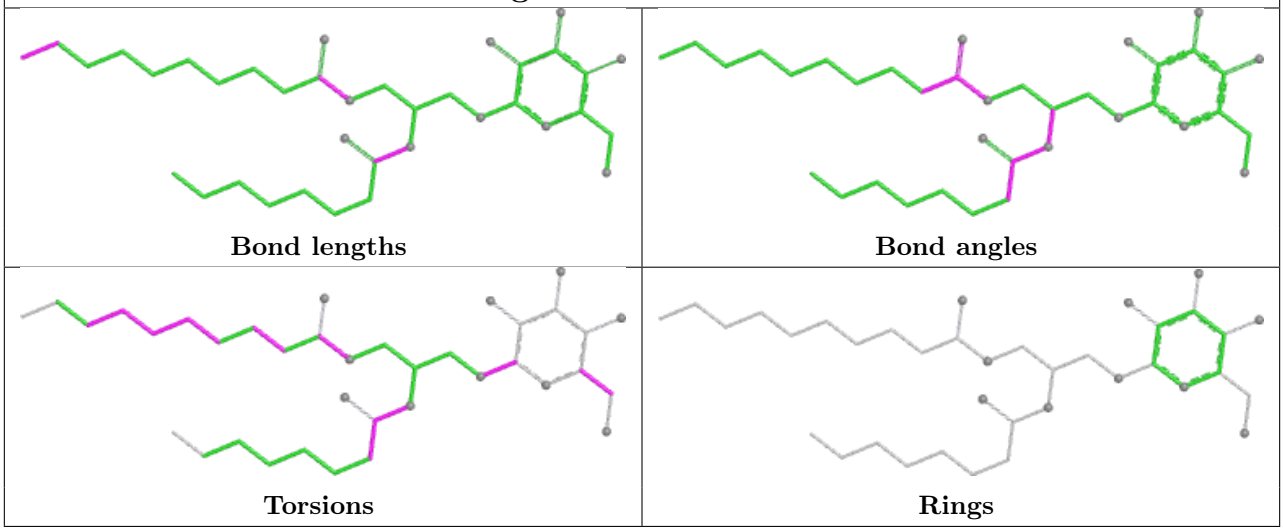
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	1023	CLA	4	0
14	a	1104	CLA	2	0
14	A	1130	CLA	2	0
13	G	1011	CL0	2	0
14	G	1129	CLA	1	0
14	G	1136	CLA	2	0
18	a	4008	BCR	1	0
14	a	1128	CLA	1	0
20	B	5002	LMG	3	0
14	A	1117	CLA	2	0
14	b	1227	CLA	1	0
14	a	1126	CLA	5	0
14	a	1127	CLA	3	0
18	B	4009	BCR	6	0
14	a	1115	CLA	1	0
14	G	1123	CLA	4	0
15	H	1230	F6C	3	0
14	G	1128	CLA	1	0
14	G	1111	CLA	3	0
14	b	1212	CLA	1	0
14	B	1206	CLA	1	0
14	H	1217	CLA	3	0
18	M	4021	BCR	3	0
14	B	1239	CLA	4	0
16	A	2001	PQN	6	0
18	L	4022	BCR	4	0
14	H	1202	CLA	7	0
14	B	1201	CLA	1	0
14	H	1207	CLA	1	0
14	a	1140	CLA	3	0
14	b	1236	CLA	1	0
14	b	1235	CLA	2	0
18	A	4007	BCR	2	0

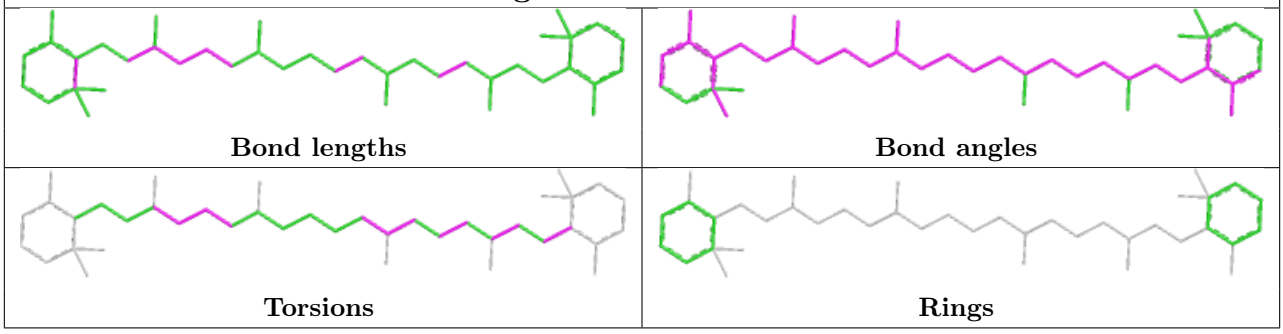
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

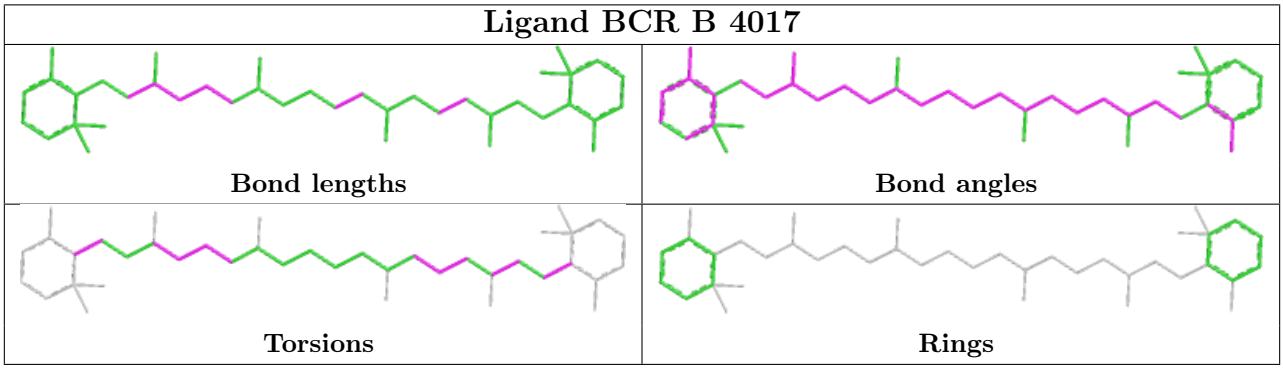
Ligand LMG R 5006

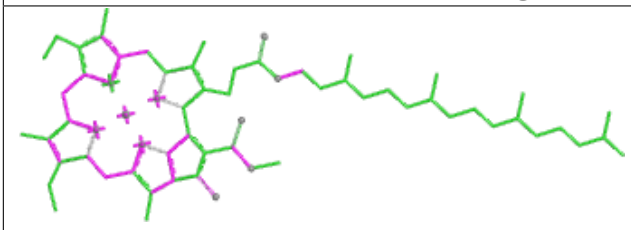
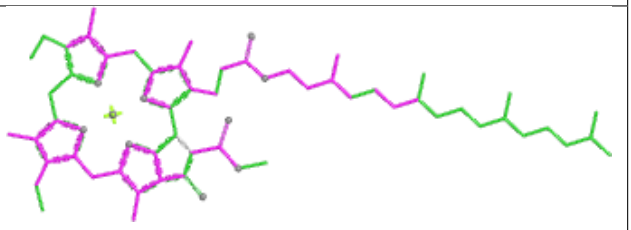
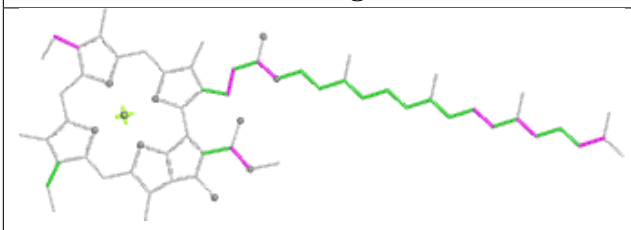
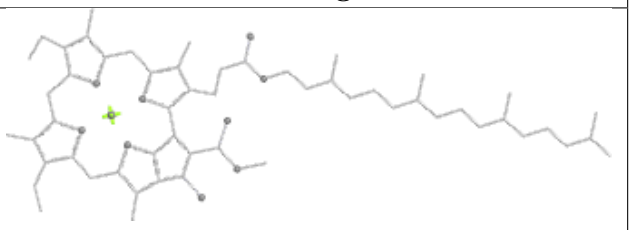


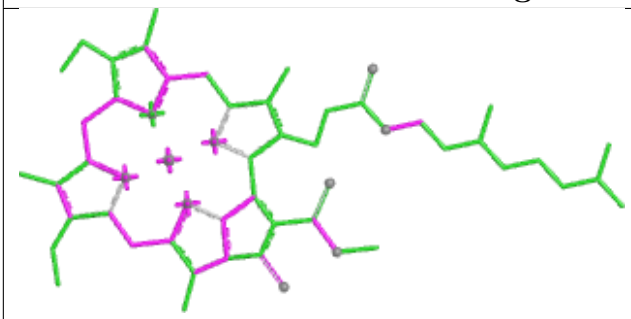
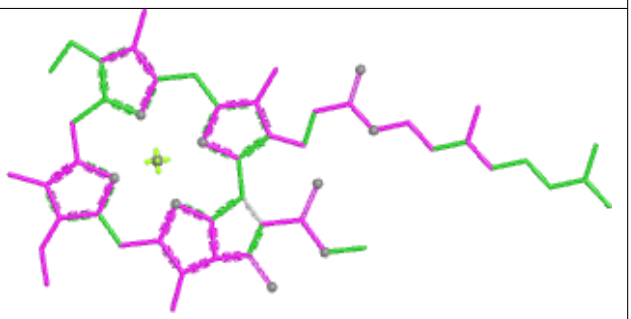
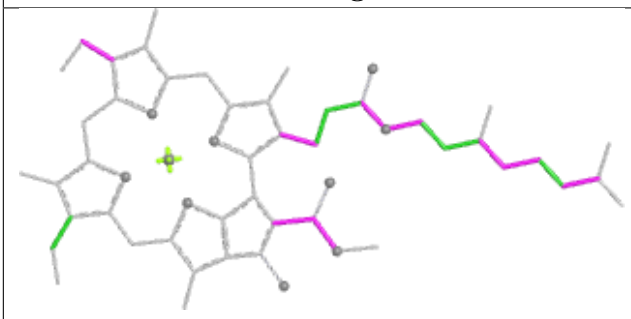
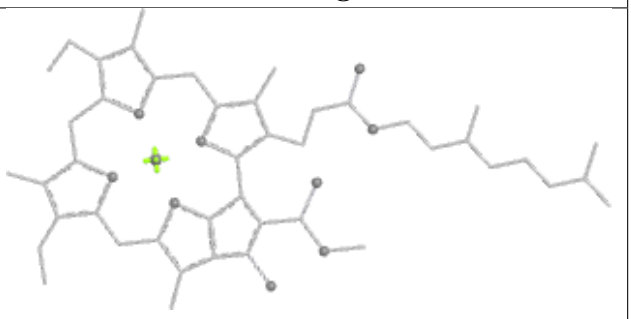
Ligand BCR G 4007



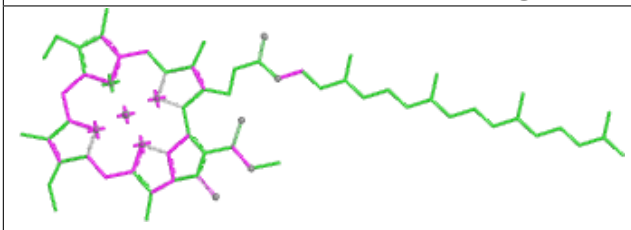
Ligand BCR B 4017



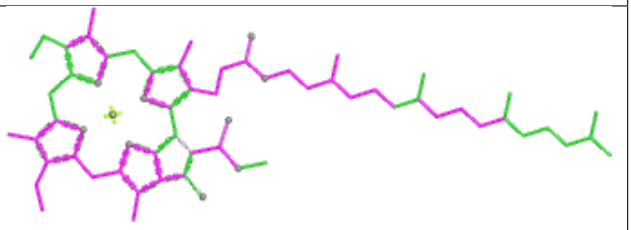
Ligand CLA H 1224	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1118	
 Bond lengths	 Bond angles
 Torsions	 Rings

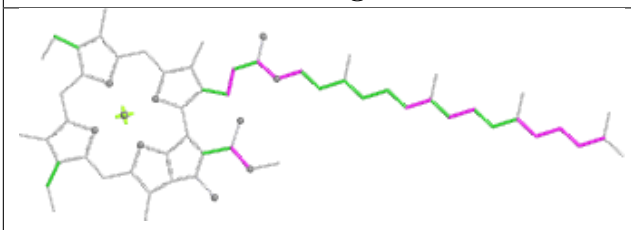
Ligand CLA B 1021



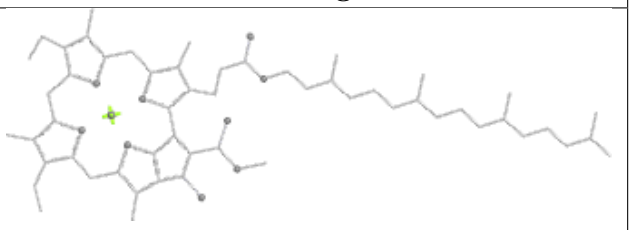
Bond lengths



Bond angles

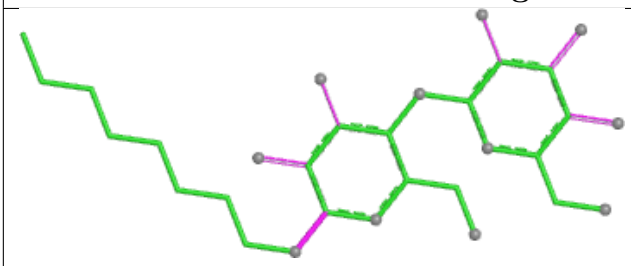


Torsions

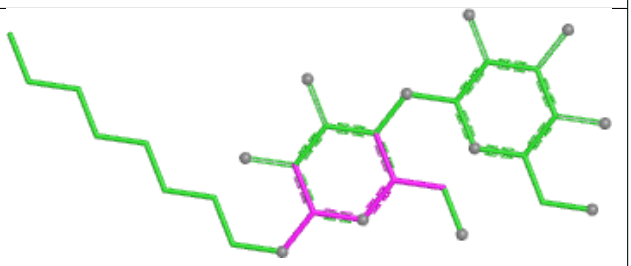


Rings

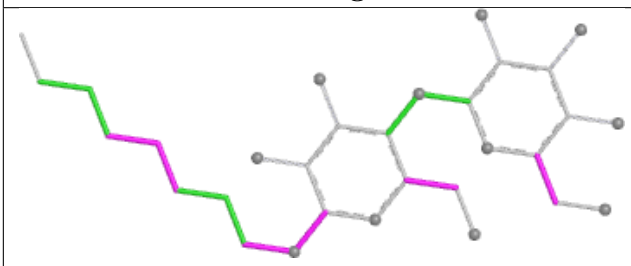
Ligand LMT A 6001



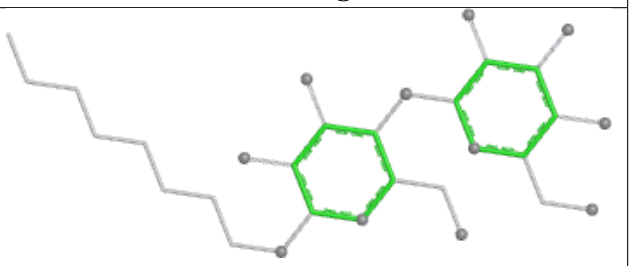
Bond lengths



Bond angles

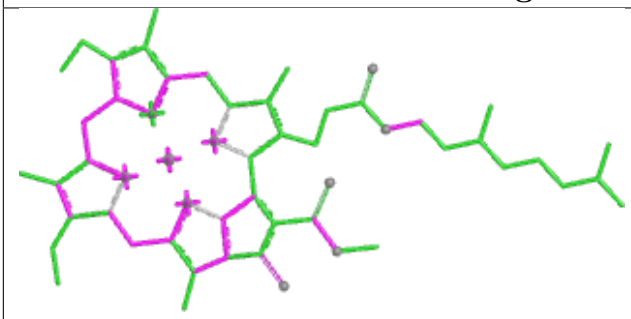


Torsions

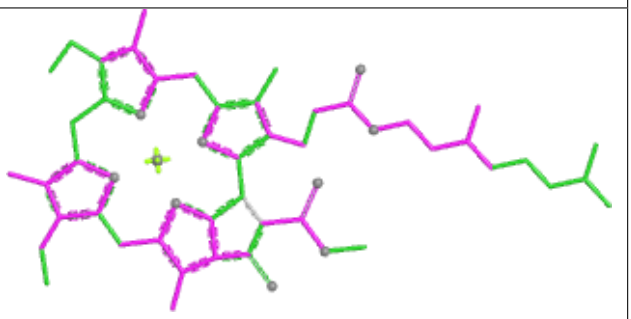


Rings

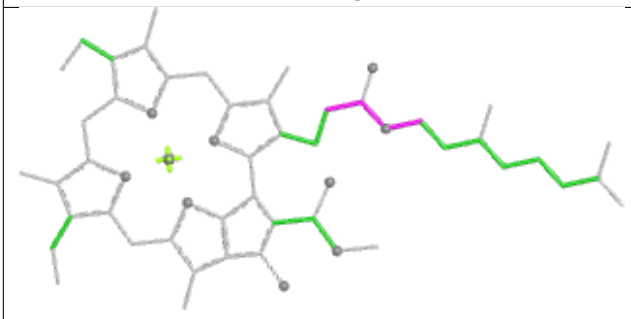
Ligand CLA B 1231



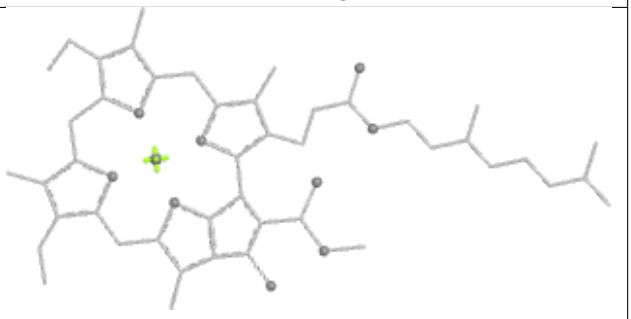
Bond lengths



Bond angles

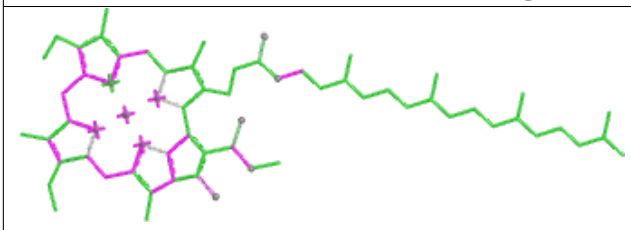


Torsions

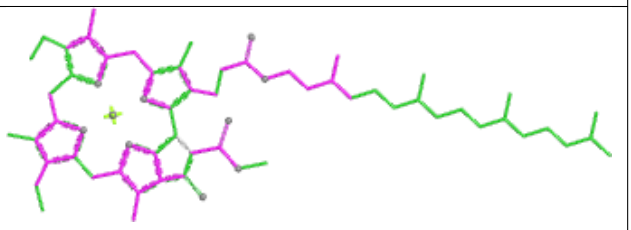


Rings

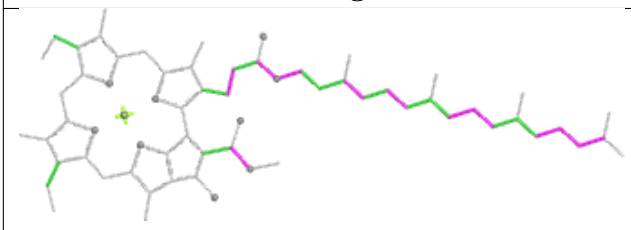
Ligand CLA a 1119



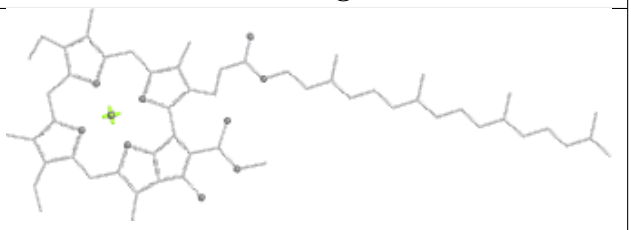
Bond lengths



Bond angles

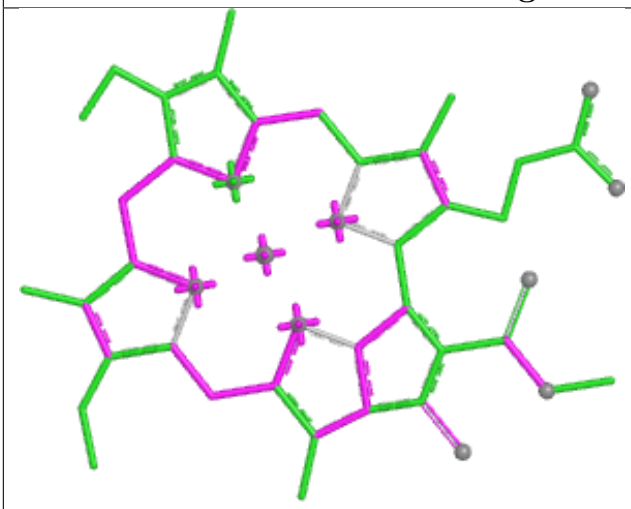


Torsions



Rings

Ligand CLA b 1206



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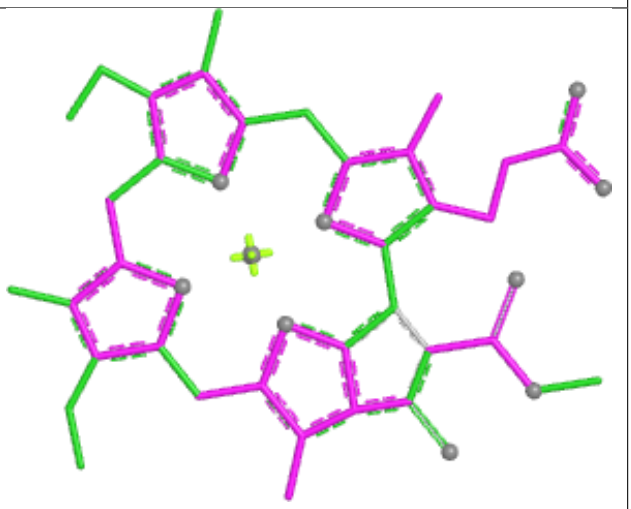
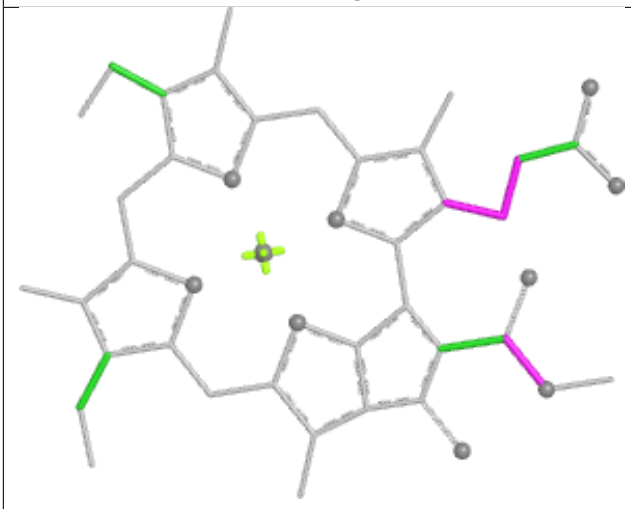


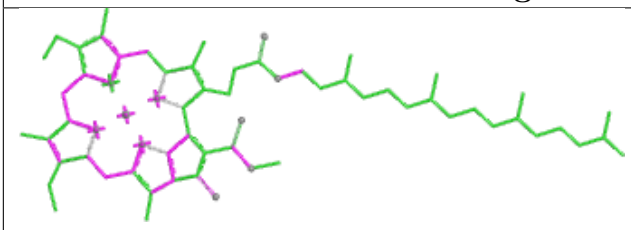
Bond angles



Torsions

Rings

Ligand CLA G 1104



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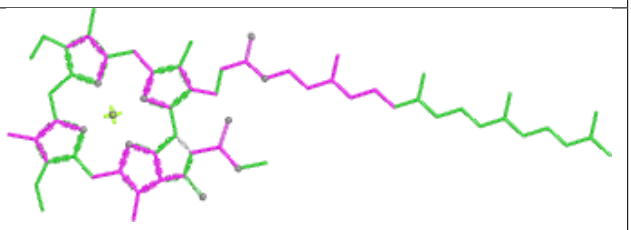
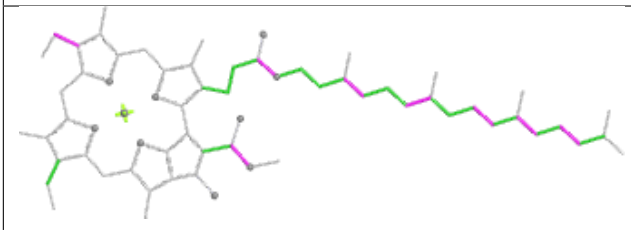


Bond angles



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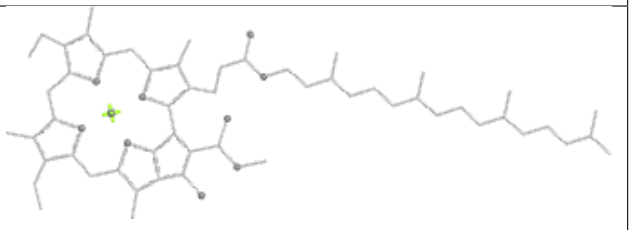
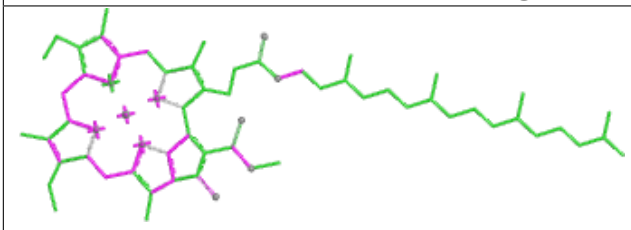


Rings

Ligand CLA B 1211



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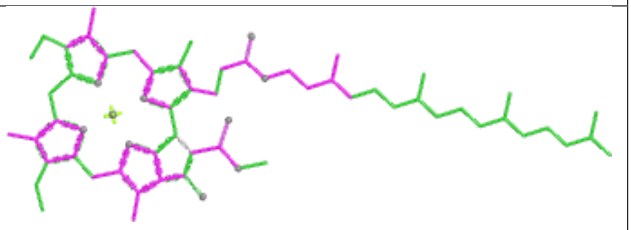

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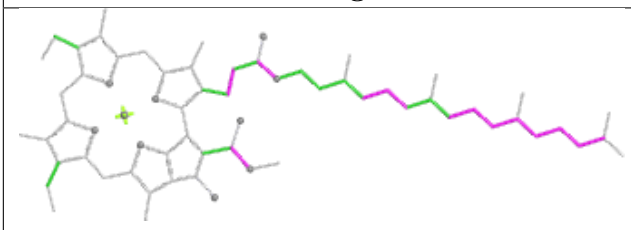
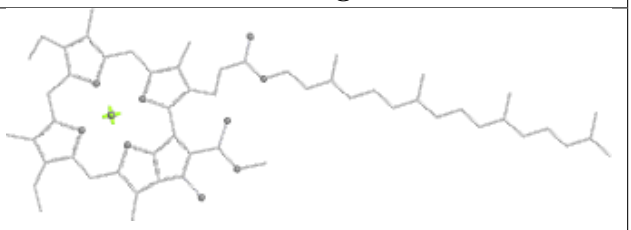
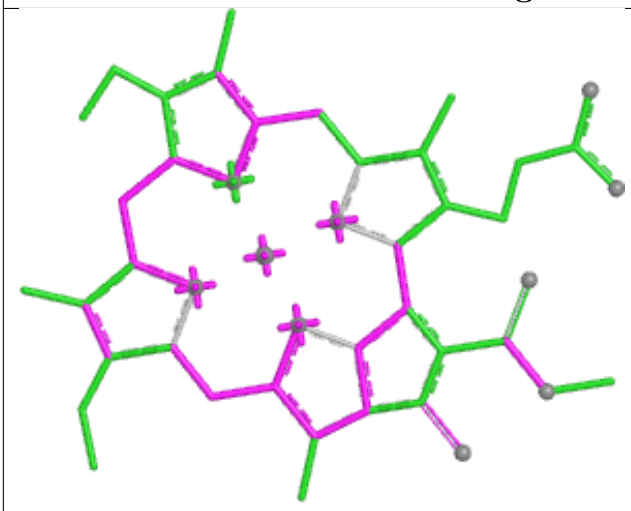


Torsions

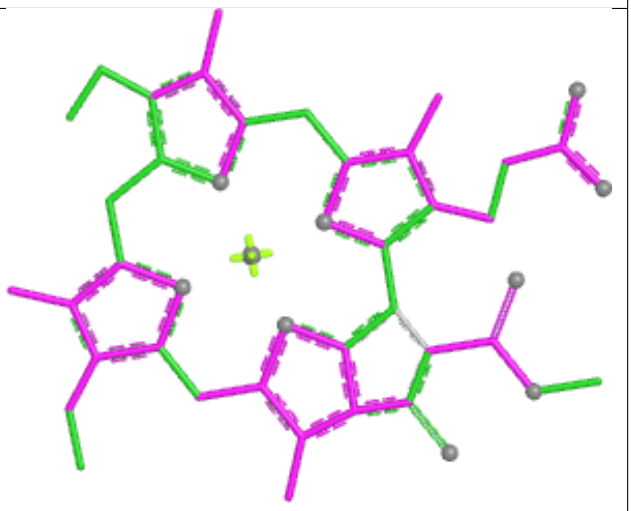


Rings

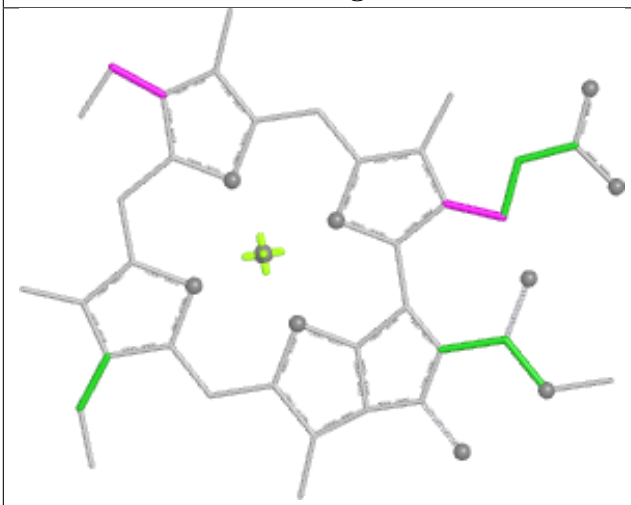
Ligand CLA B 1209



Bond lengths



Bond angles



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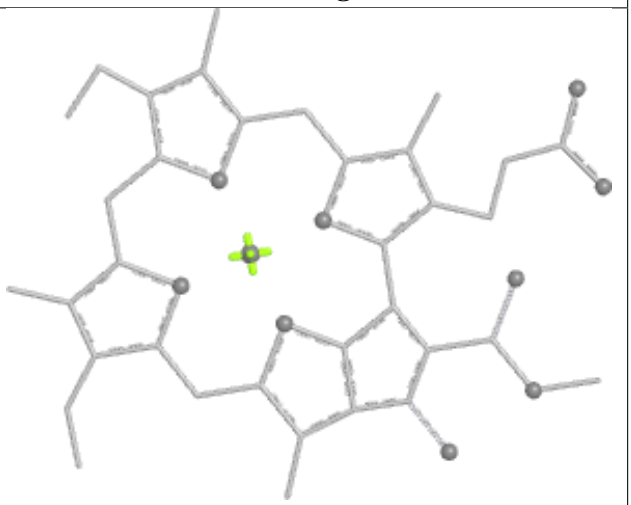
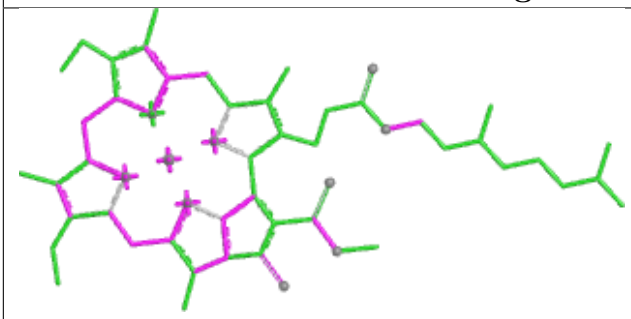


Rings

Ligand CLA H 1234



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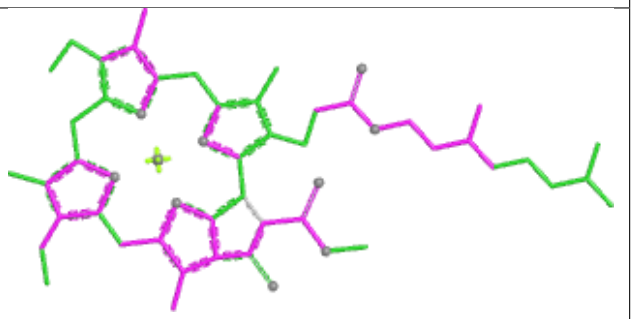
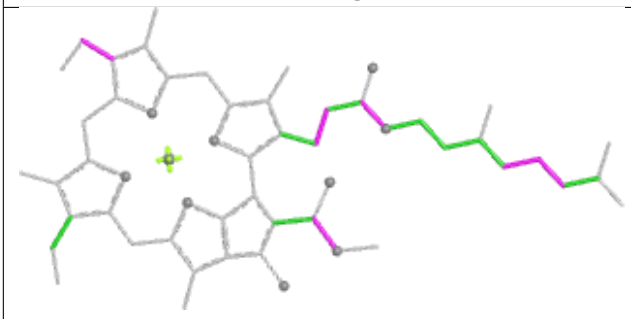
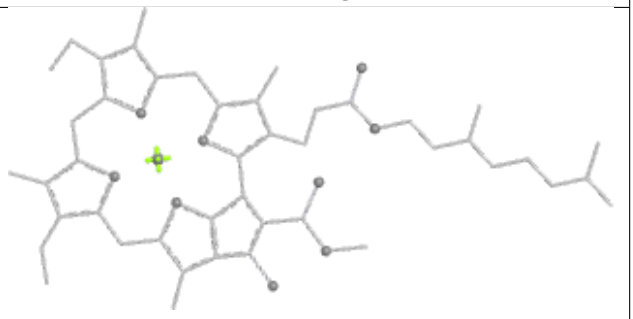


Bond angles

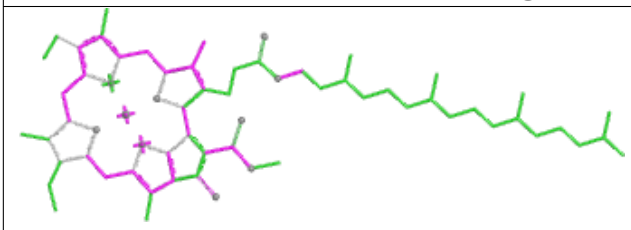


Torsions



Rings

Ligand CL0 A 1011



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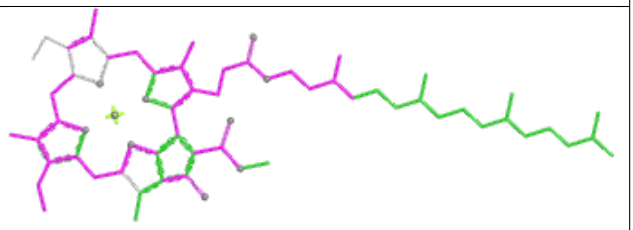
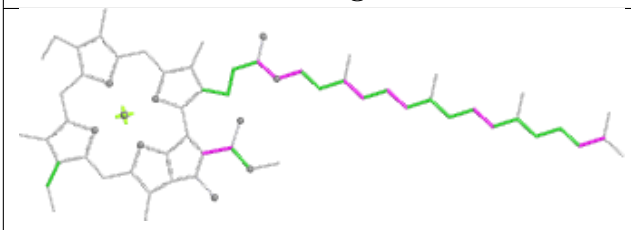


Bond angles



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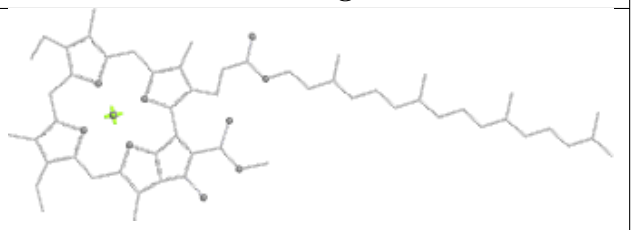
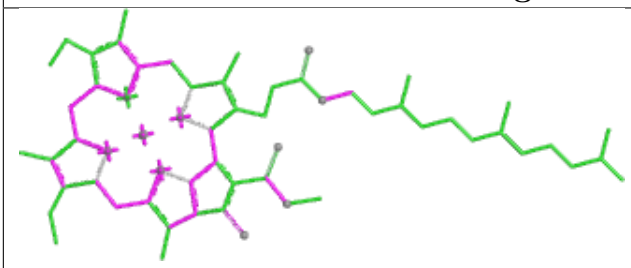


Rings

Ligand CLA G 1131



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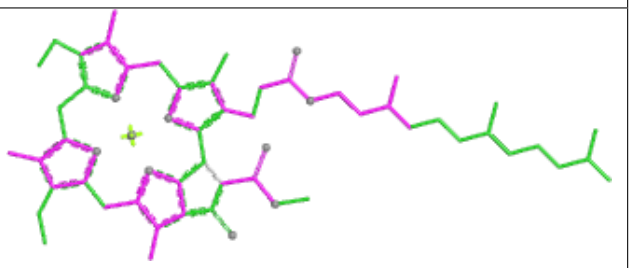
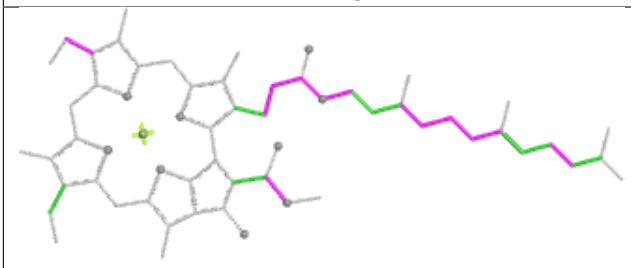


Bond angles



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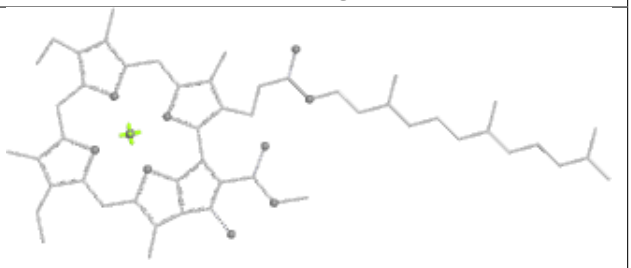
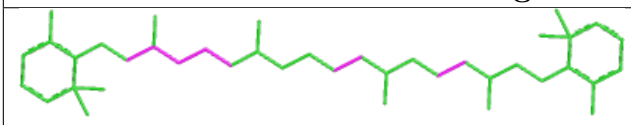


Rings

Ligand BCR B 4010



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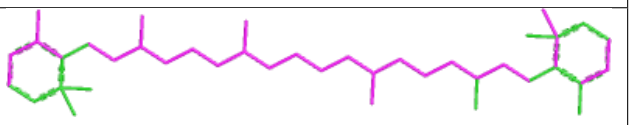
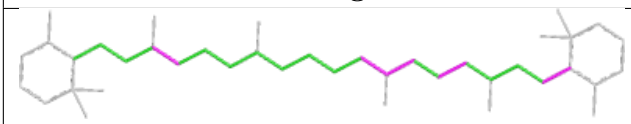
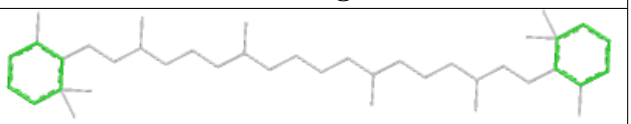


Bond angles

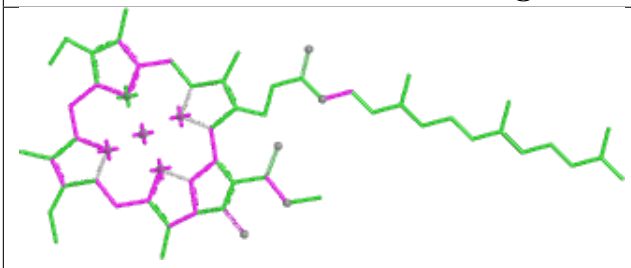


Torsions



Rings

Ligand CLA A 1138



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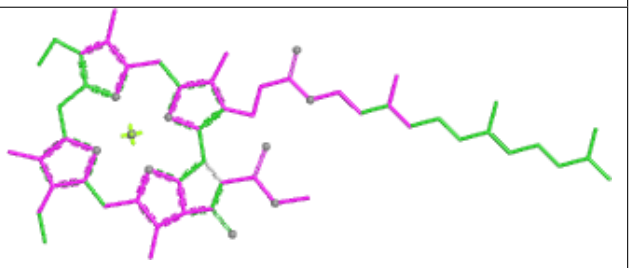
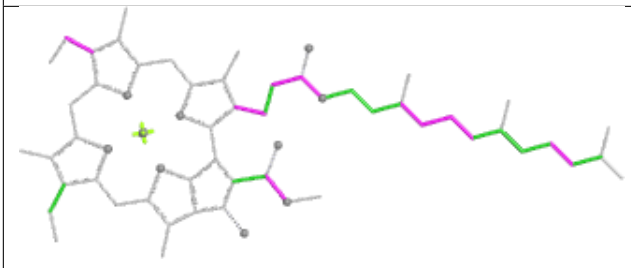


Bond angles



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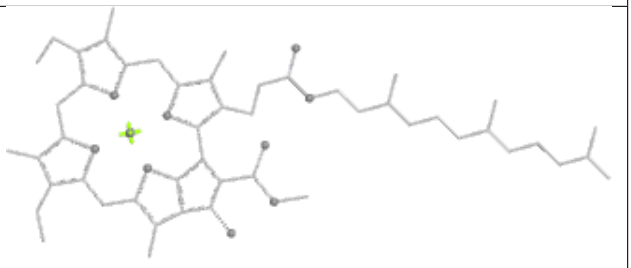
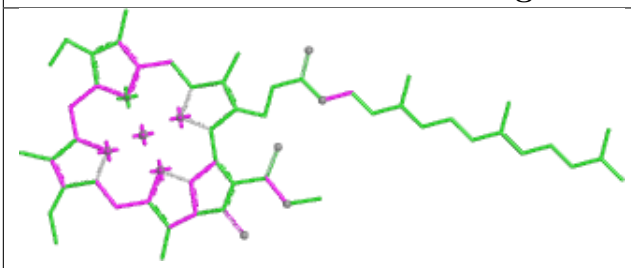


Rings

Ligand CLA B 1221



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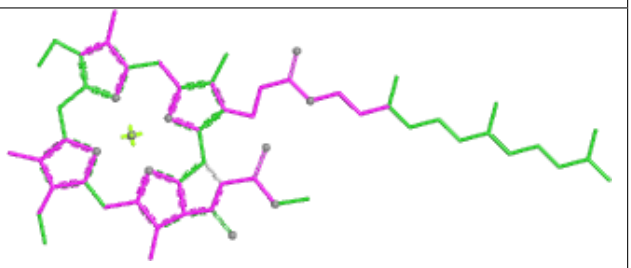
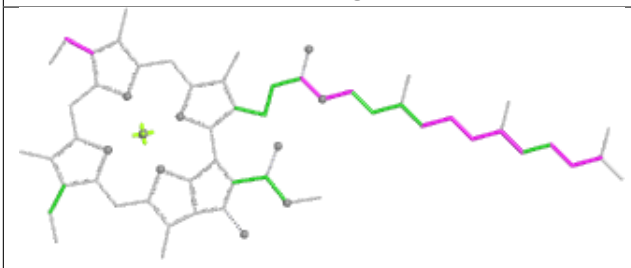


Bond angles



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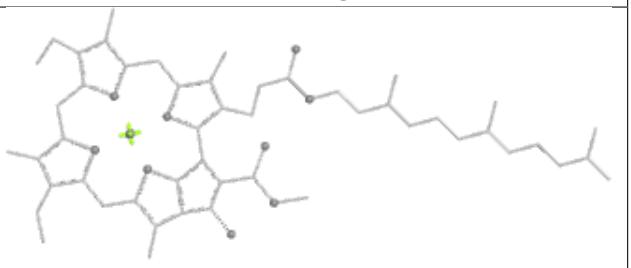
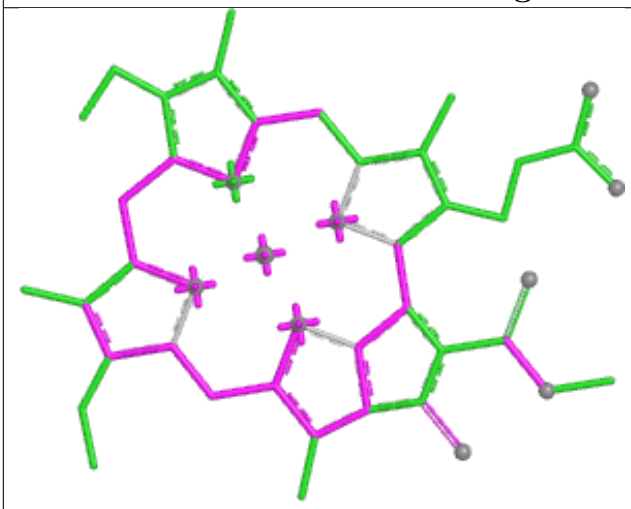


Rings

Ligand CLA G 1114



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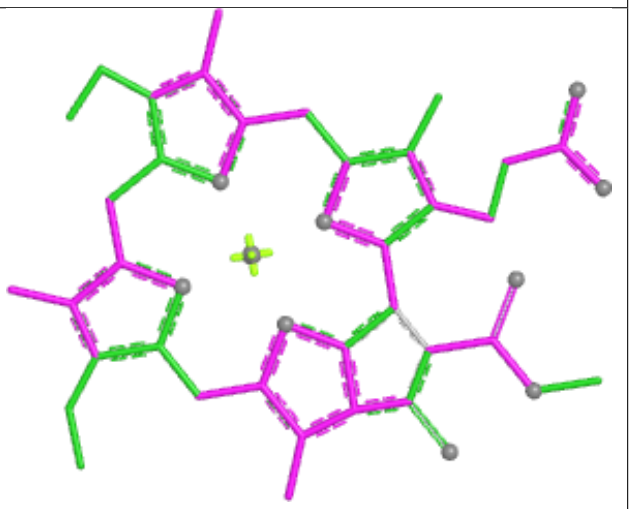
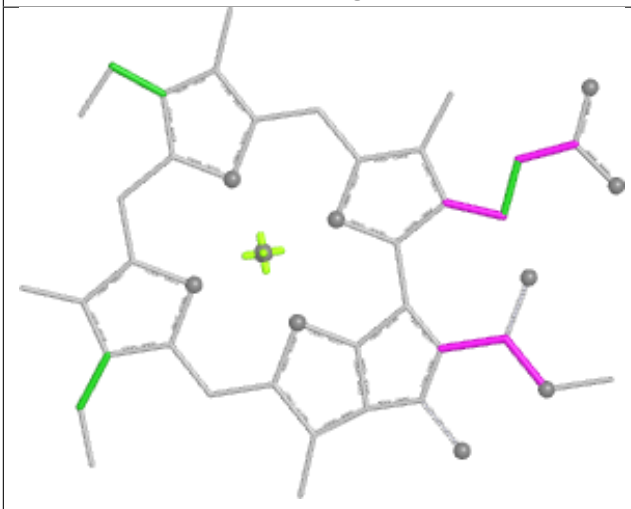


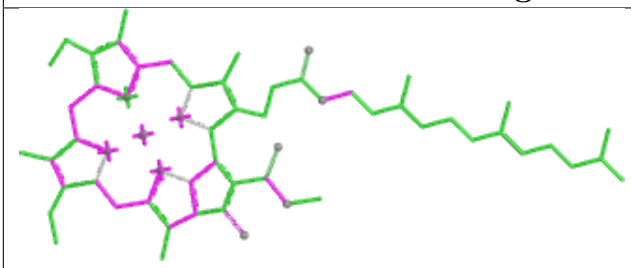
Bond angles



Torsions

Rings

Ligand CLA A 1126



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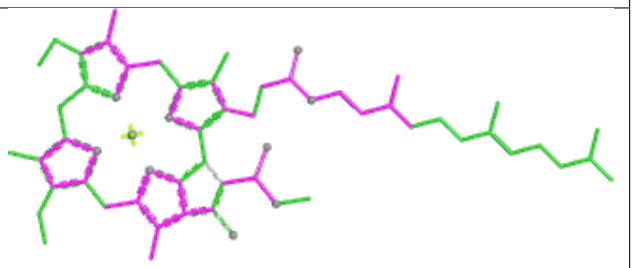
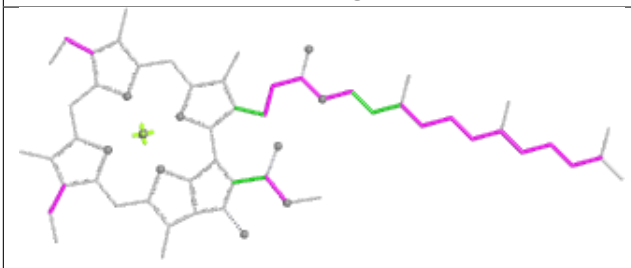
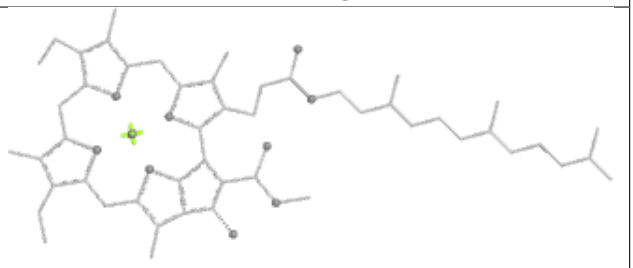


Bond angles

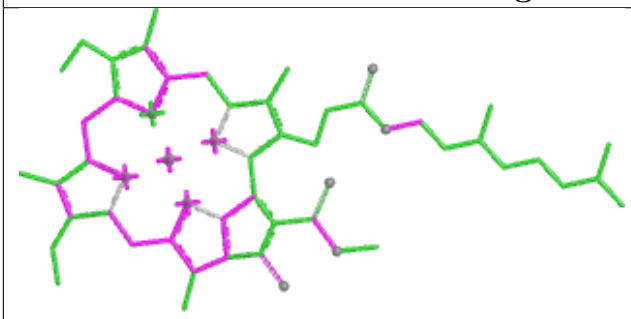


Torsions



Rings

Ligand CLA A 1115



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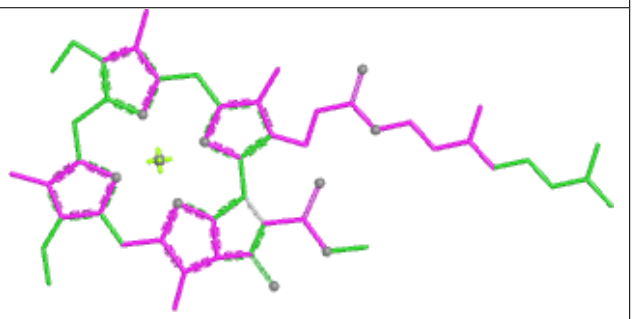
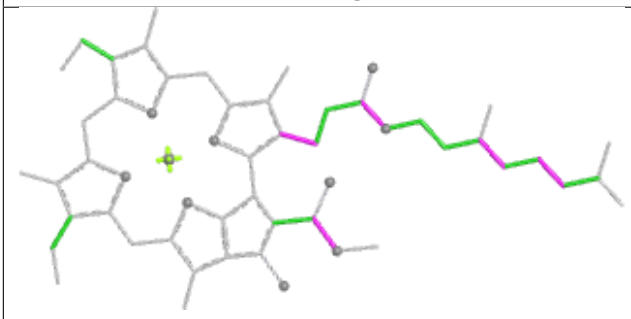
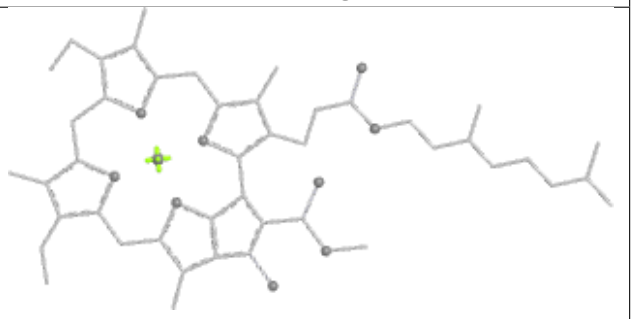


Bond angles

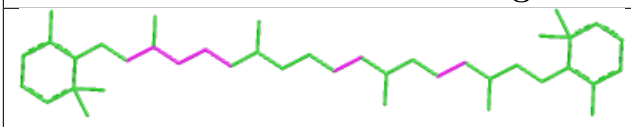


Torsions

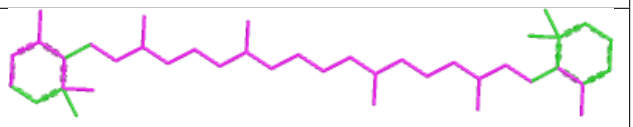


Rings

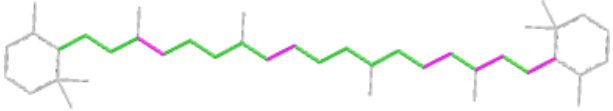
Ligand BCR U 4019



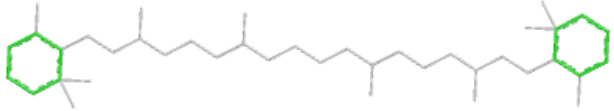
Bond lengths



Bond angles

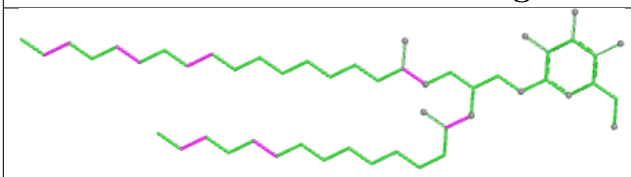


Torsions



Rings

Ligand LMG L 5007



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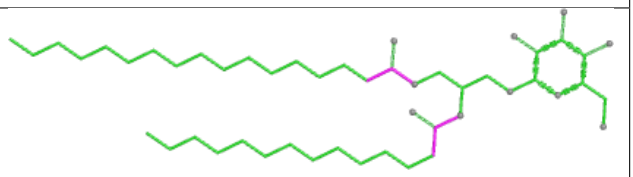

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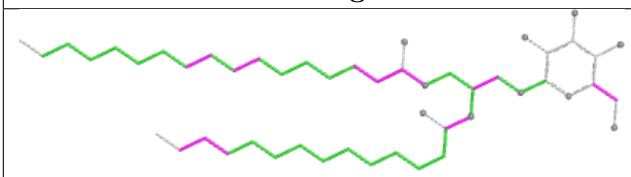

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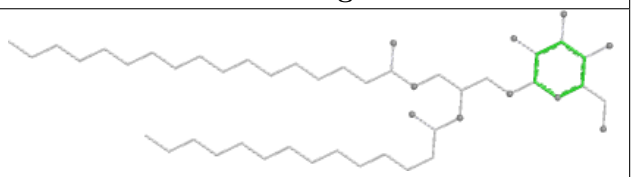
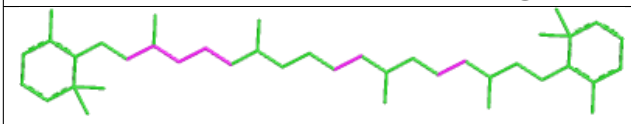


Rings

Ligand BCR b 4012



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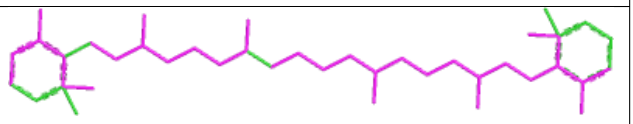
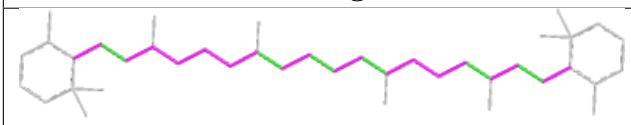
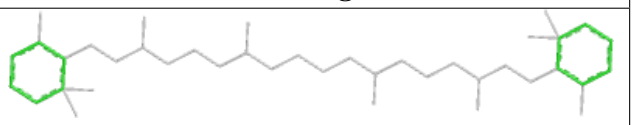


Bond angles

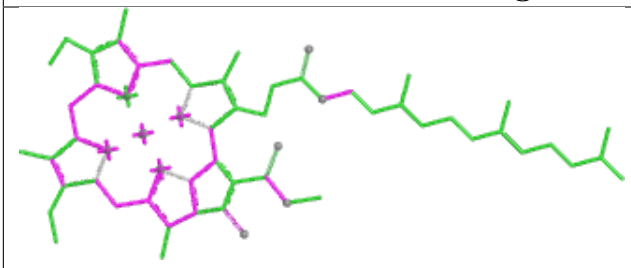


Torsions



Rings

Ligand CLA G 1138



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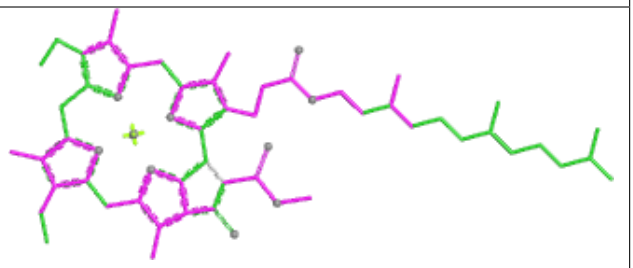
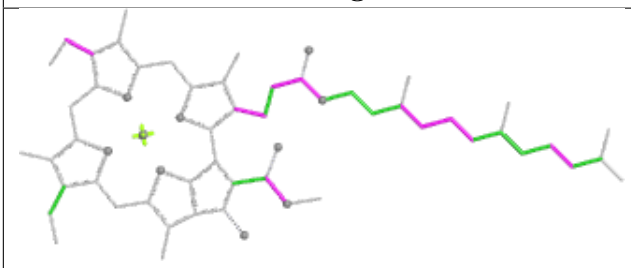


Bond angles



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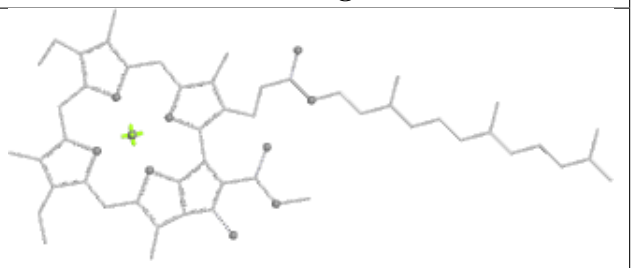
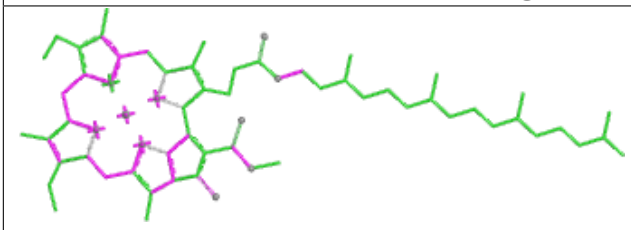


Rings

Ligand CLA b 1211



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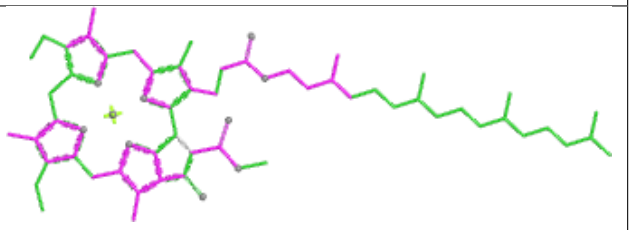
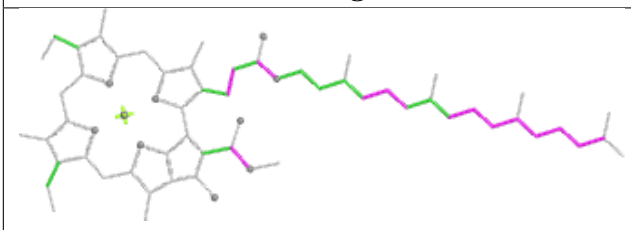
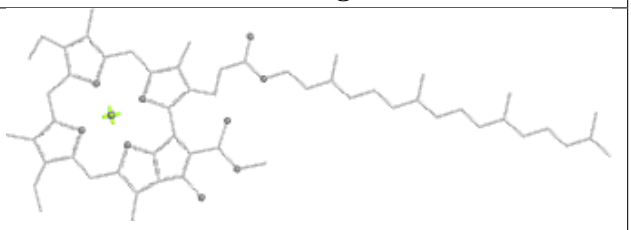


Bond angles

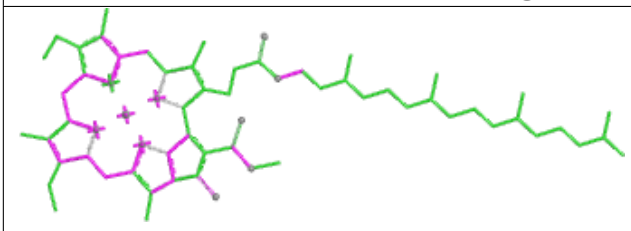


Torsions



Rings

Ligand CLA b 1210



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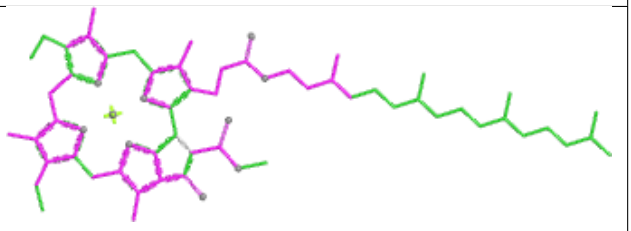
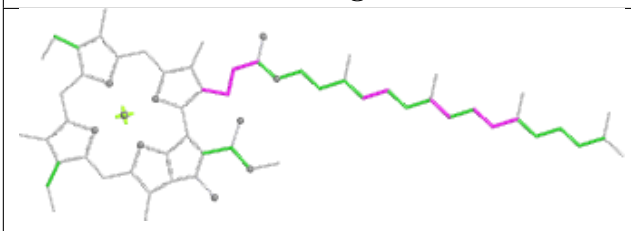
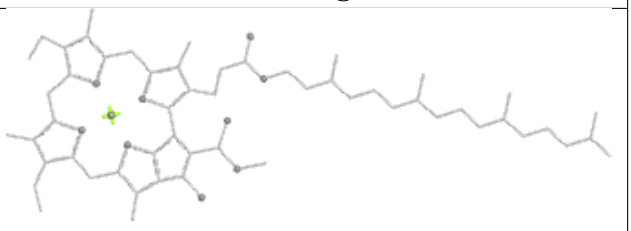


Bond angles

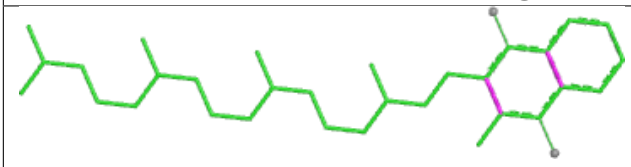


Torsions



Rings

Ligand PQN b 2002



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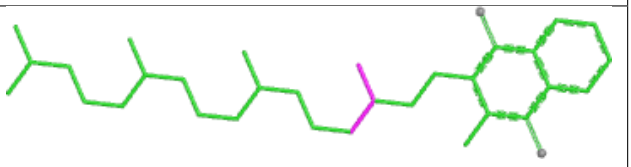
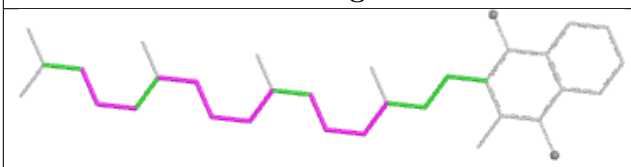
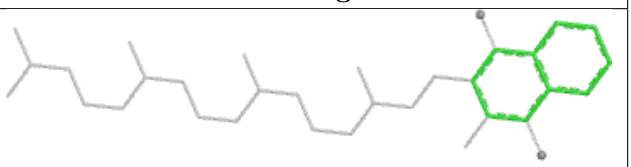


Bond angles

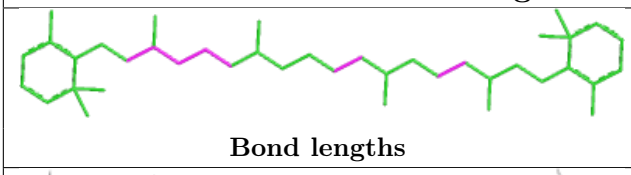


Torsions



Rings

Ligand BCR B 4006



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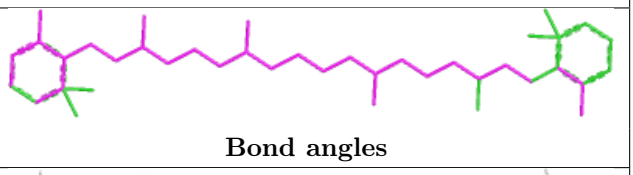
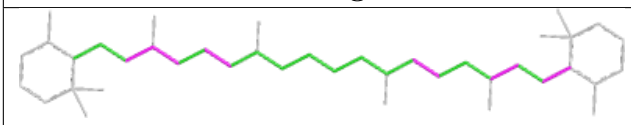


Bond angles



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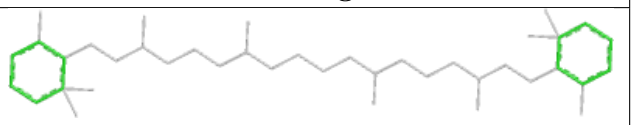
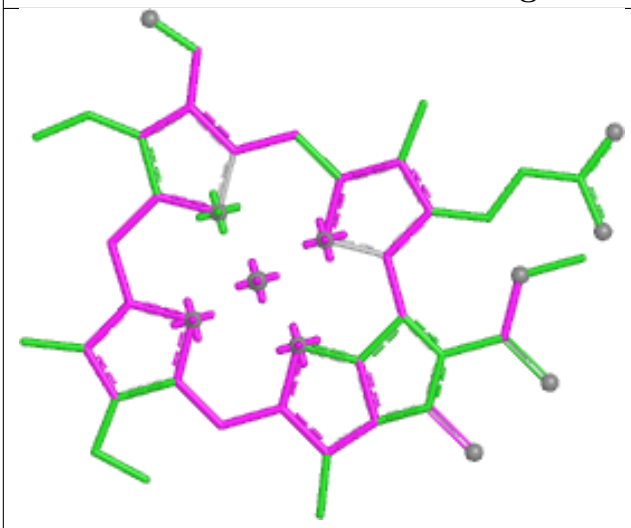
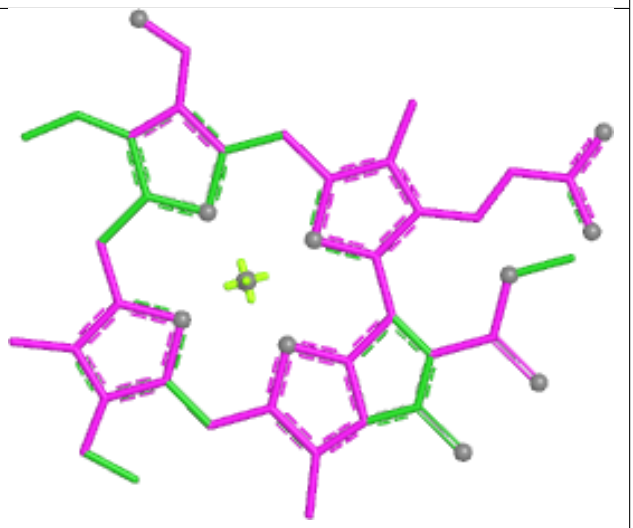


Rings

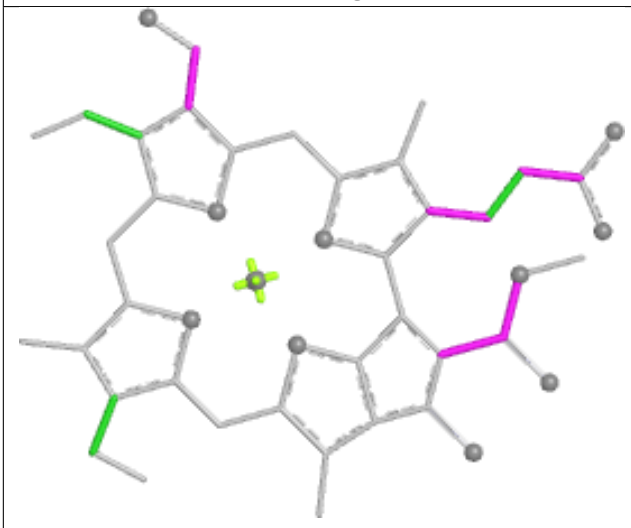
Ligand F6C B 1230



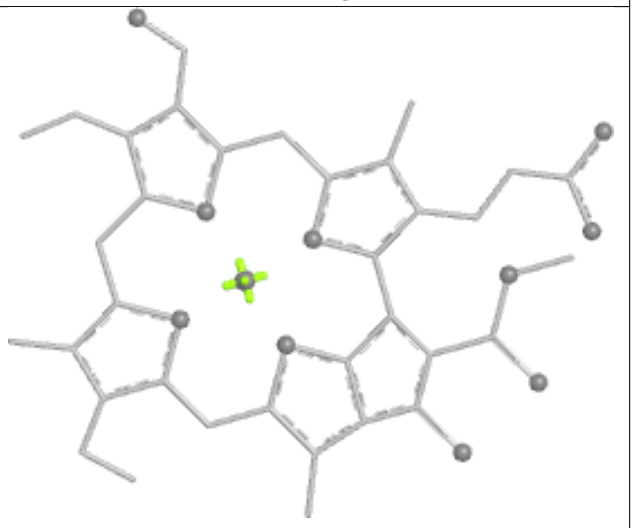
Bond lengths



Bond angles

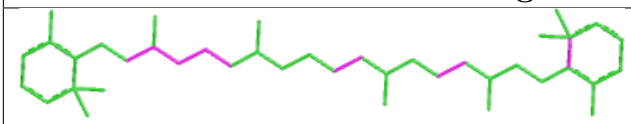


Torsions



Rings

Ligand BCR b 4005



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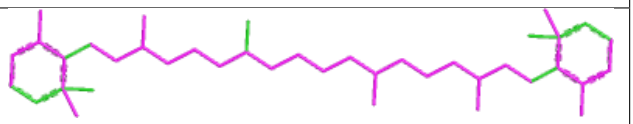
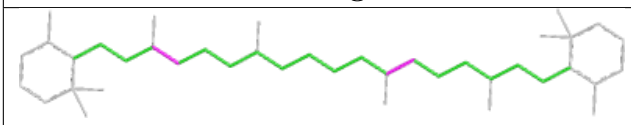


Bond angles



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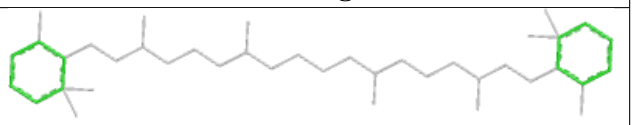
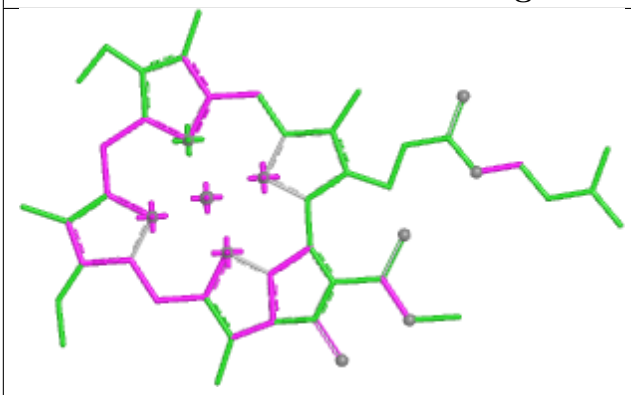


Rings

Ligand CLA A 1135



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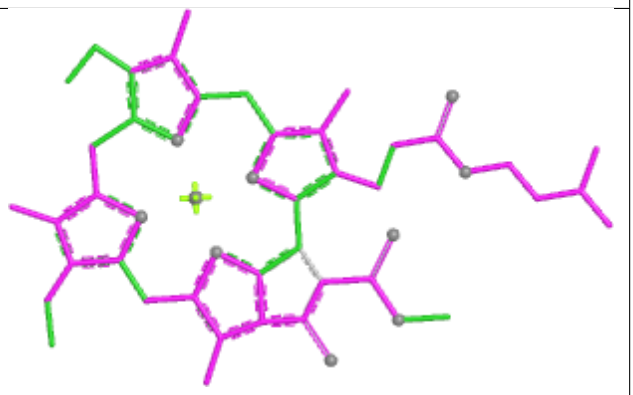
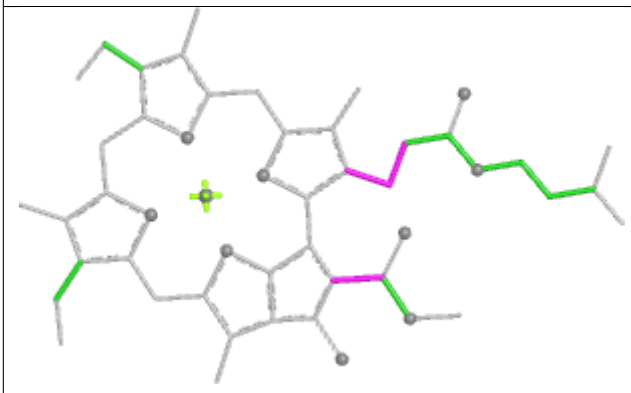


Bond angles



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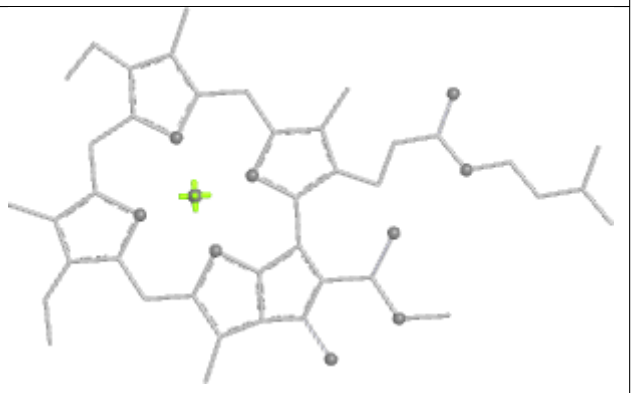
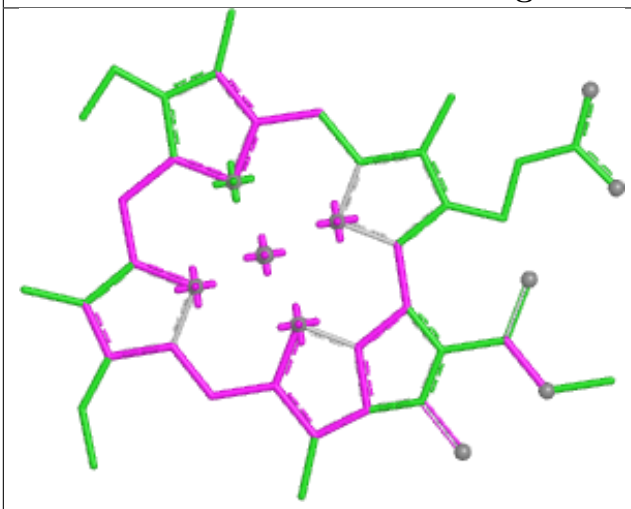


Rings

Ligand CLA T 1401



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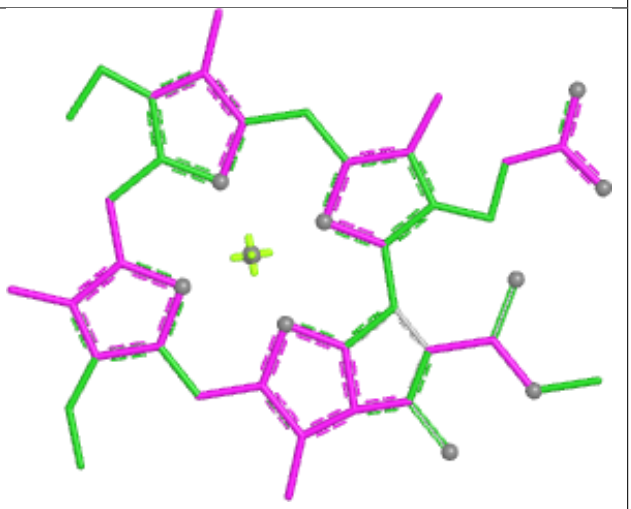
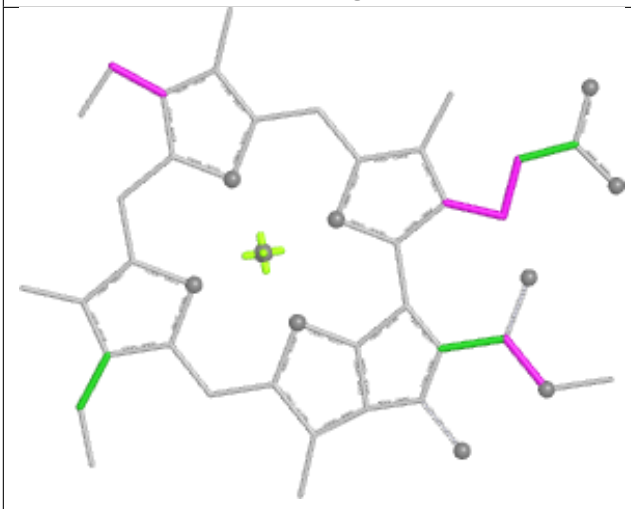


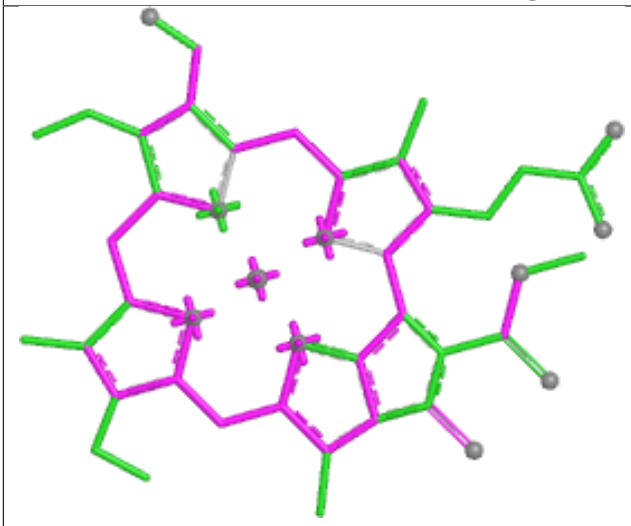
Bond angles



Torsions

Rings

Ligand F6C a 1121



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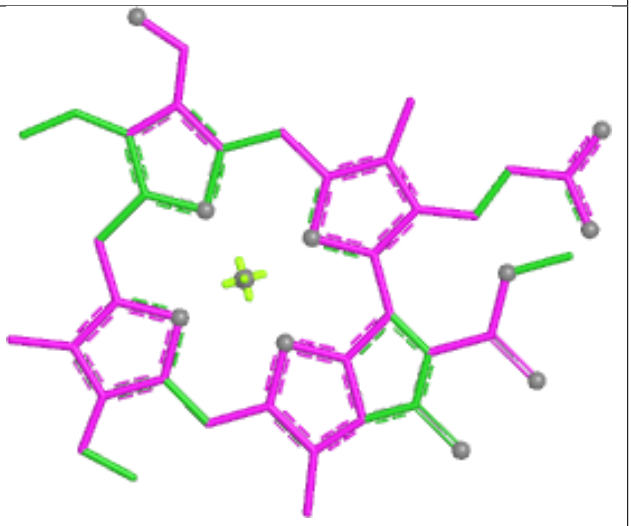
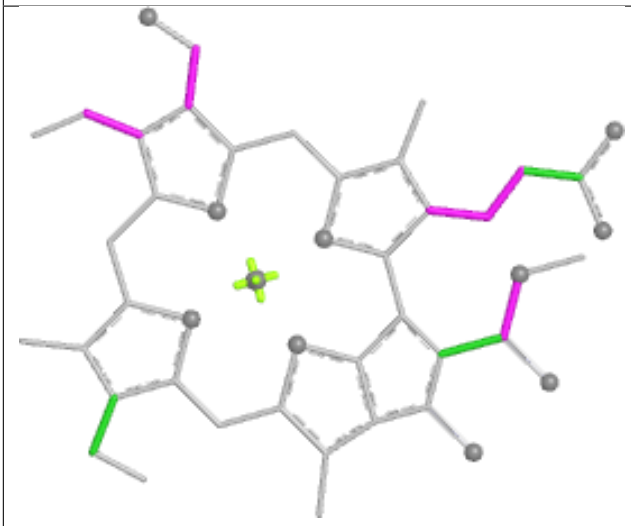
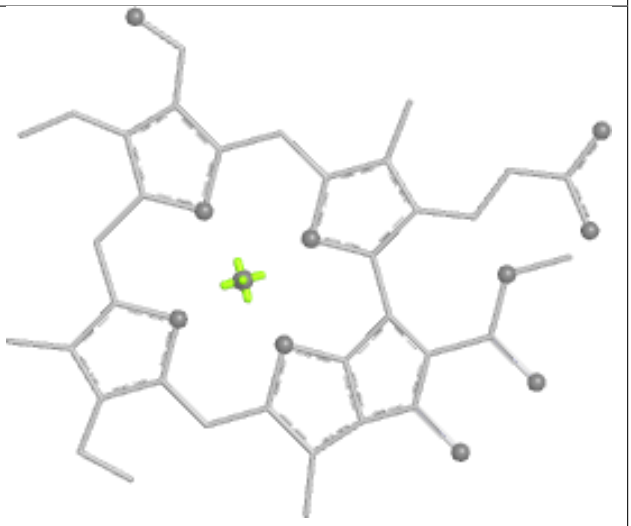


Bond angles

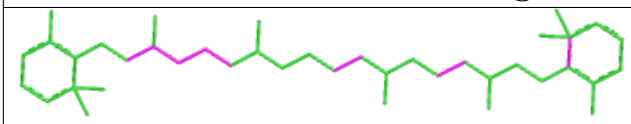


Torsions



Rings

Ligand BCR B 4004



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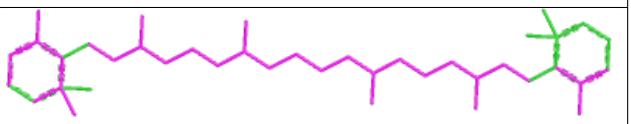
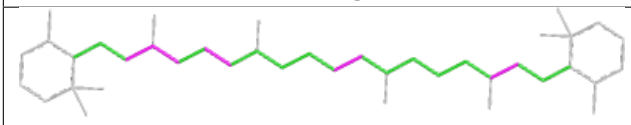
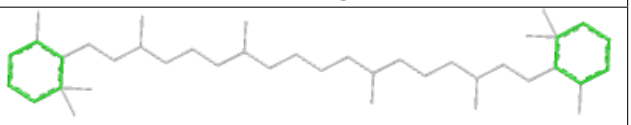


Bond angles

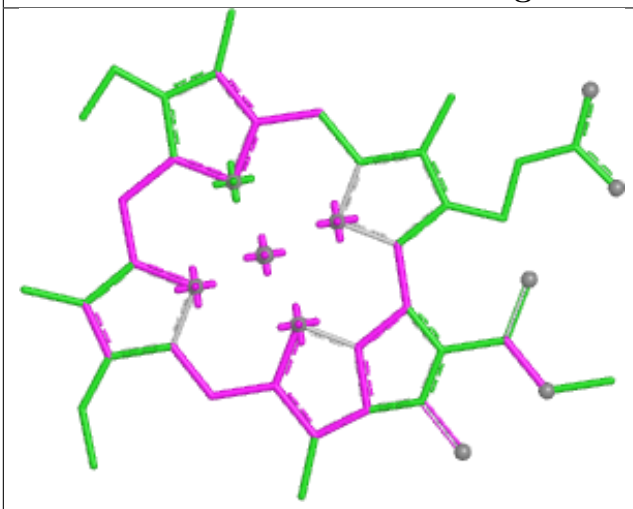


Torsions

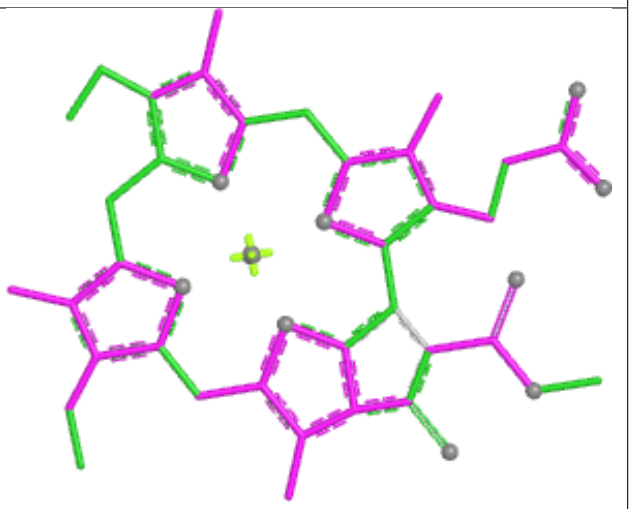


Rings

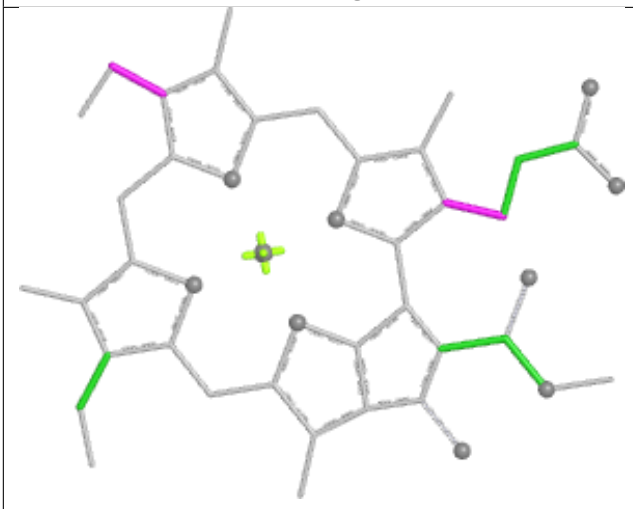
Ligand CLA H 1209



Bond lengths



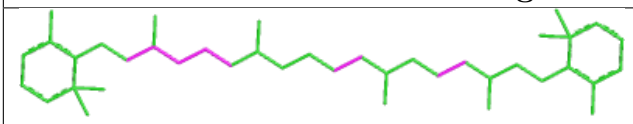
Bond angles



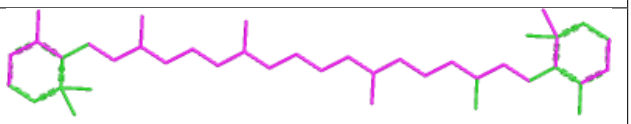
Torsions

Rings

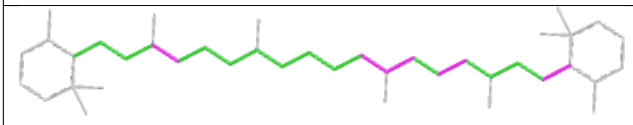
Ligand BCR b 4010



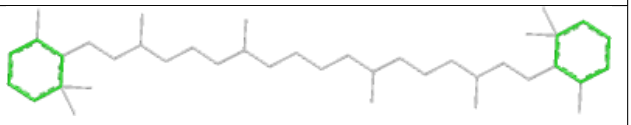
Bond lengths



Bond angles

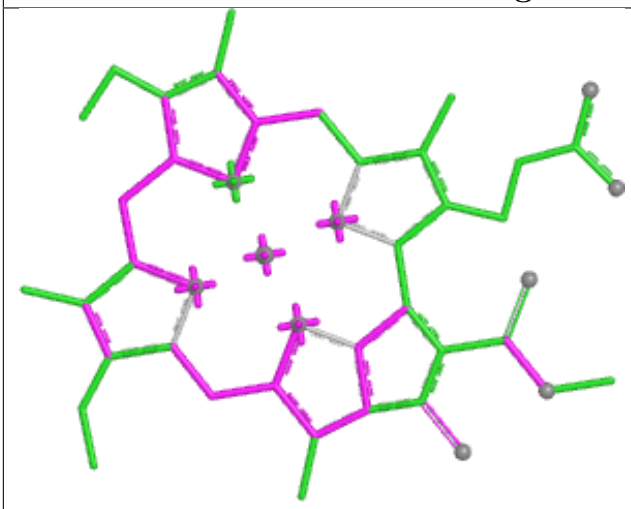


Torsions

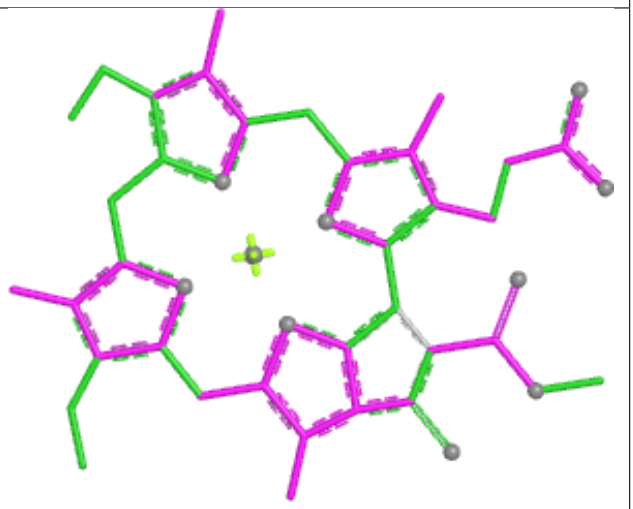


Rings

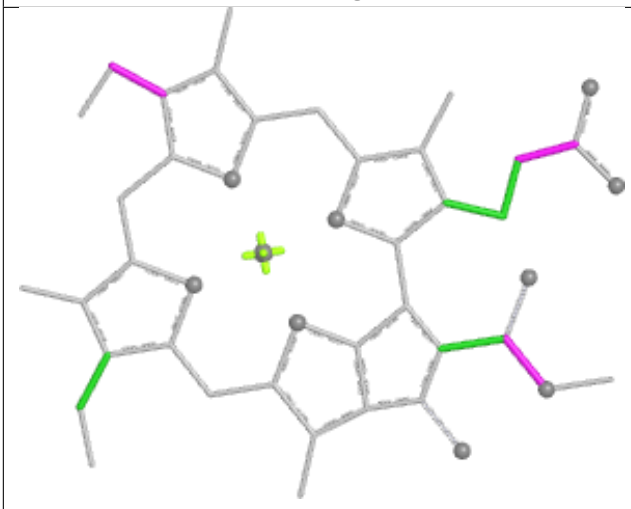
Ligand CLA A 1108



Bond lengths



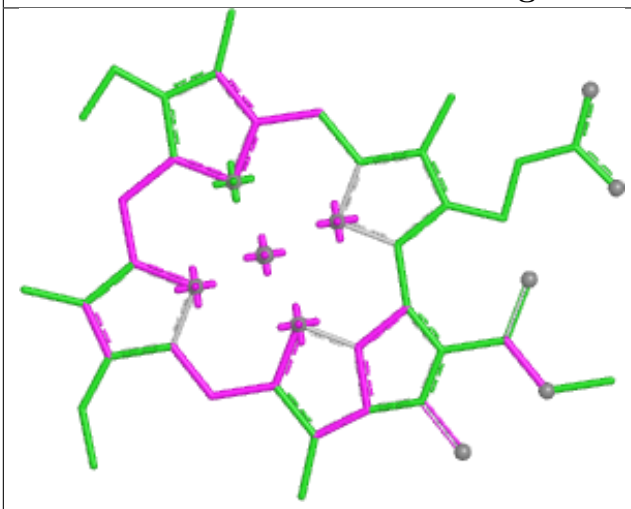
Bond angles



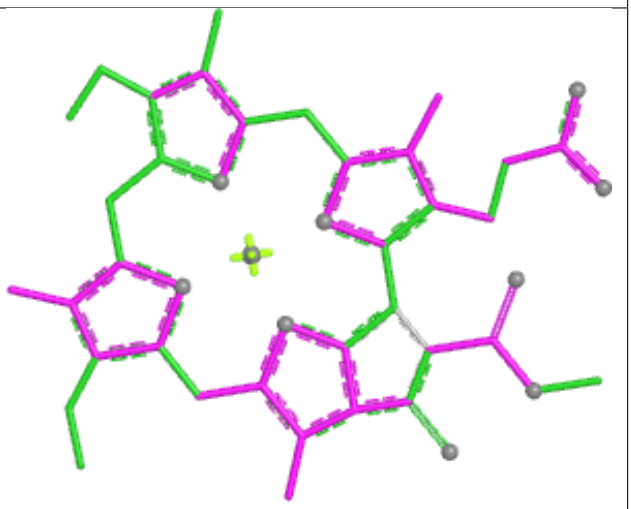
Torsions

Rings

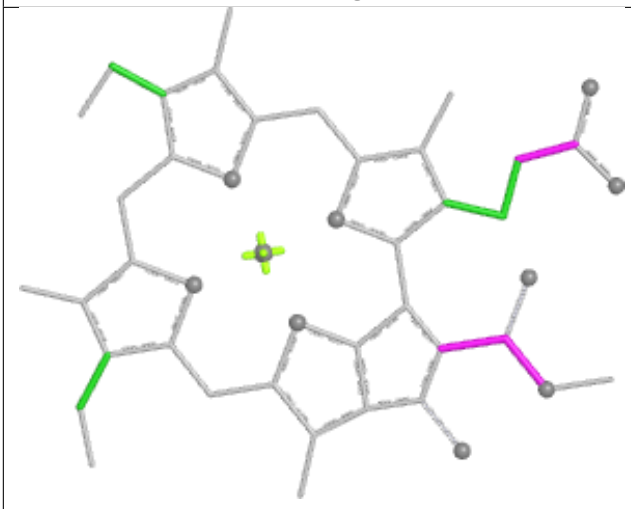
Ligand CLA b 1218



Bond lengths



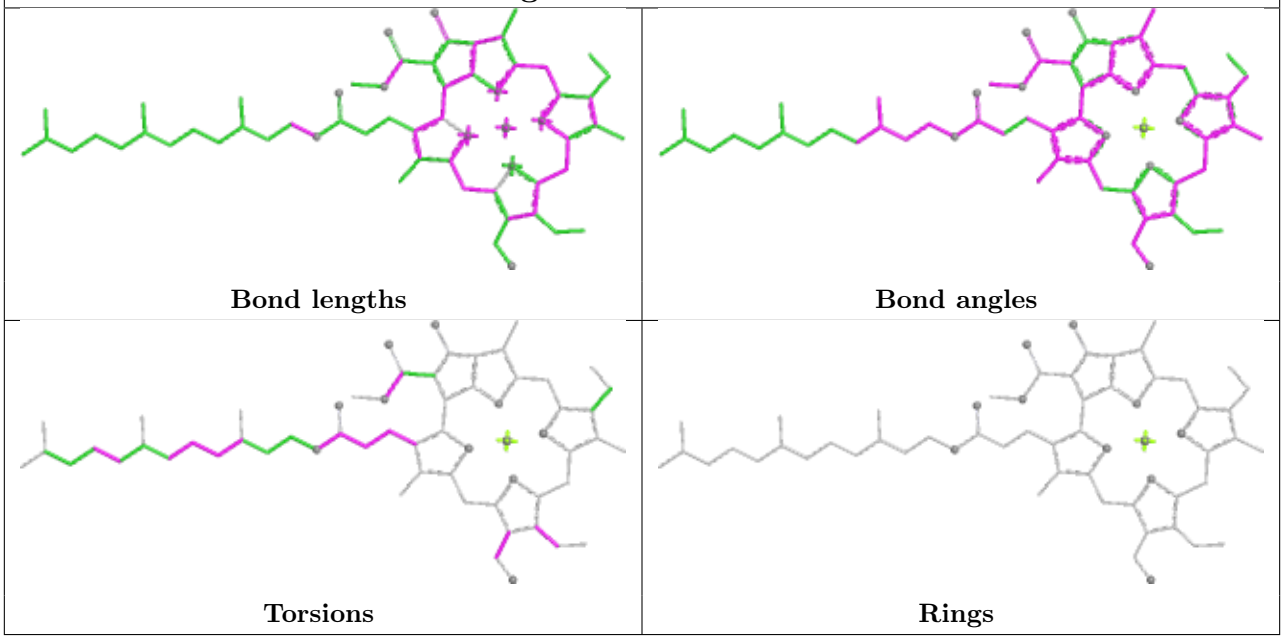
Bond angles



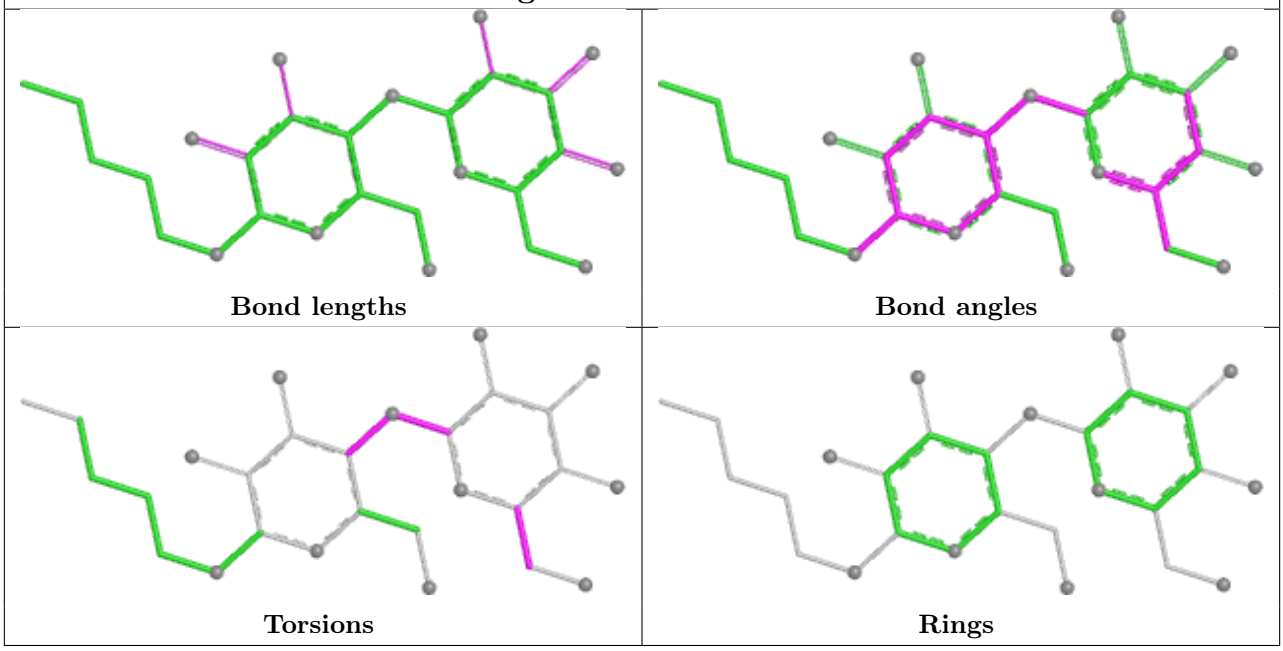
Torsions

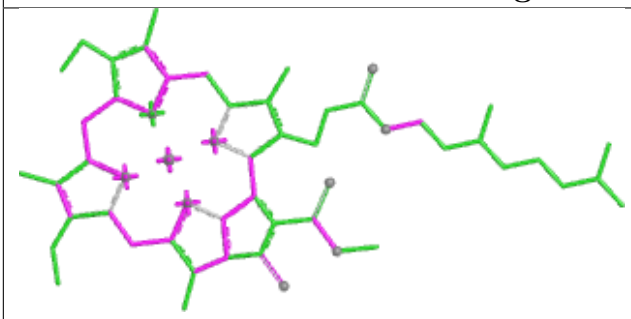
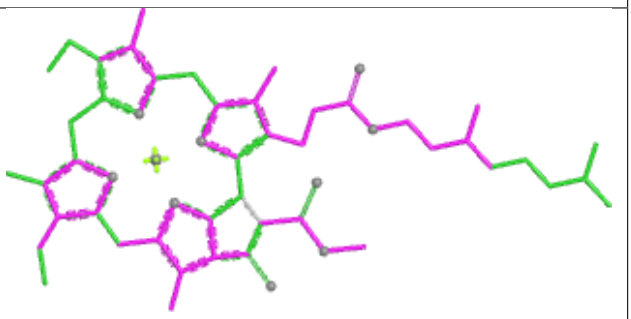
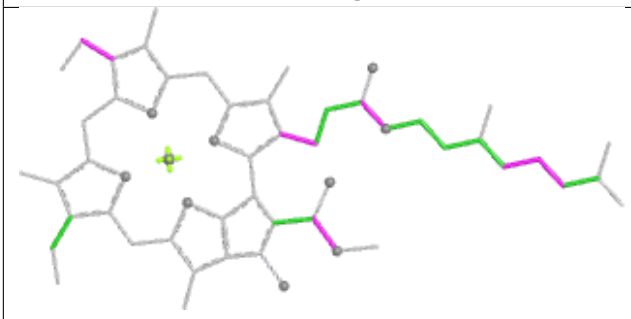
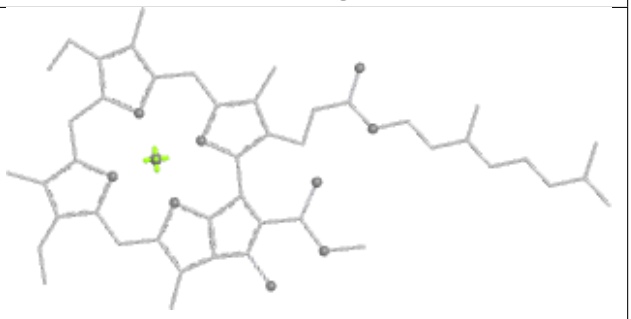
Rings

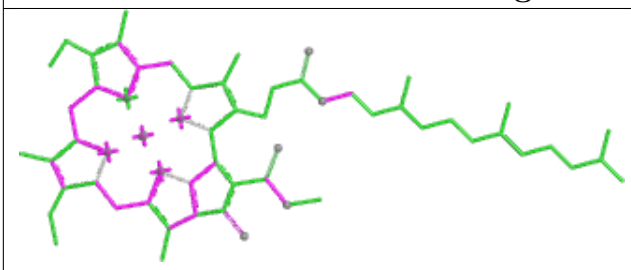
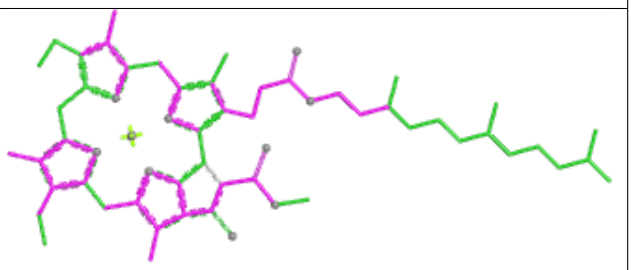
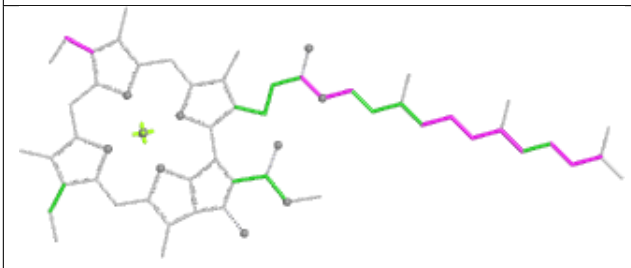
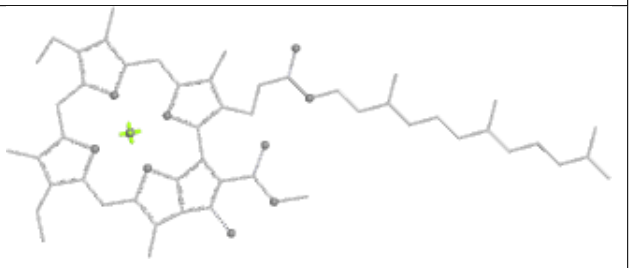
Ligand F6C B 1237



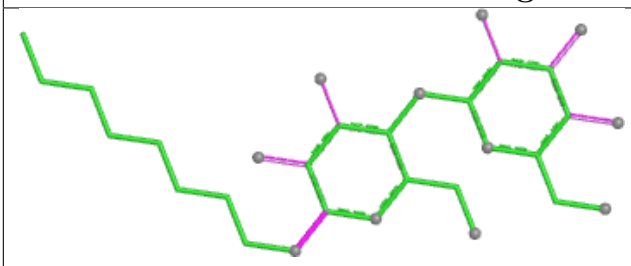
Ligand LMT a 6002



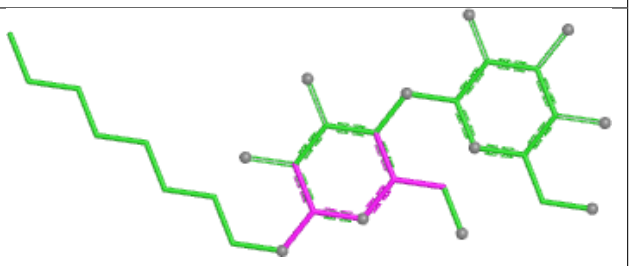
Ligand CLA G 1122	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1221	
	
Bond lengths	Bond angles
	
Torsions	Rings

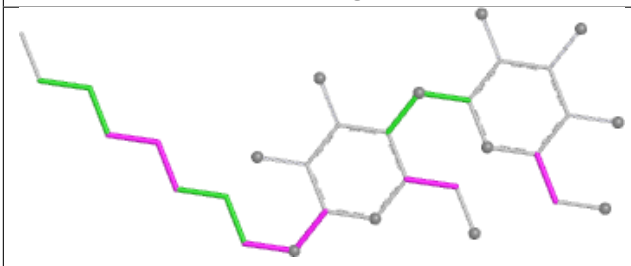
Ligand LMT a 6001



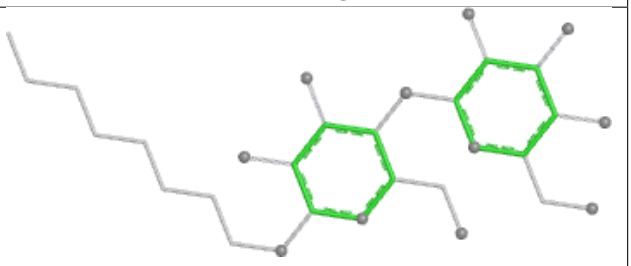
Bond lengths



Bond angles

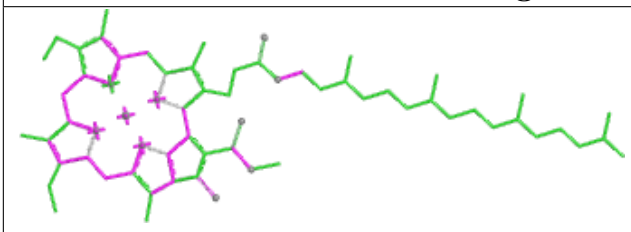


Torsions

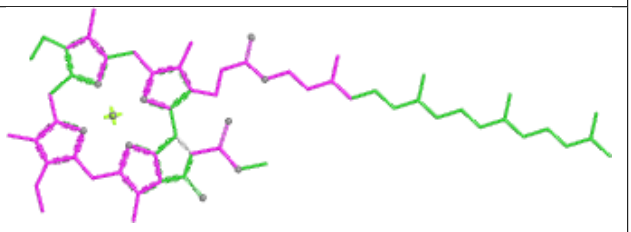


Rings

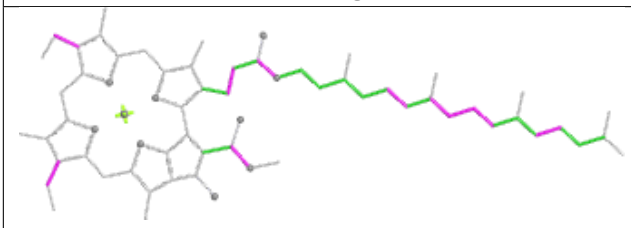
Ligand CLA B 1023



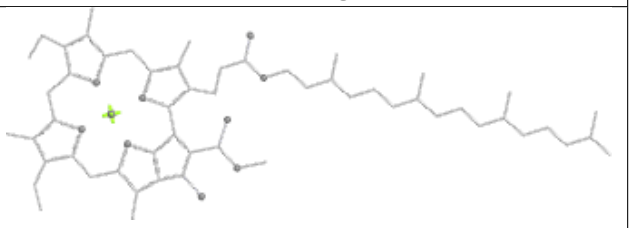
Bond lengths



Bond angles

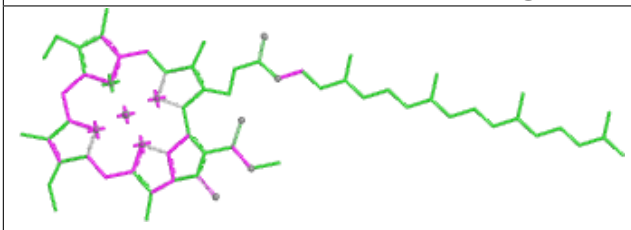


Torsions

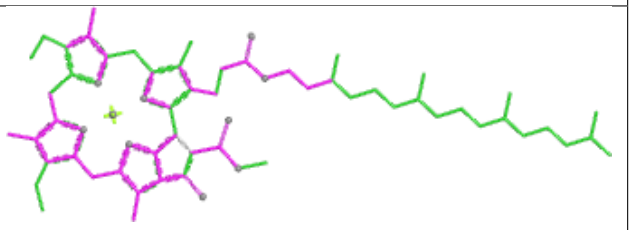


Rings

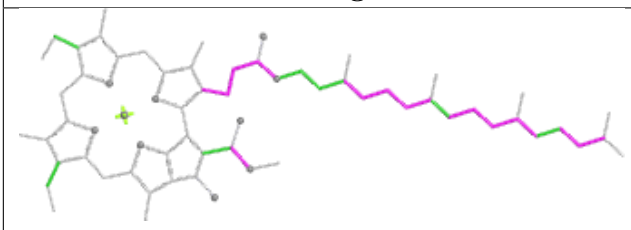
Ligand CLA a 1125



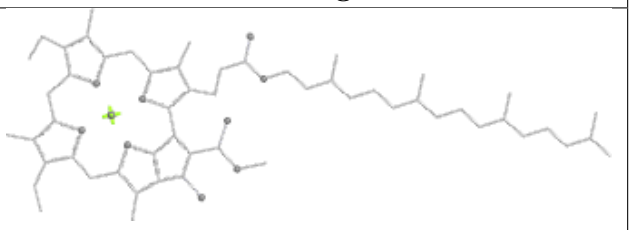
Bond lengths



Bond angles

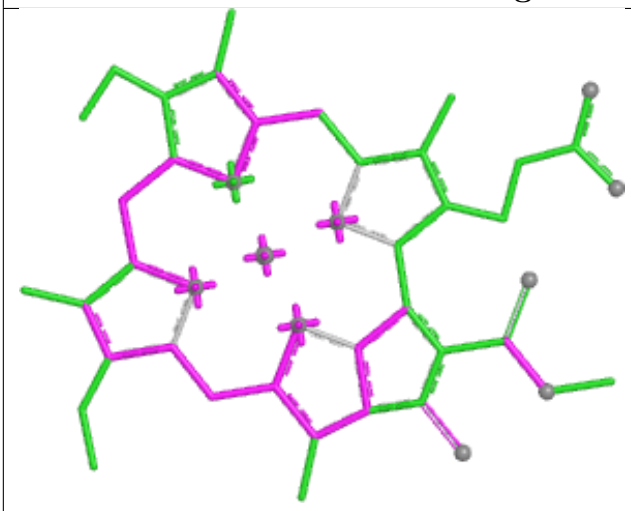


Torsions

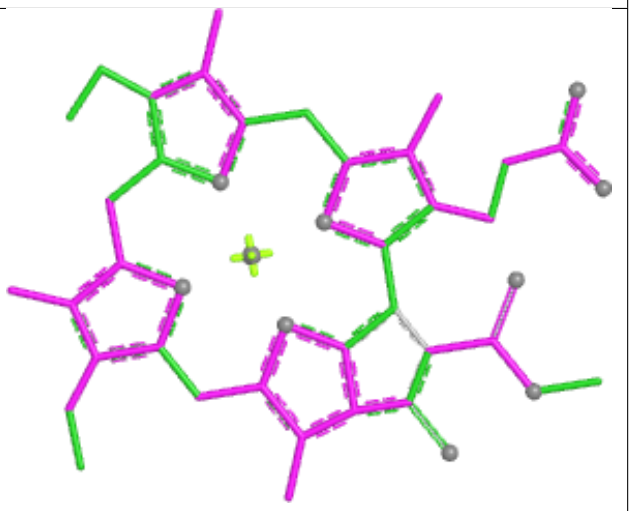


Rings

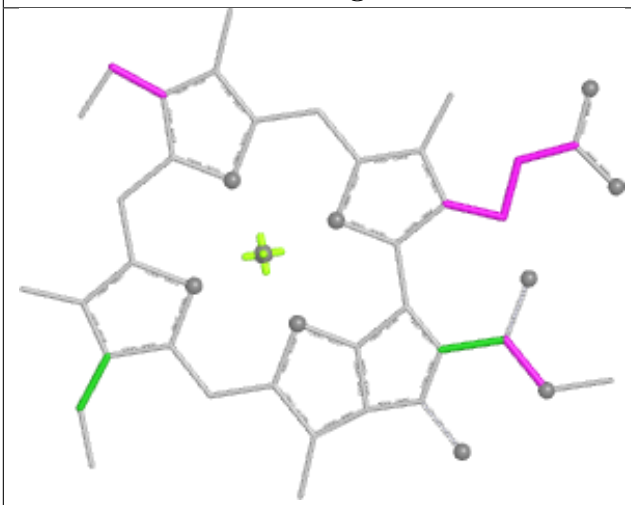
Ligand CLA H 1233



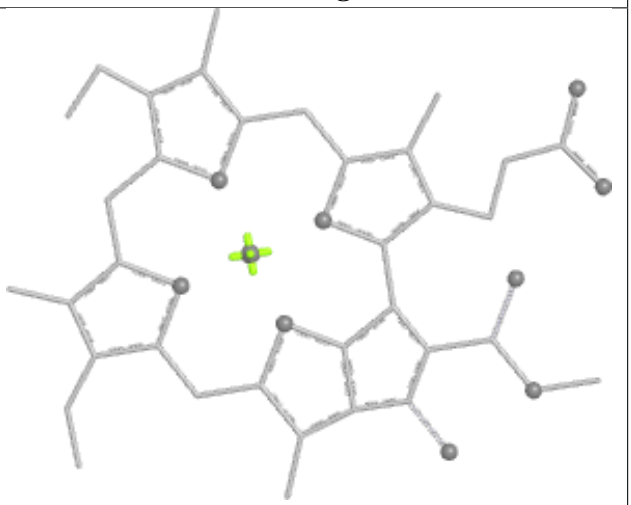
Bond lengths



Bond angles

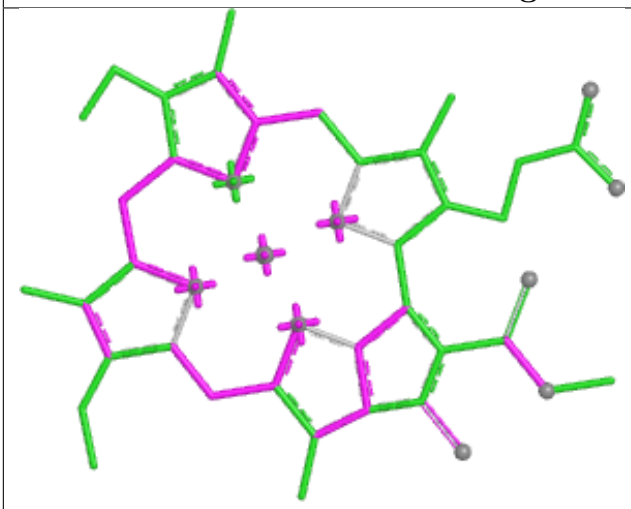


Torsions

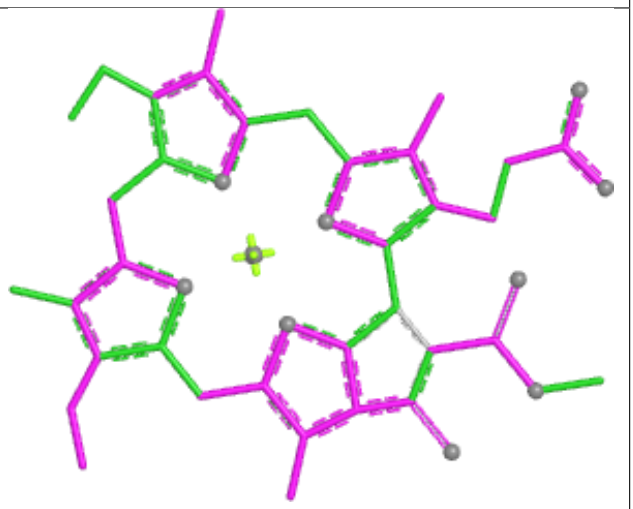


Rings

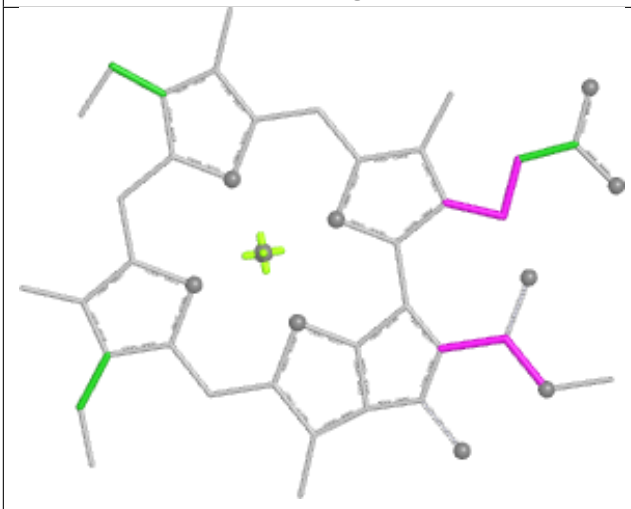
Ligand CLA a 1113



Bond lengths



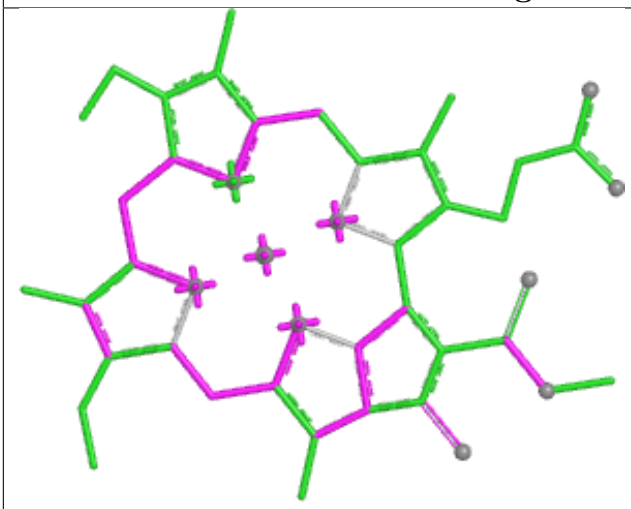
Bond angles



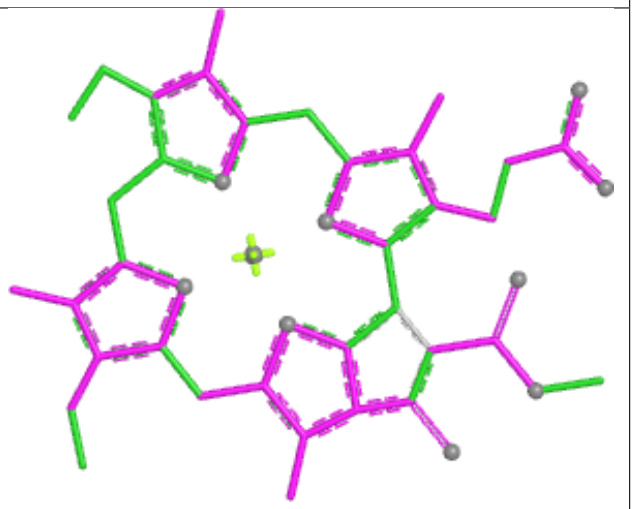
Torsions

Rings

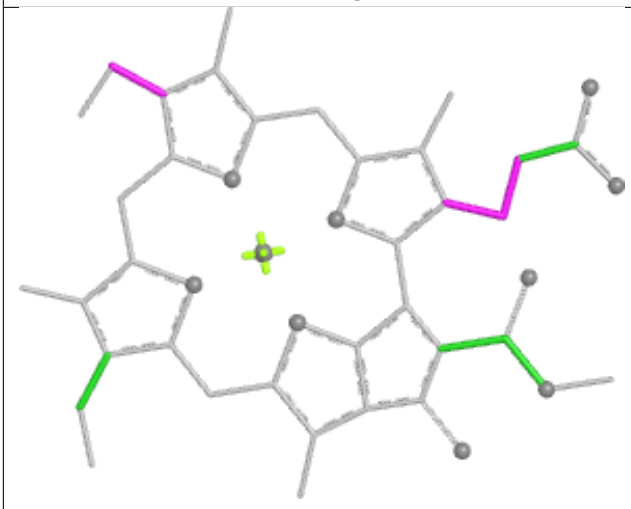
Ligand CLA A 1129



Bond lengths



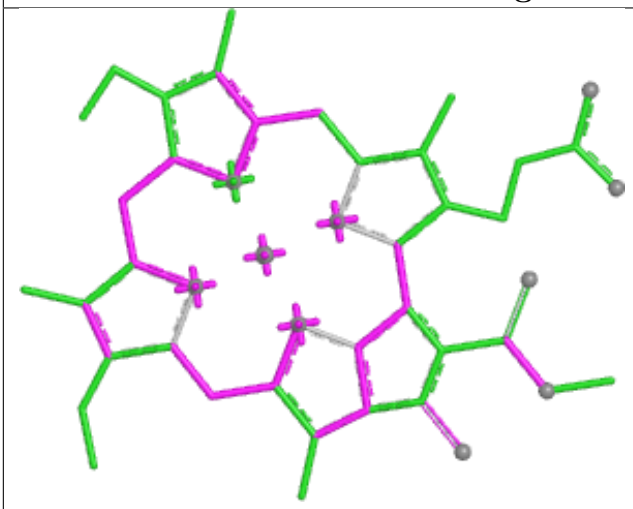
Bond angles



Torsions

Rings

Ligand CLA A 1110



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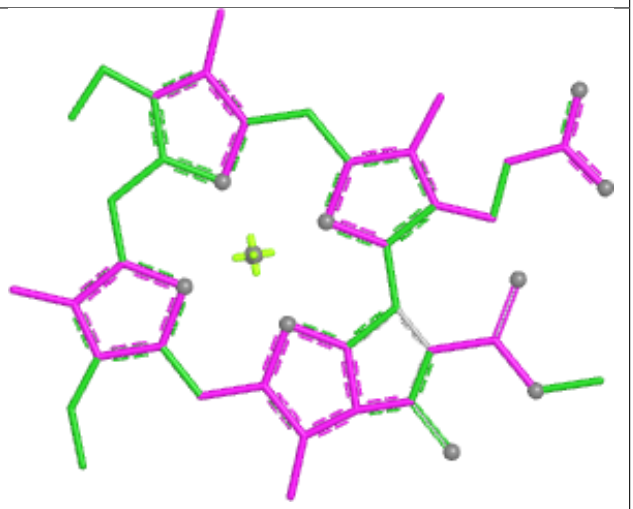
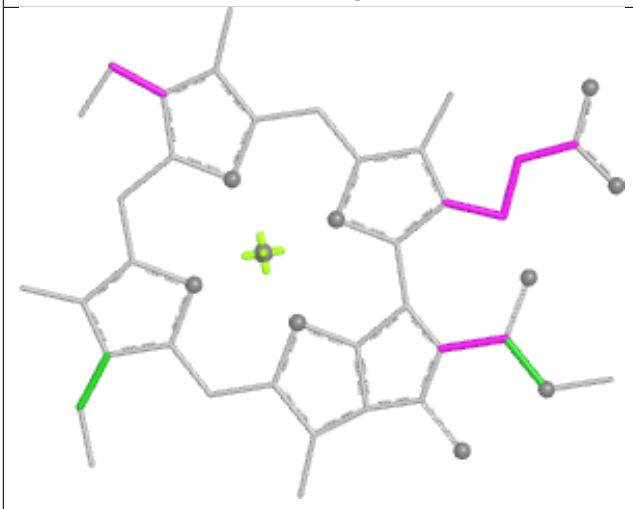


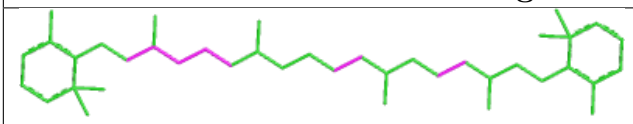
Bond angles



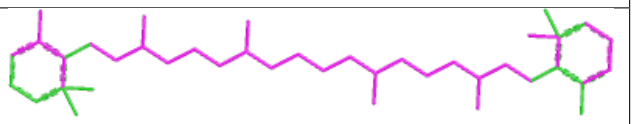
Torsions

Rings

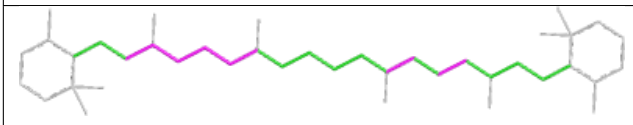
Ligand BCR b 4014



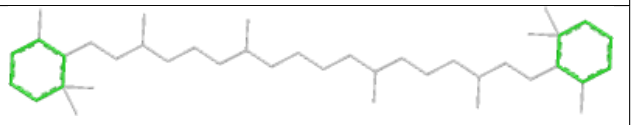
Bond lengths



Bond angles

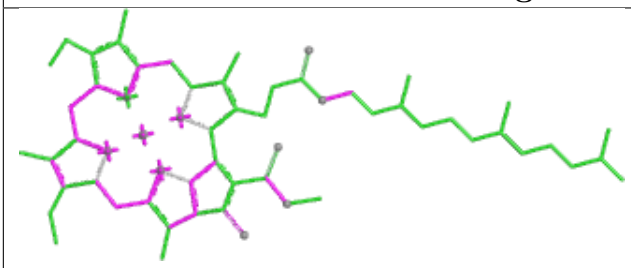


Torsions

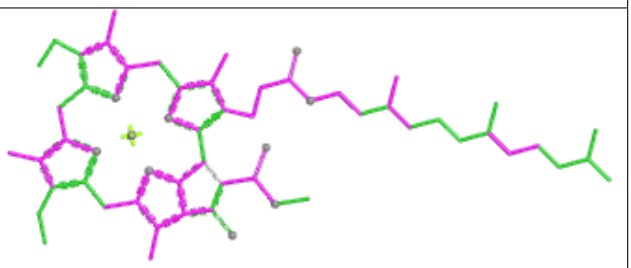


Rings

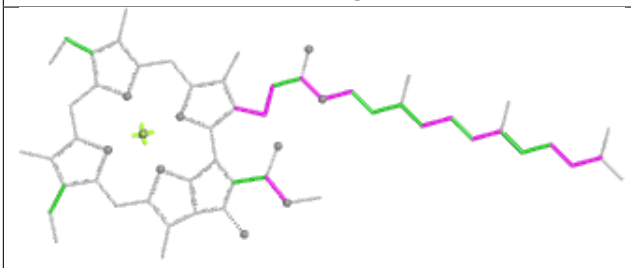
Ligand CLA B 1215



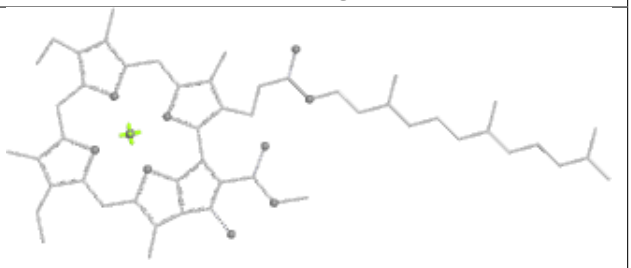
Bond lengths



Bond angles

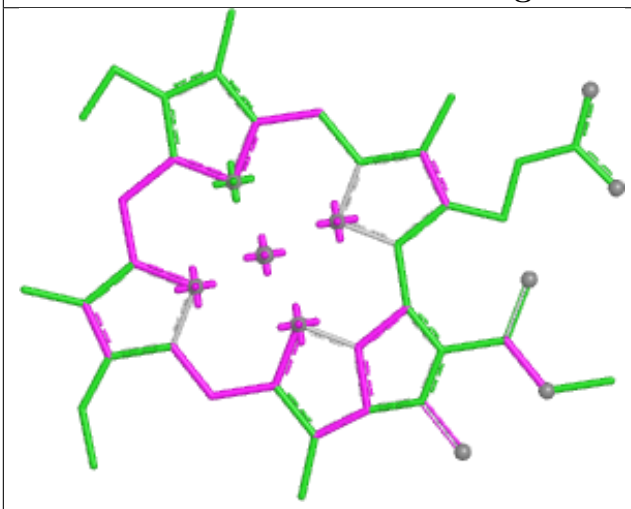


Torsions

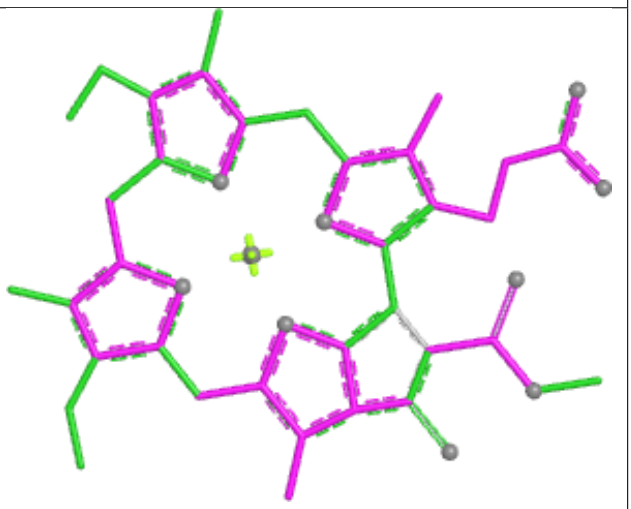


Rings

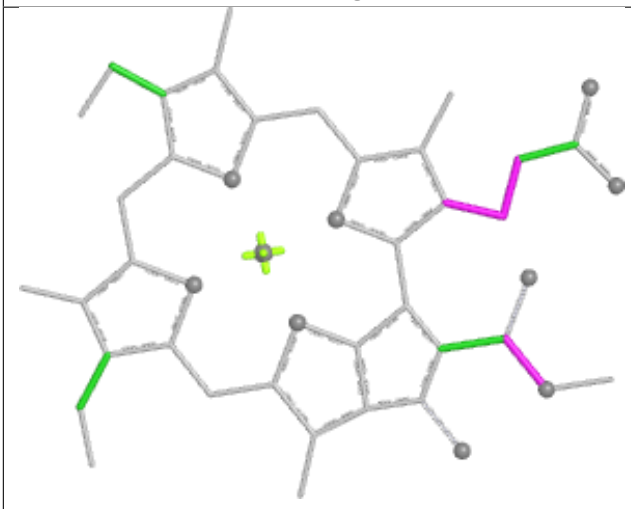
Ligand CLA H 1206



Bond lengths



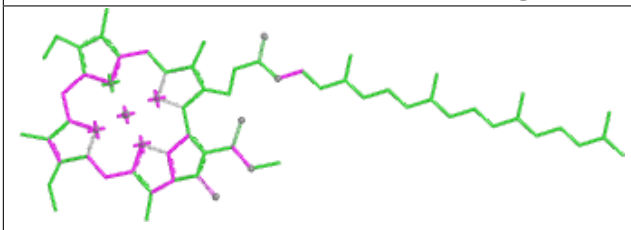
Bond angles



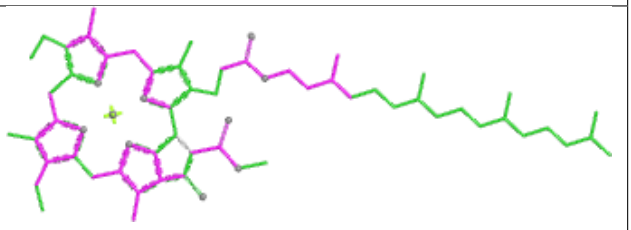
Torsions

Rings

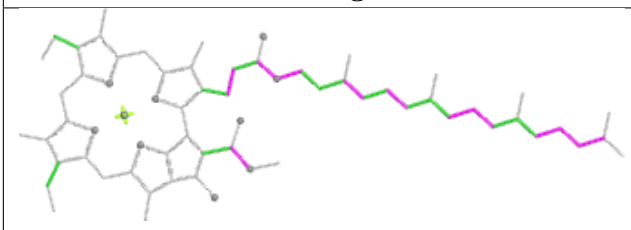
Ligand CLA A 1119



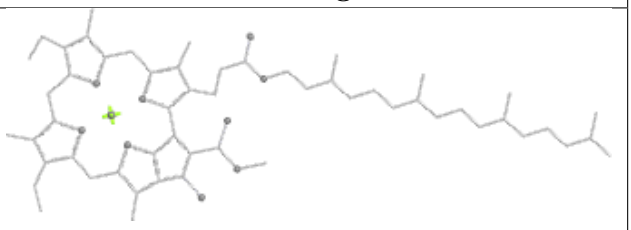
Bond lengths



Bond angles

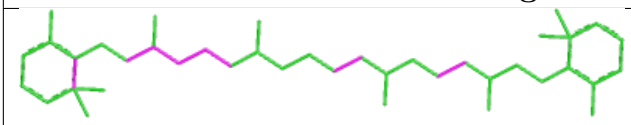


Torsions



Rings

Ligand BCR I 4018



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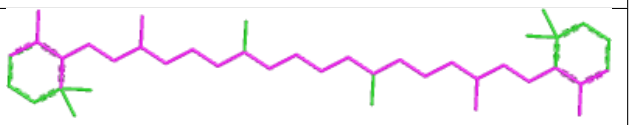
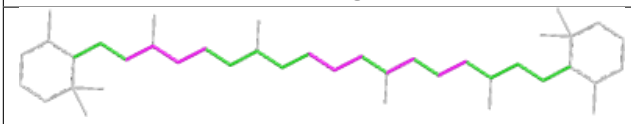
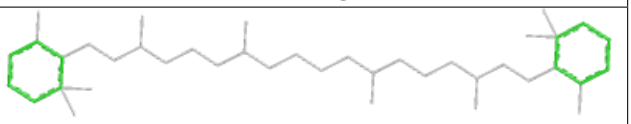


Bond angles

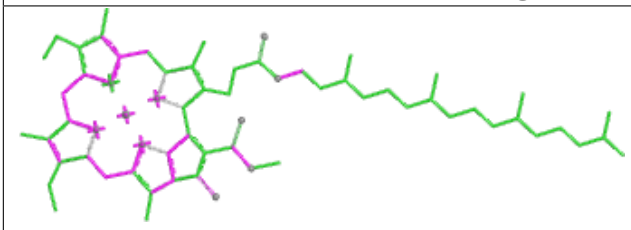


Torsions



Rings

Ligand CLA G 1125



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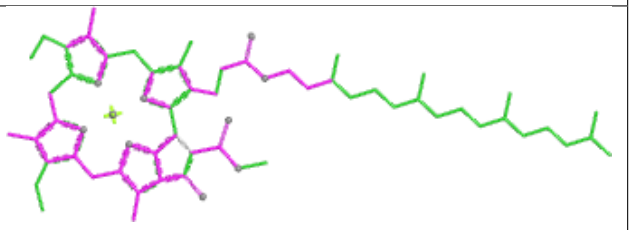
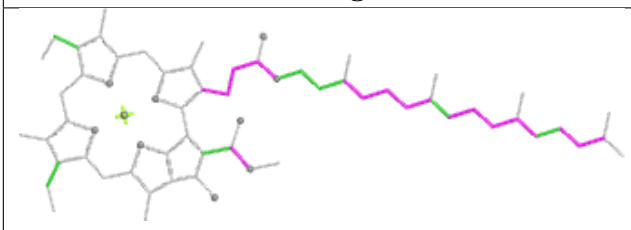
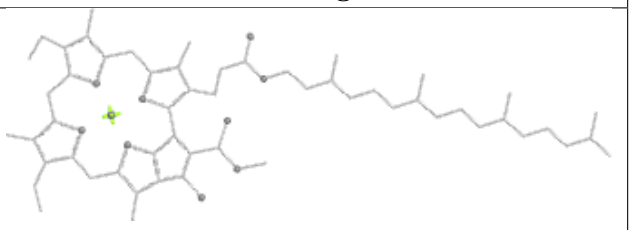


Bond angles

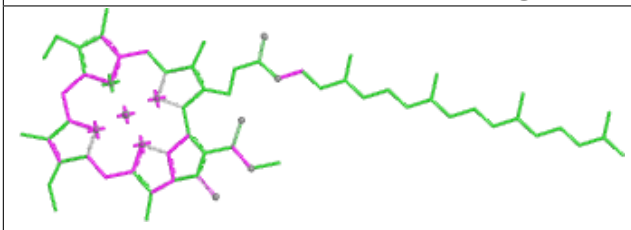


Torsions

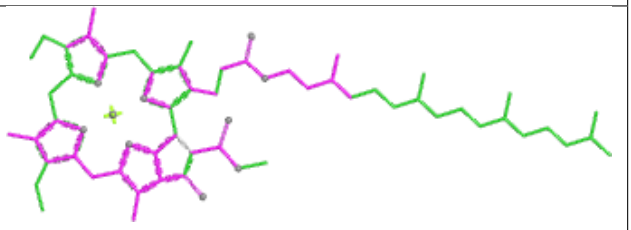


Rings

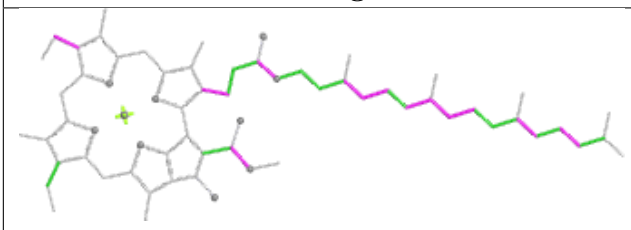
Ligand CLA B 1203



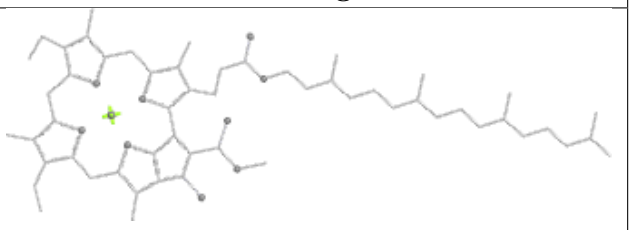
Bond lengths



Bond angles

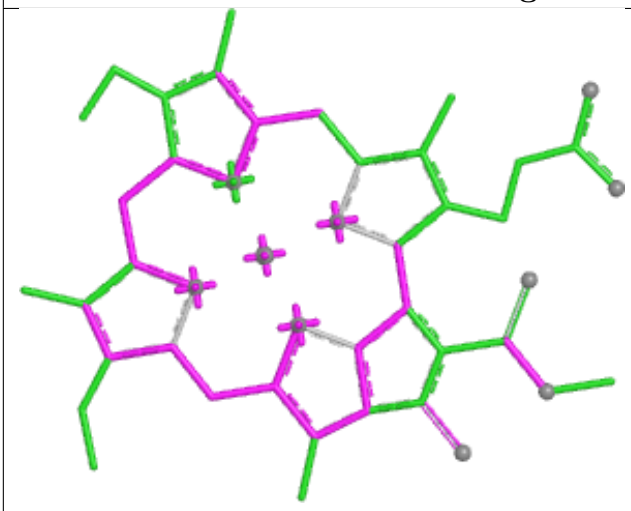


Torsions



Rings

Ligand CLA a 1112



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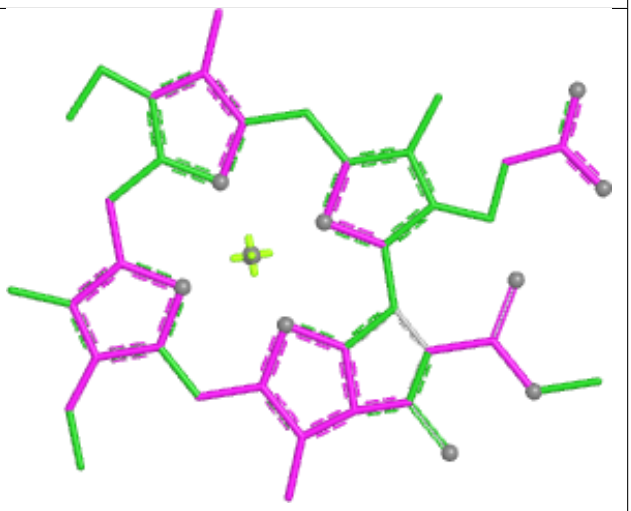
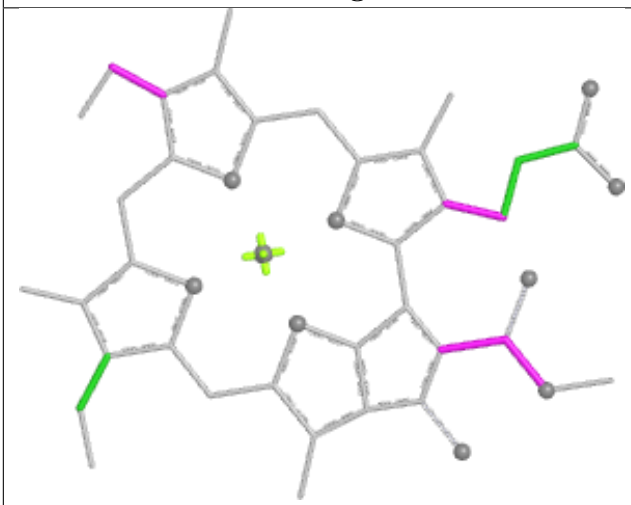


Bond angles



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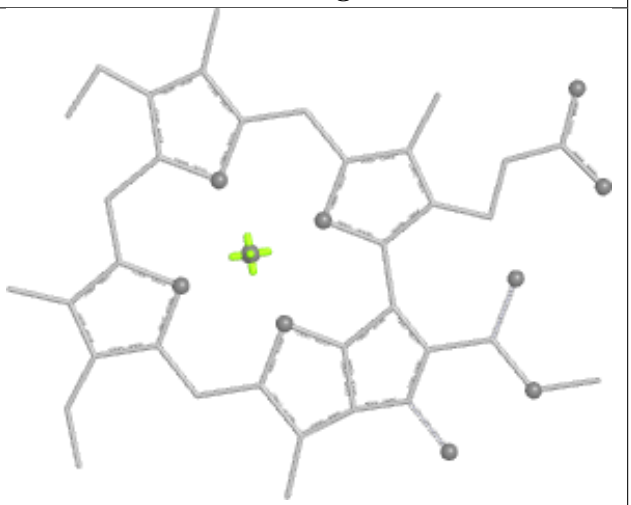
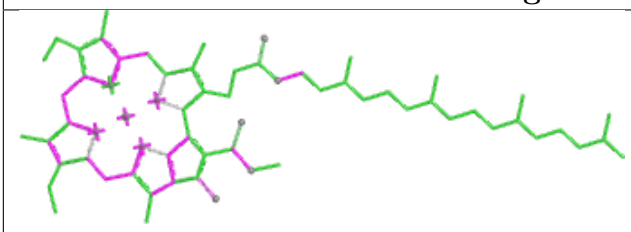


Rings

Ligand CLA l 1503



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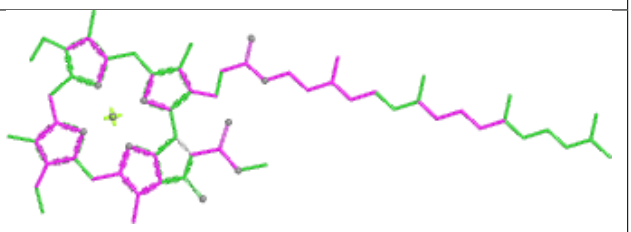
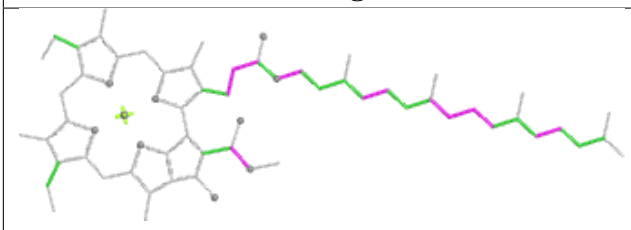


Bond angles



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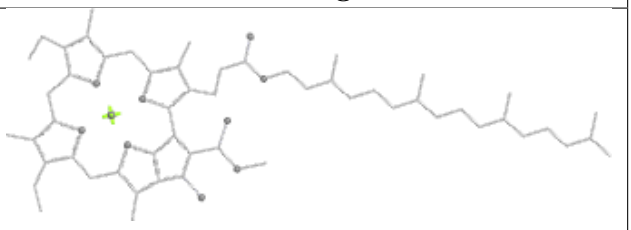
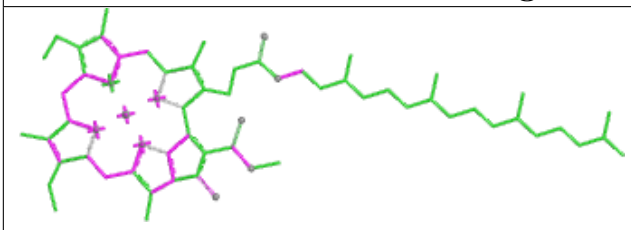


Rings

Ligand CLA b 1204



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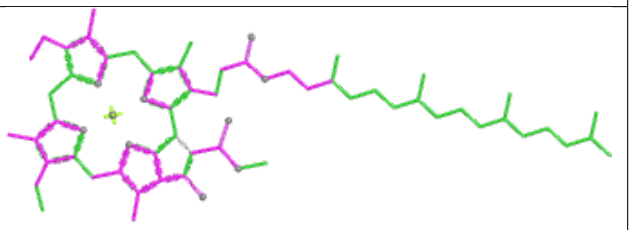
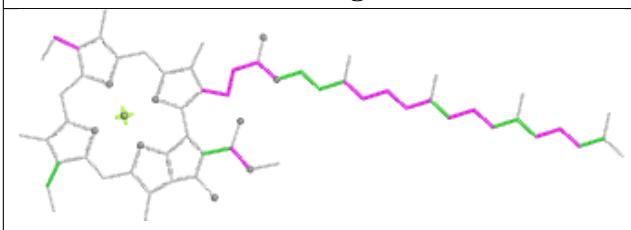


Bond angles



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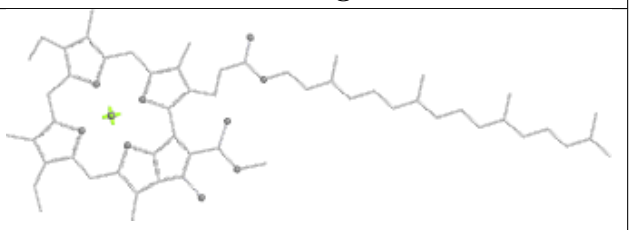
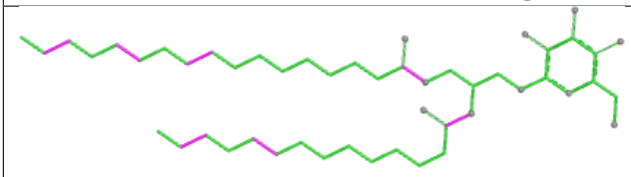
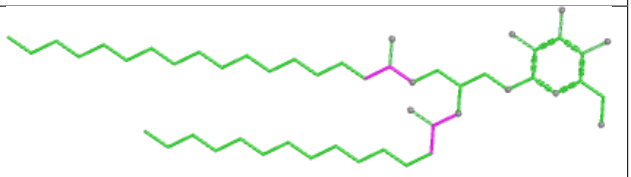


Rings

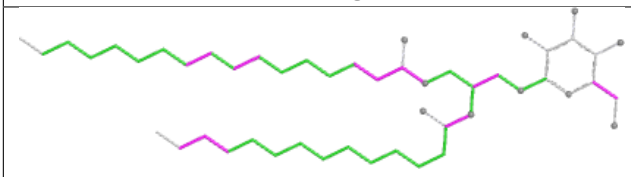
Ligand LMG l 5007



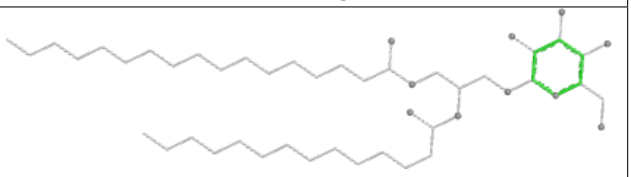
Bond lengths



Bond angles

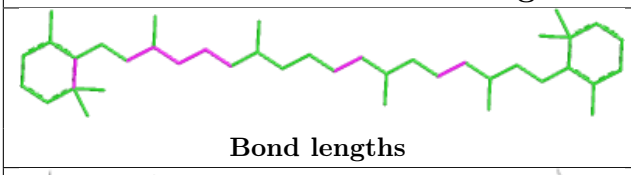


Torsions



Rings

Ligand BCR a 4007



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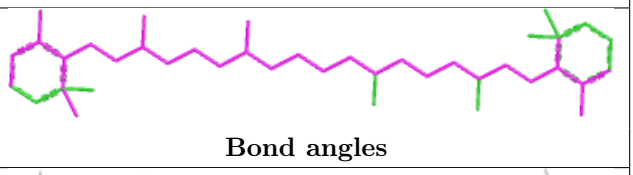
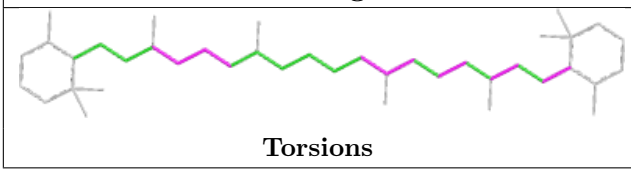


Bond angles



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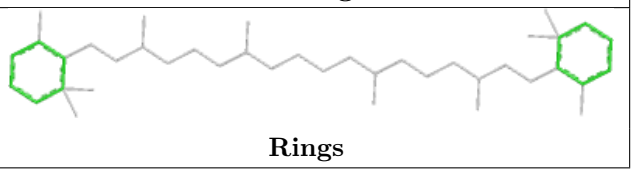
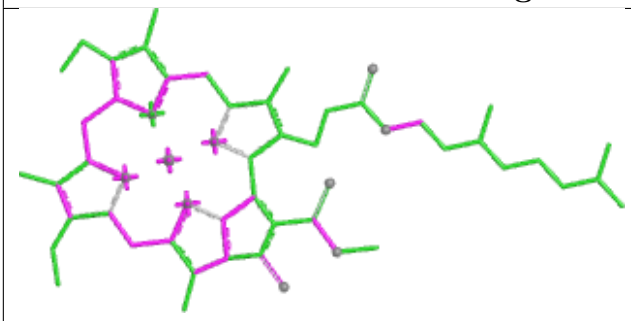


Rings

Ligand CLA A 1124



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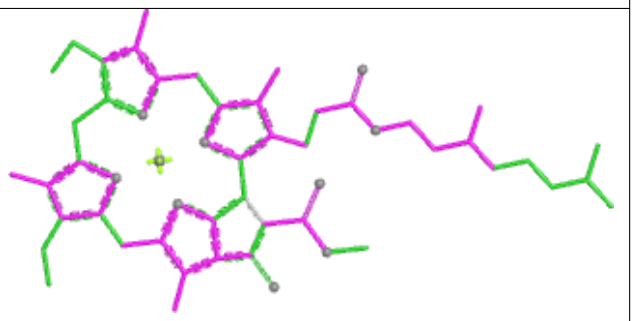
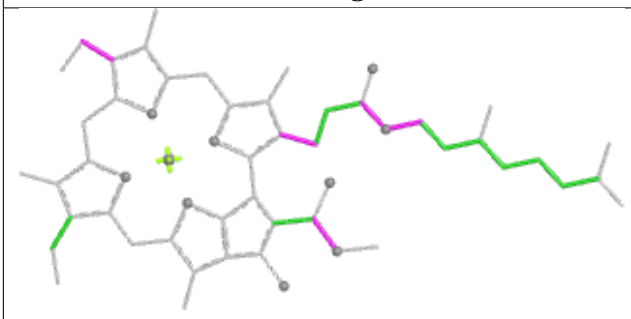
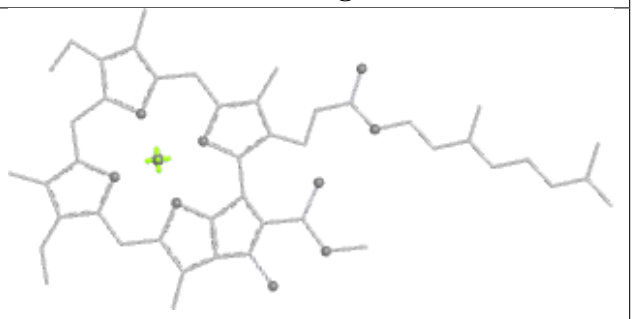


Bond angles

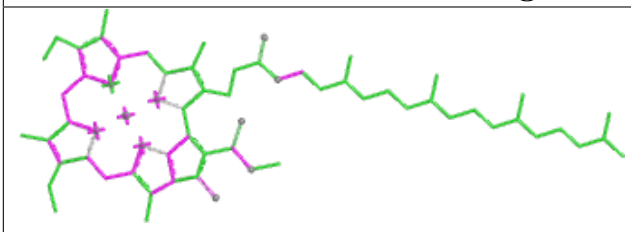


Torsions

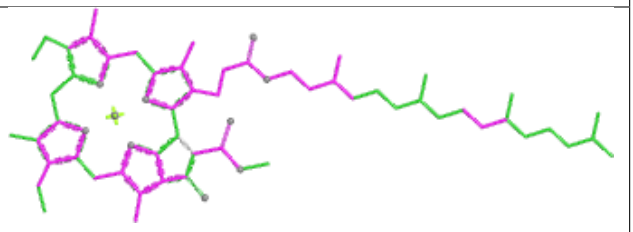


Rings

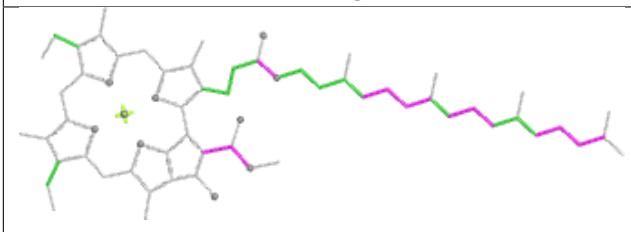
Ligand CLA b 1222



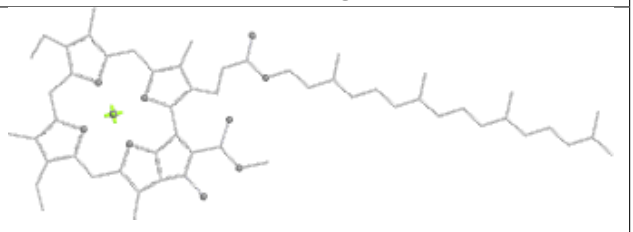
Bond lengths



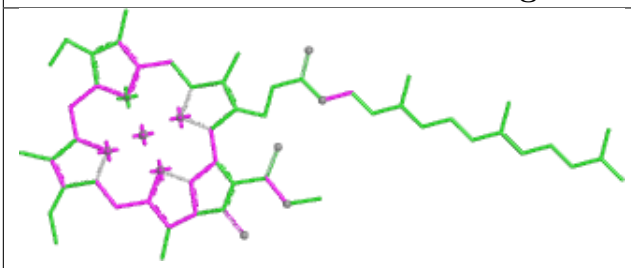
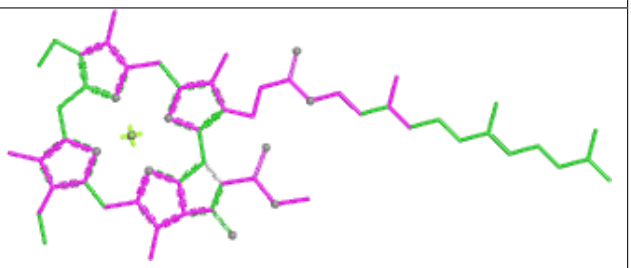
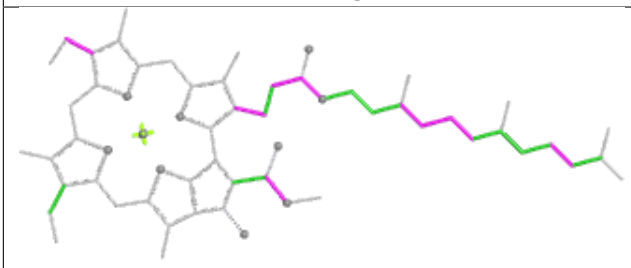
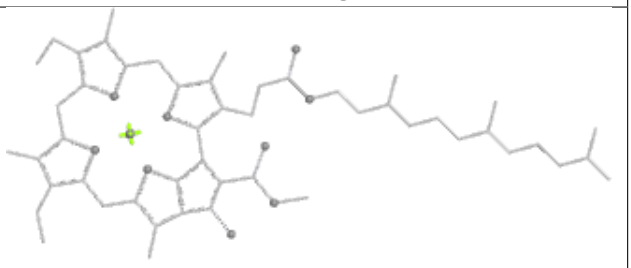
Bond angles

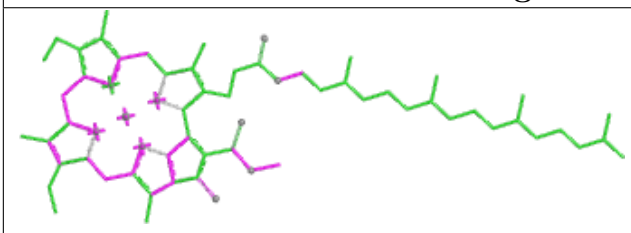
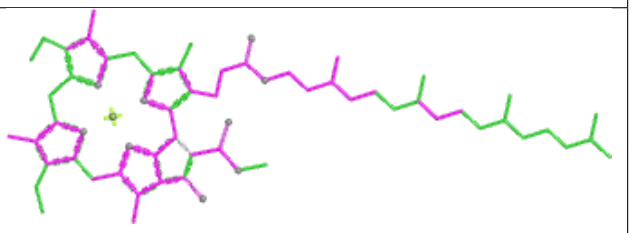
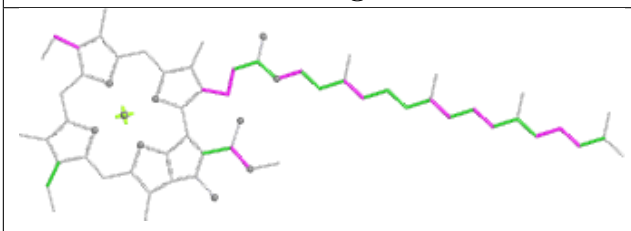
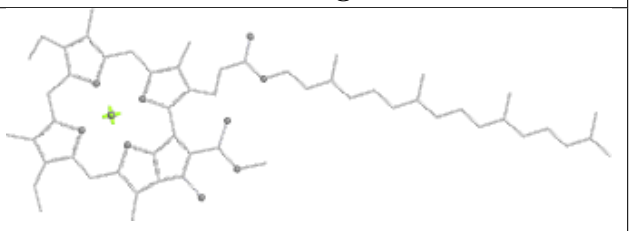


Torsions

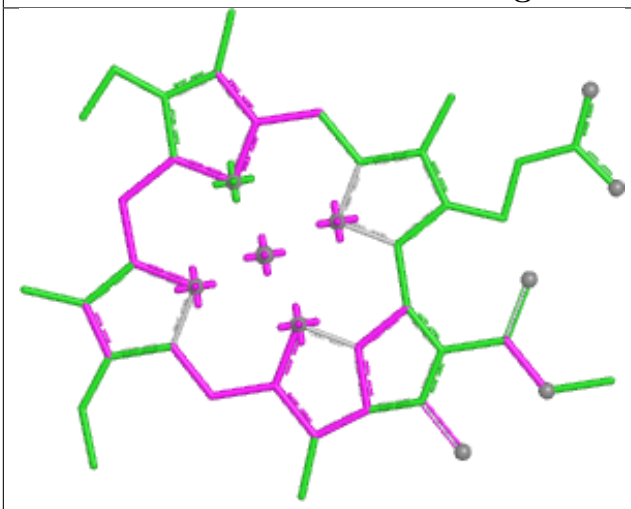


Rings

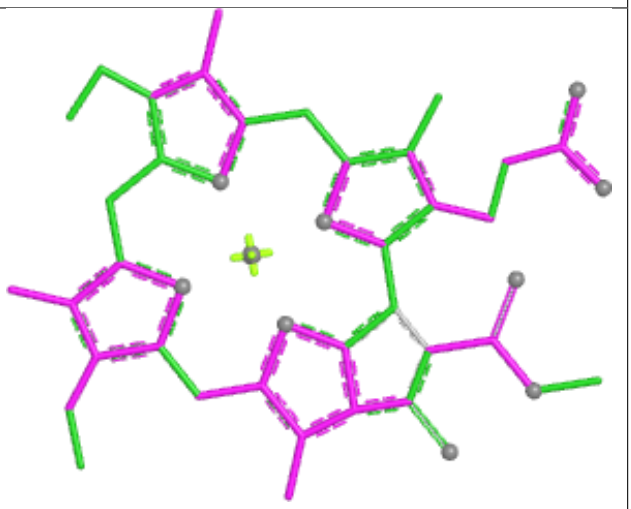
Ligand CLA a 1138	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1012	
	
Bond lengths	Bond angles
	
Torsions	Rings

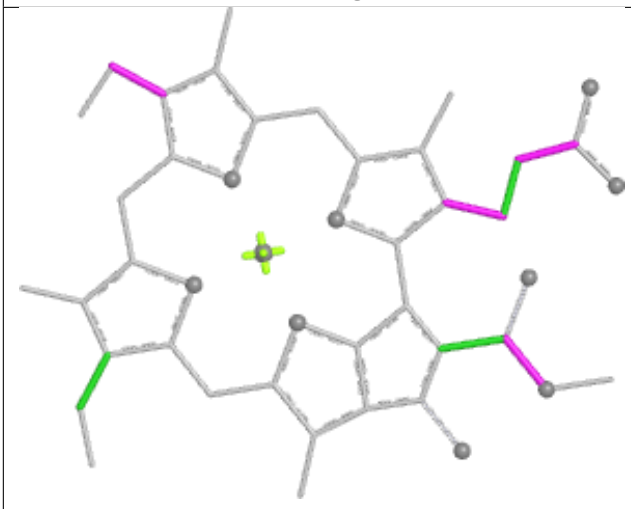
Ligand CLA G 1105



Bond lengths



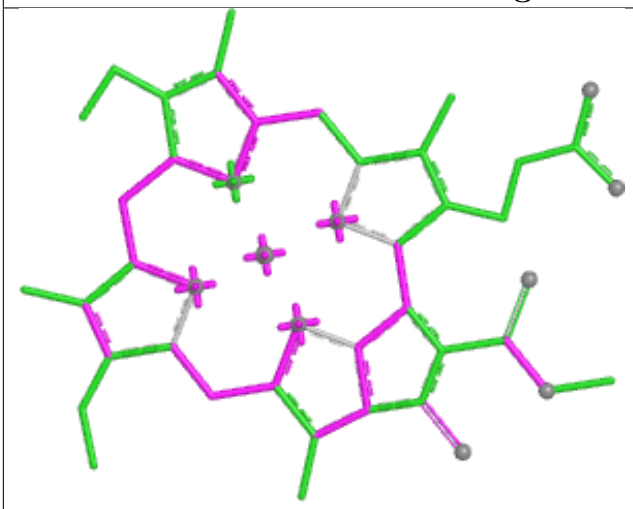
Bond angles



Torsions

Rings

Ligand CLA G 1106



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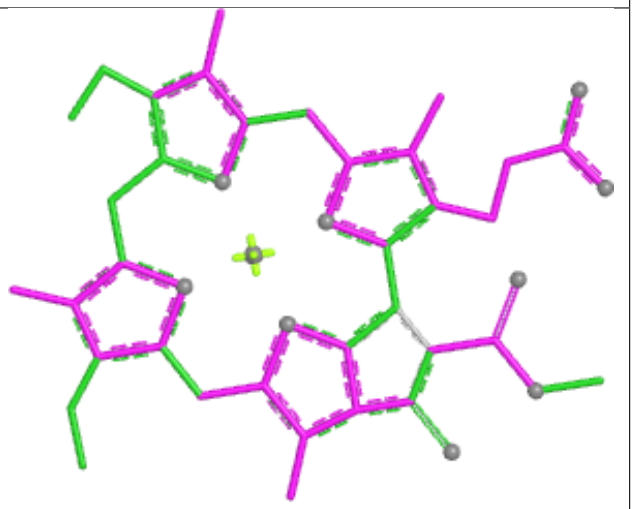
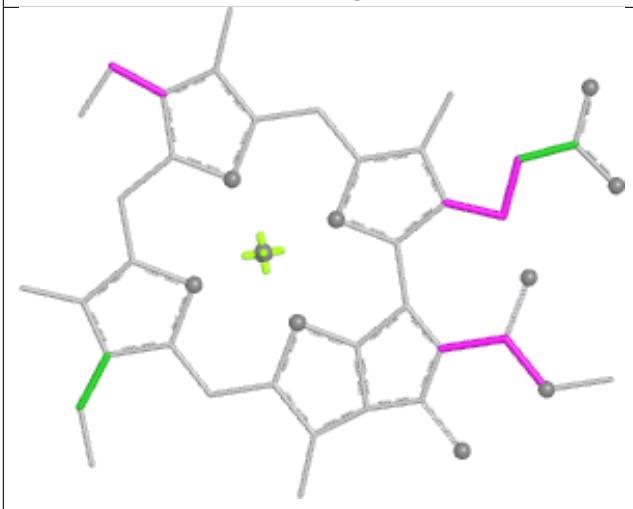


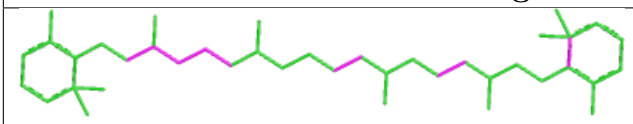
Bond angles



Torsions

Rings

Ligand BCR H 4004



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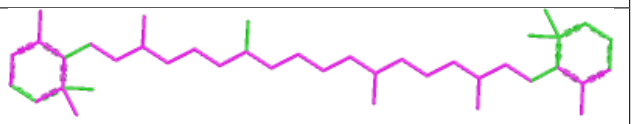
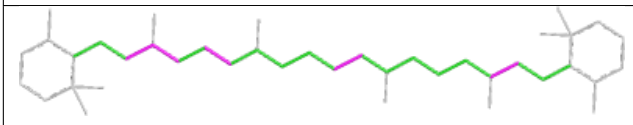
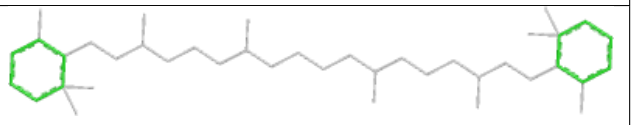


Bond angles

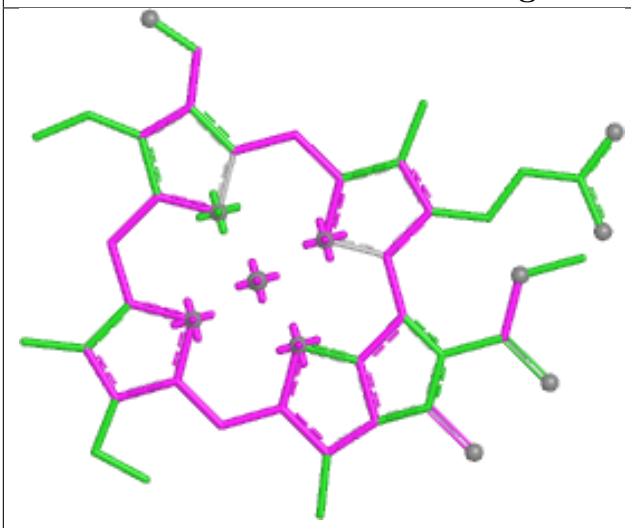


Torsions



Rings

Ligand F6C A 1121



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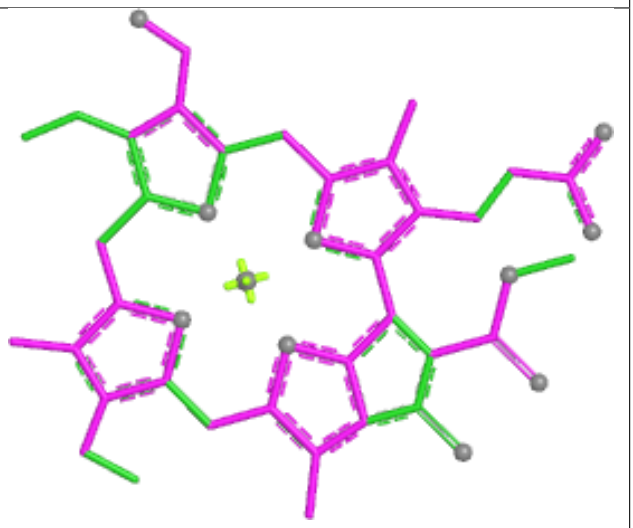
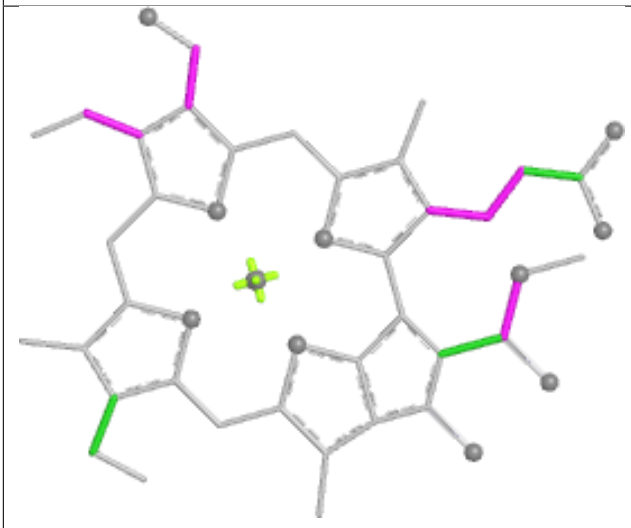
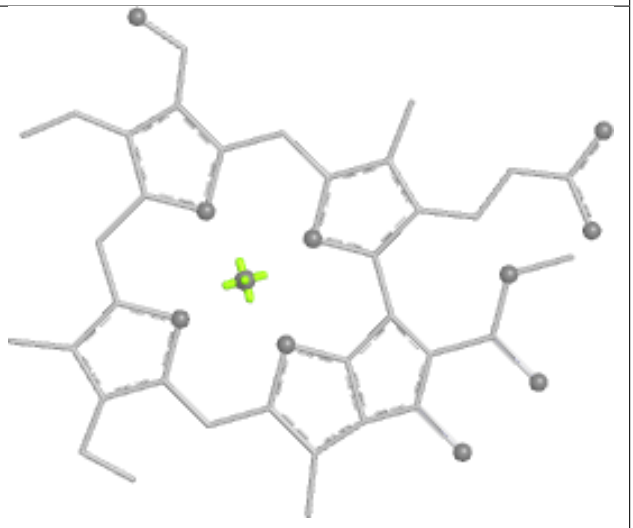


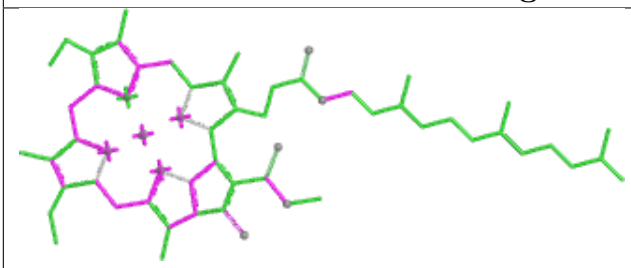
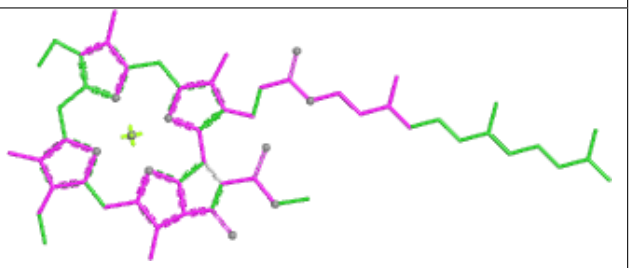
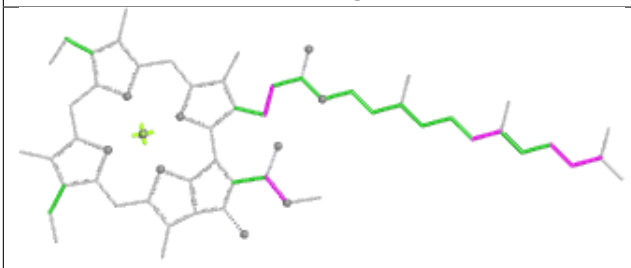
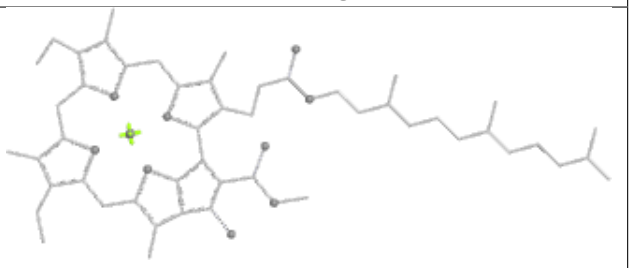
Bond angles

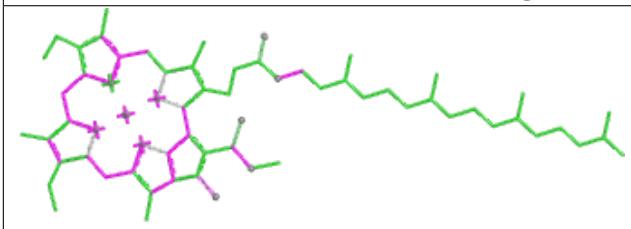
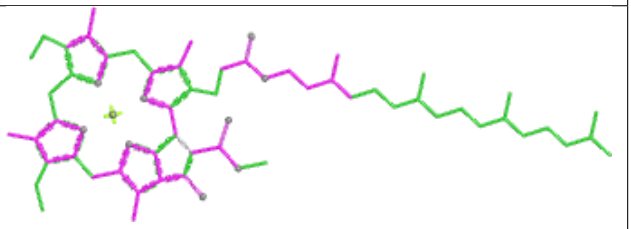
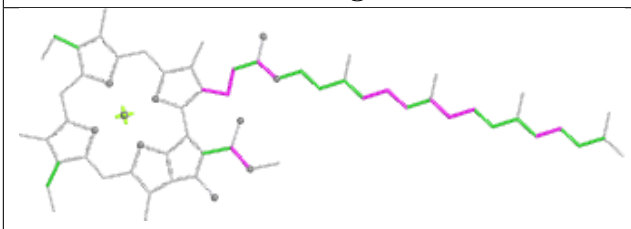
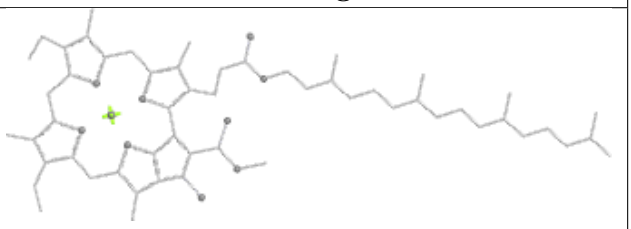


Torsions

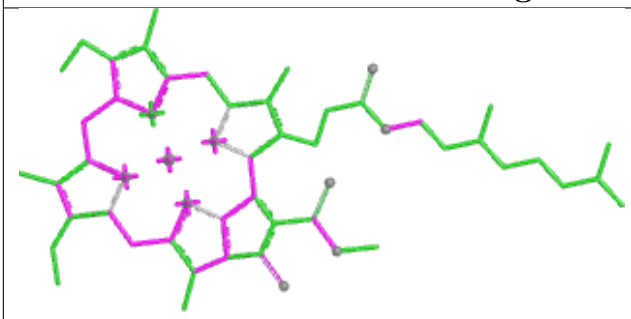


Rings

Ligand CLA a 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1136



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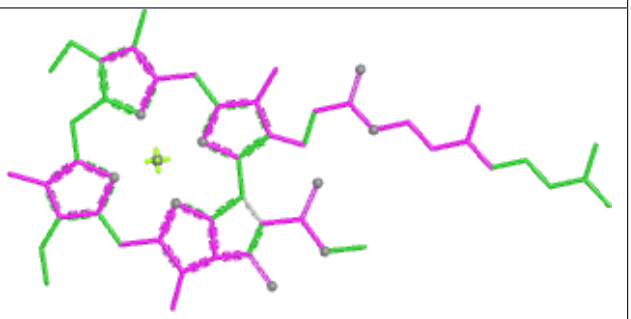
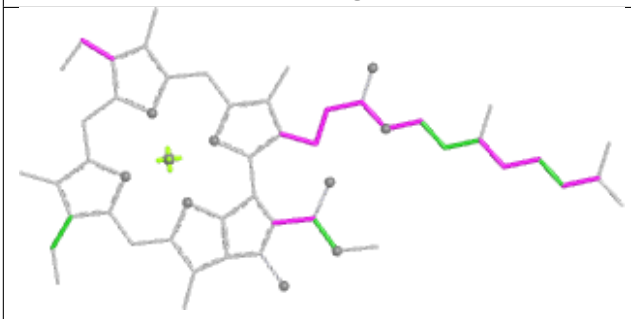
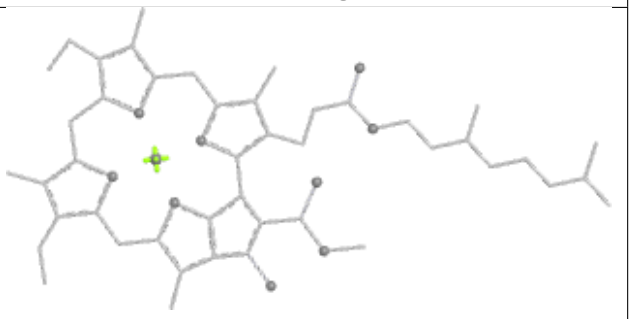


Bond angles

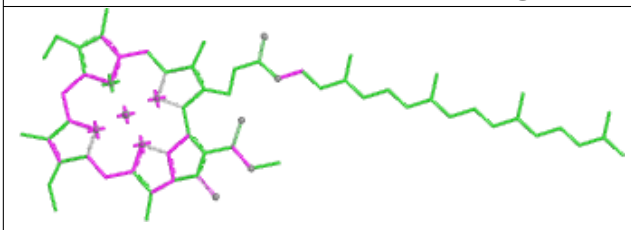


Torsions

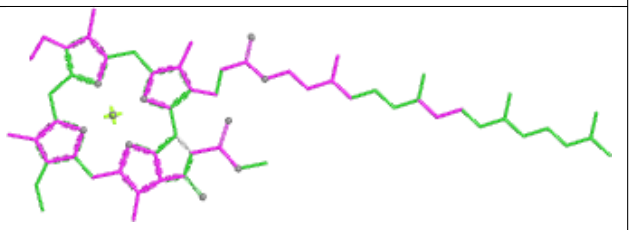


Rings

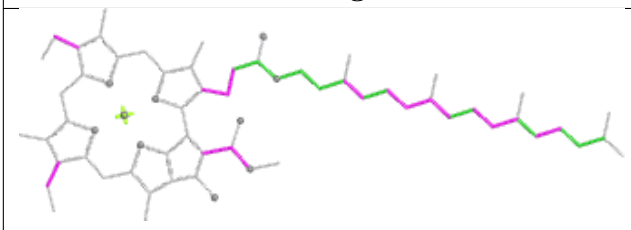
Ligand CLA G 1132



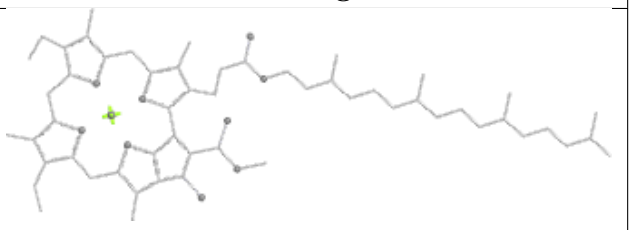
Bond lengths



Bond angles

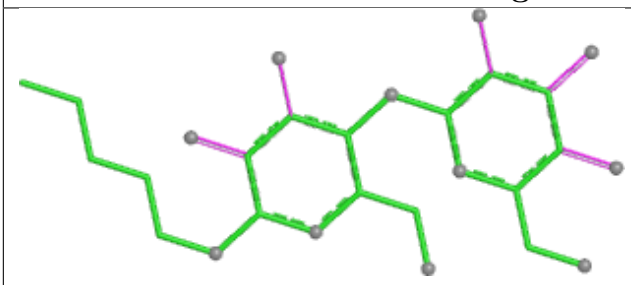


Torsions



Rings

Ligand LMT A 6002



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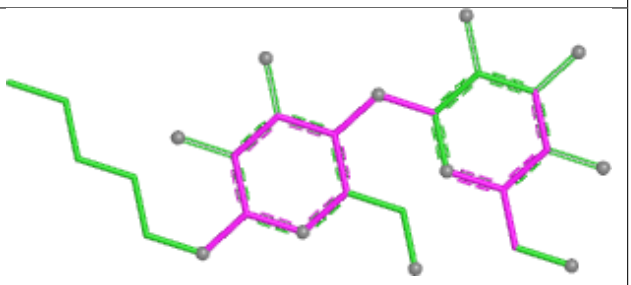
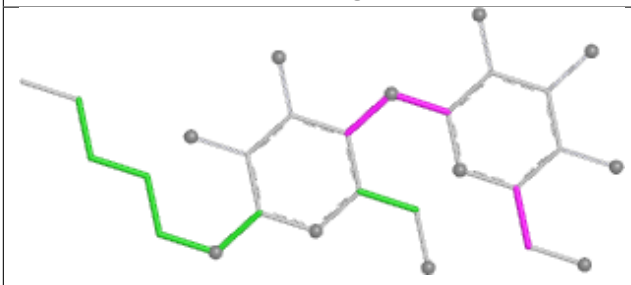
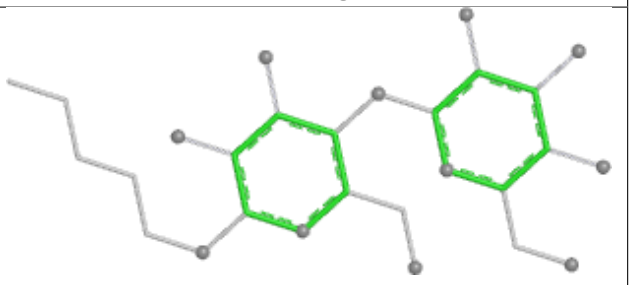


Bond angles

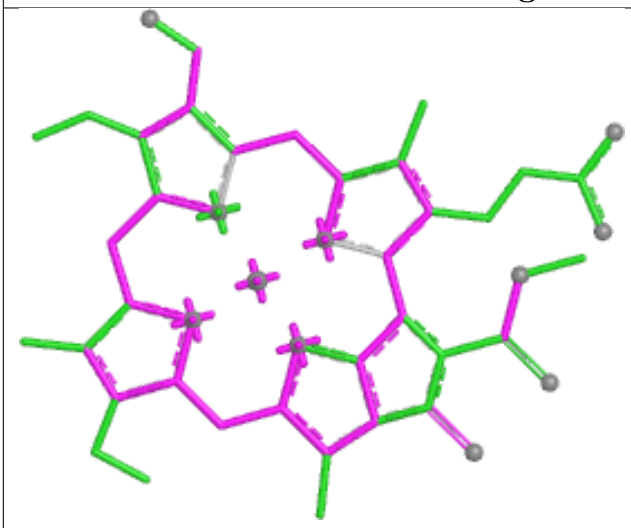


Torsions



Rings

Ligand F6C G 1121



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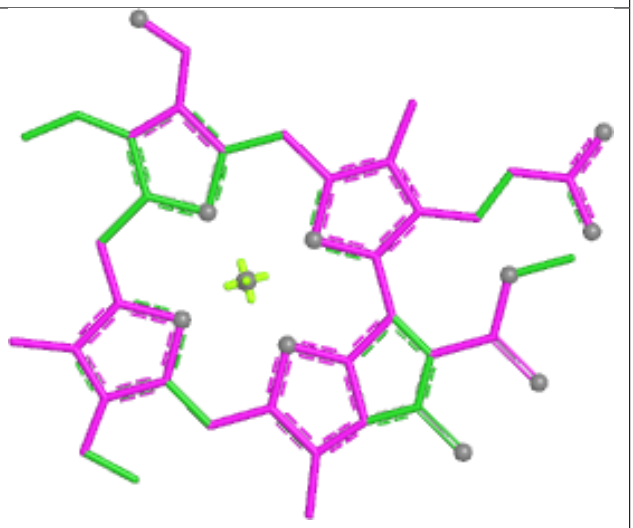
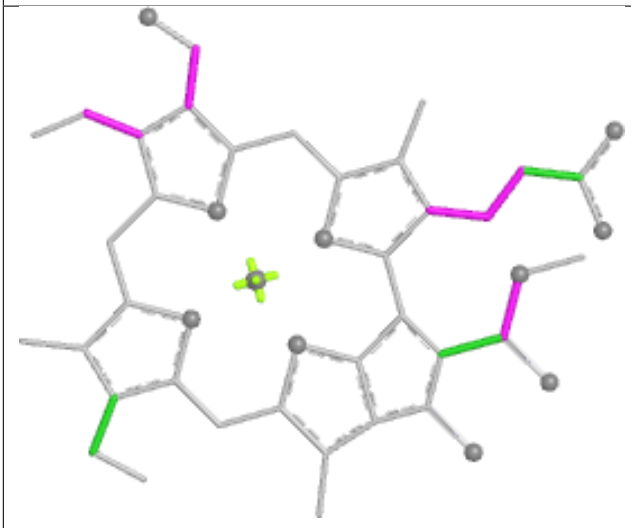


Bond angles



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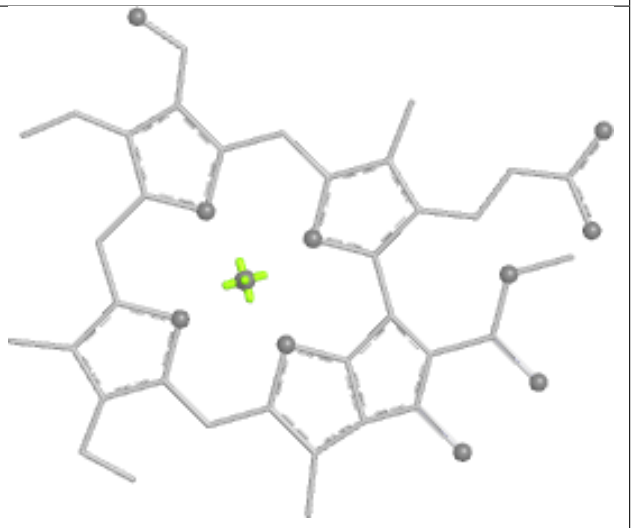
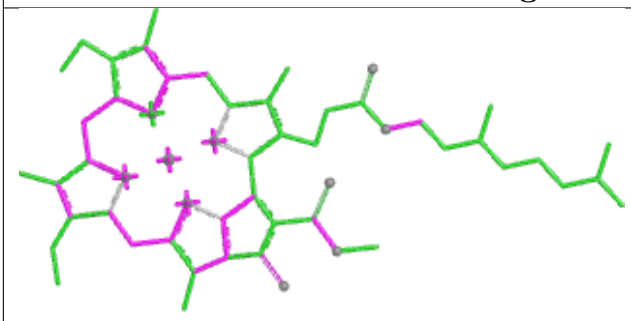


Rings

Ligand CLA a 1118



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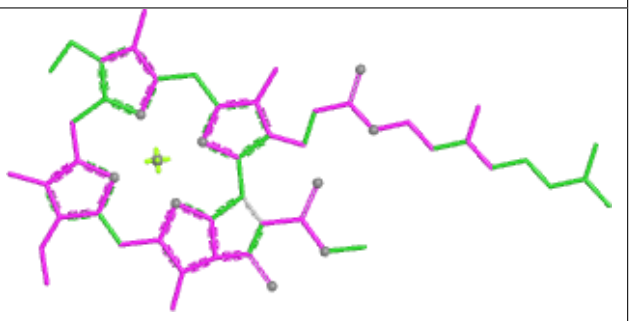
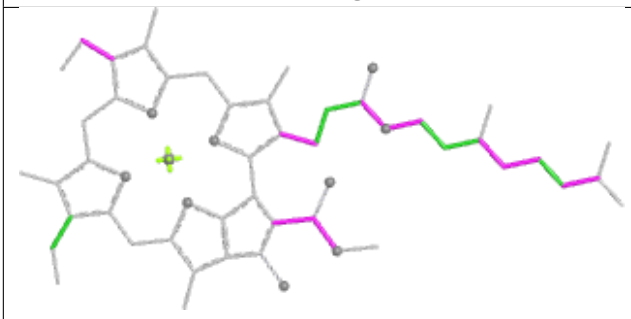
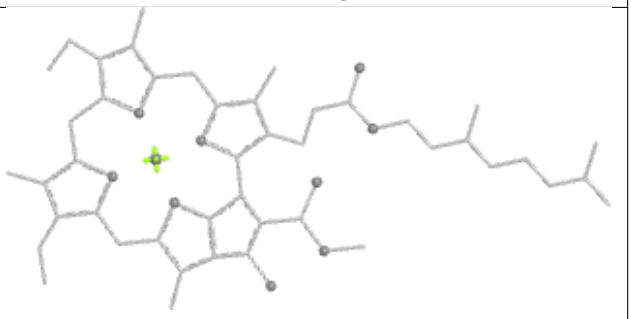


Bond angles

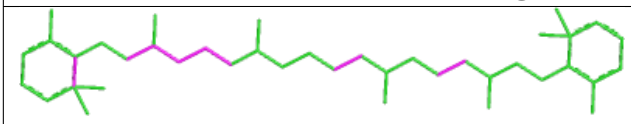


Torsions

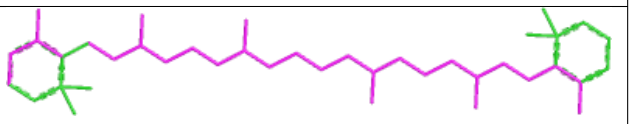


Rings

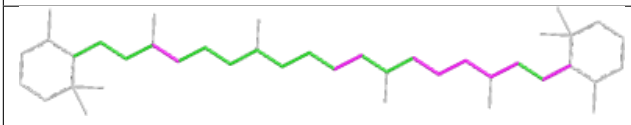
Ligand BCR R 4020



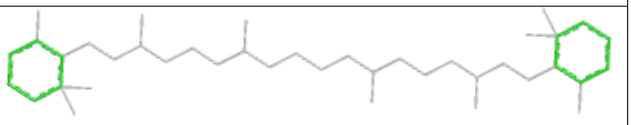
Bond lengths



Bond angles

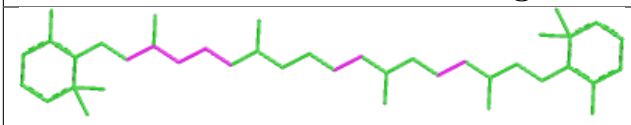


Torsions

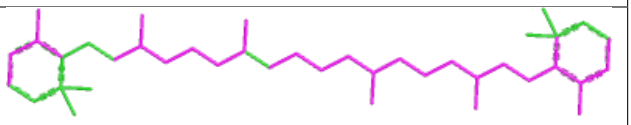


Rings

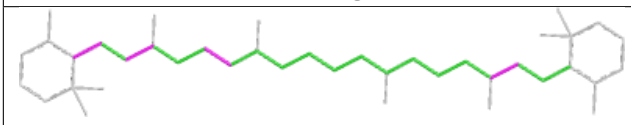
Ligand BCR A 4002



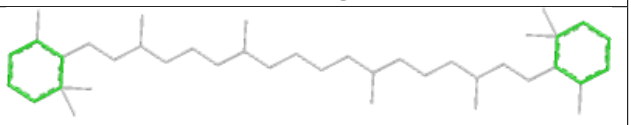
Bond lengths



Bond angles

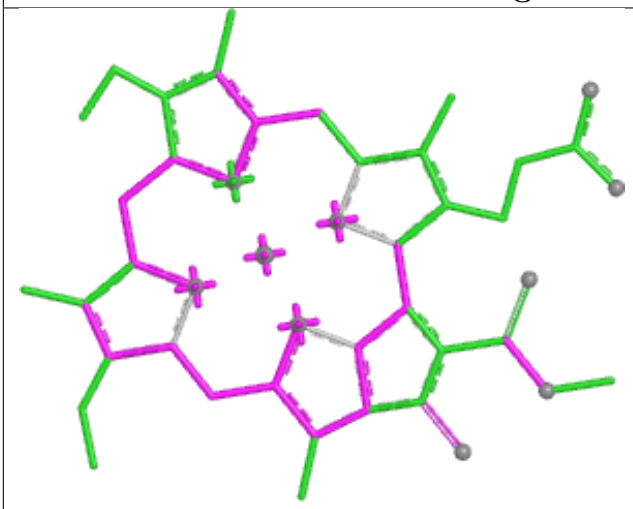


Torsions



Rings

Ligand CLA G 1112



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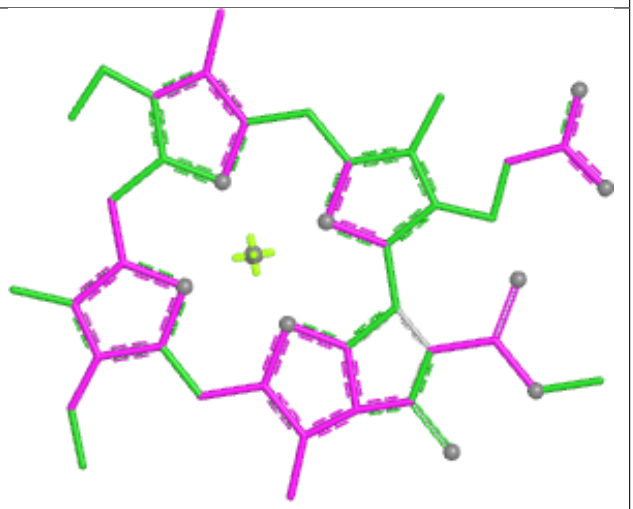
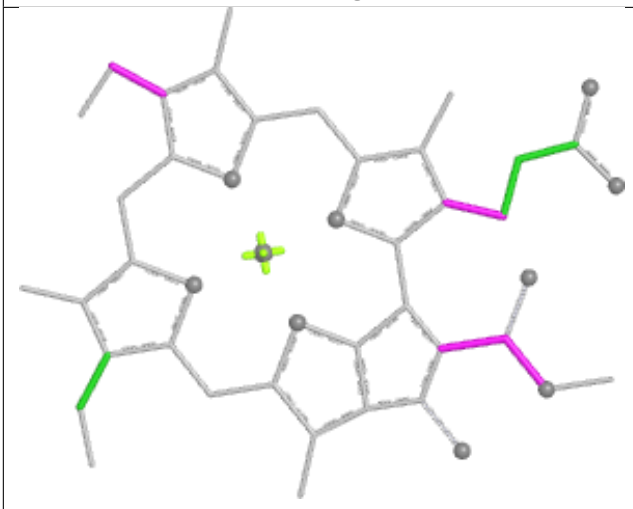


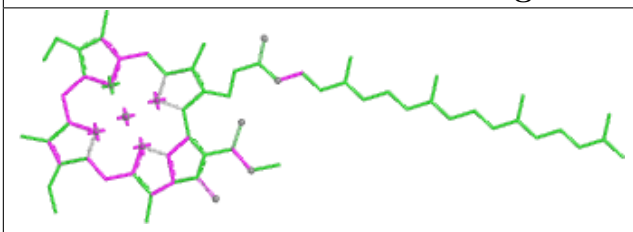
Bond angles



Torsions

Rings

Ligand CLA A 1125



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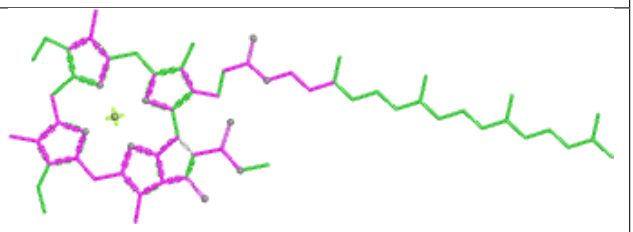
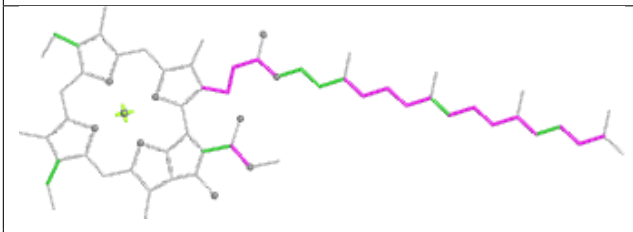
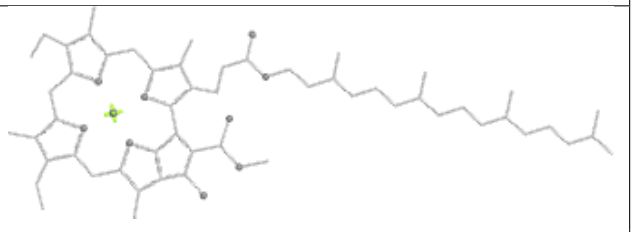


Bond angles

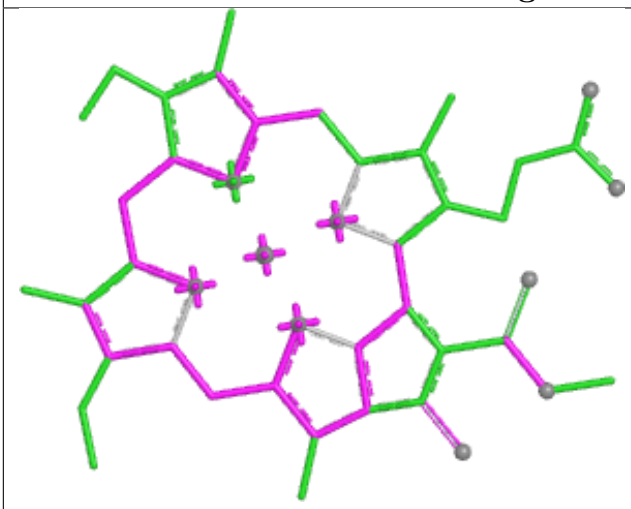


Torsions

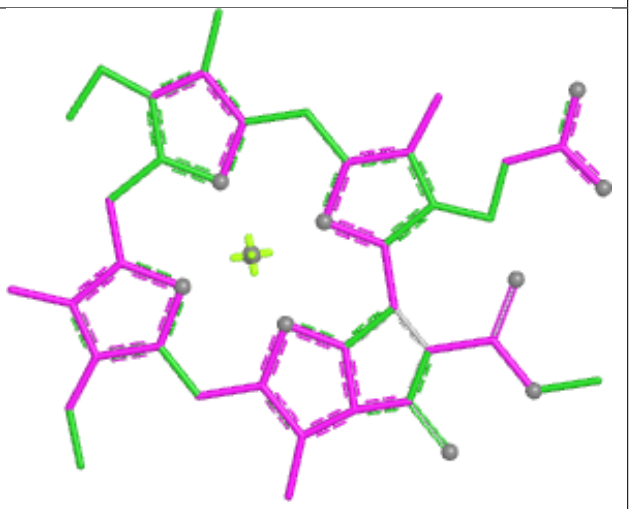


Rings

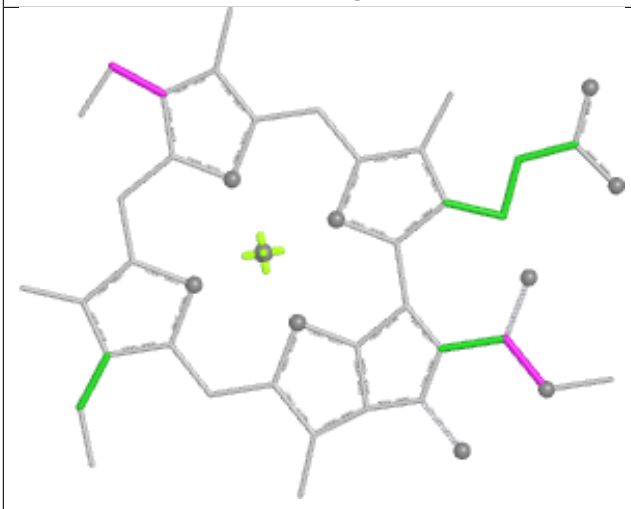
Ligand CLA b 1232



Bond lengths



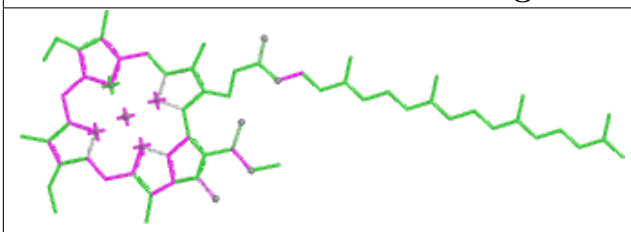
Bond angles



Torsions

Rings

Ligand CLA G 1140



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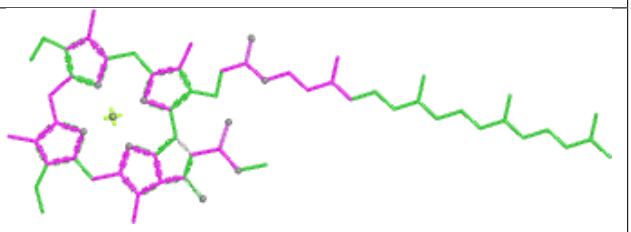
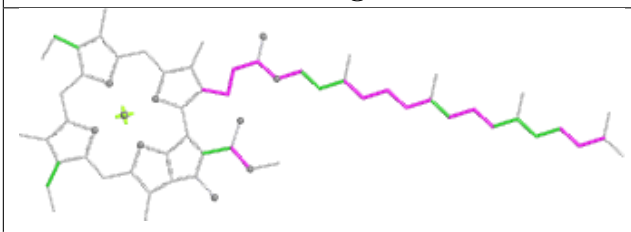
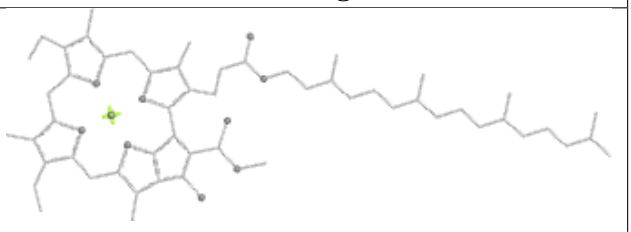


Bond angles

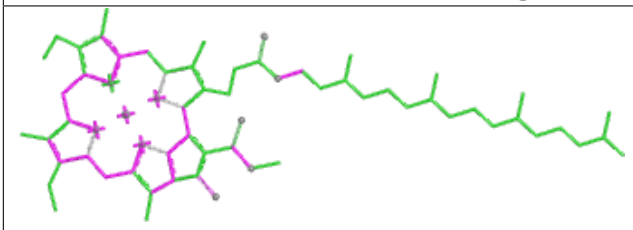


Torsions



Rings

Ligand CLA H 1023



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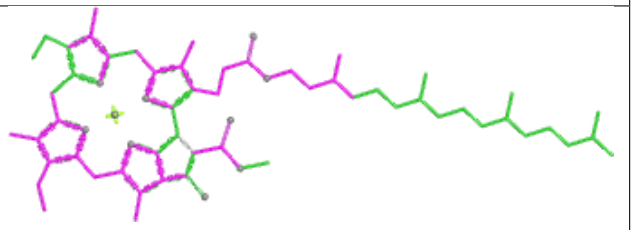
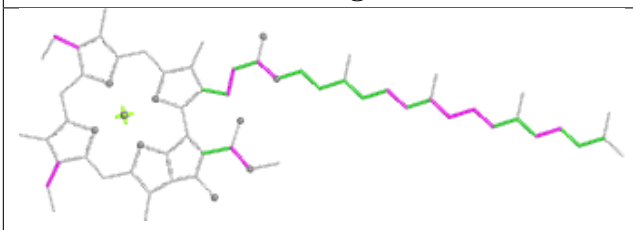
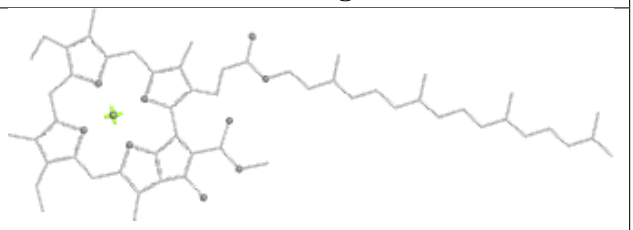


Bond angles

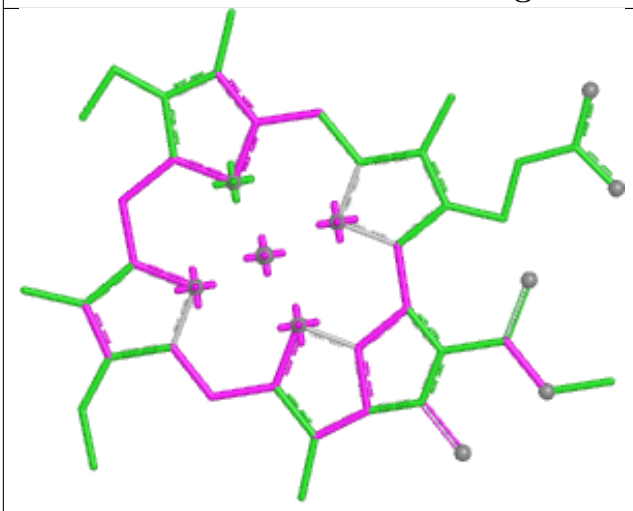


Torsions



Rings

Ligand CLA H 1232



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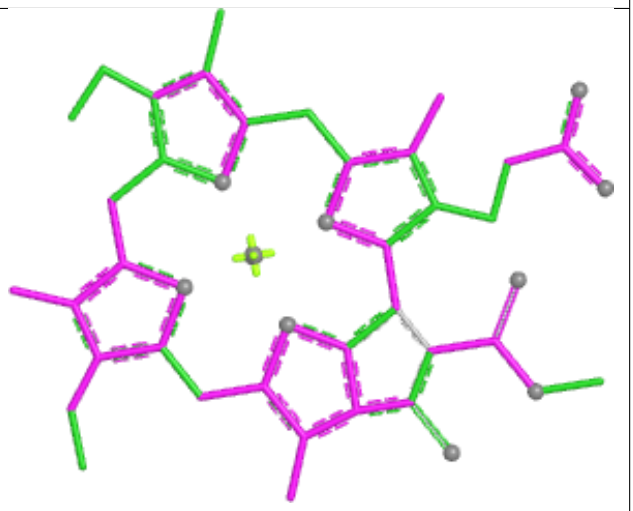
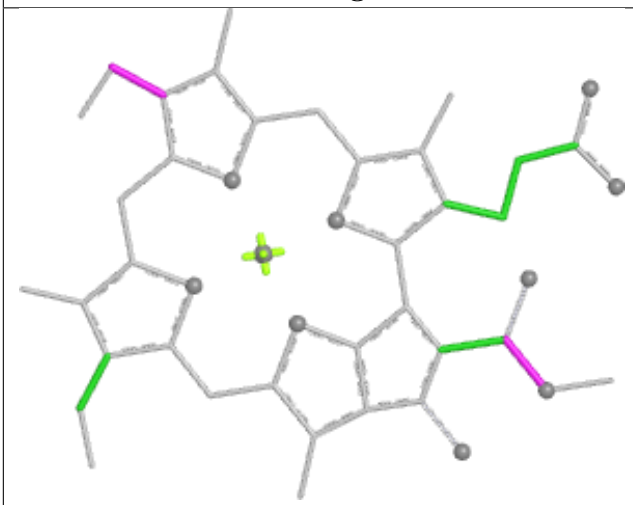
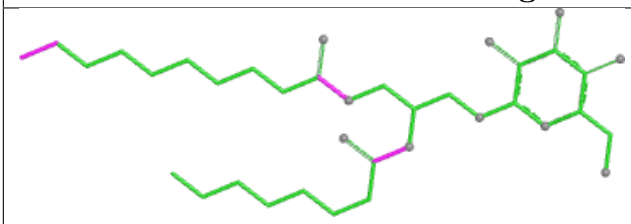
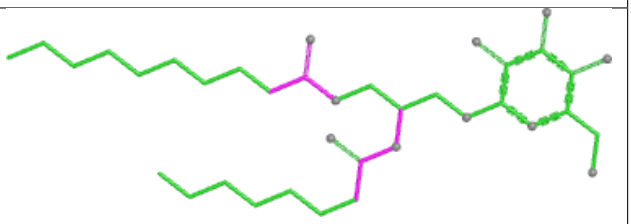
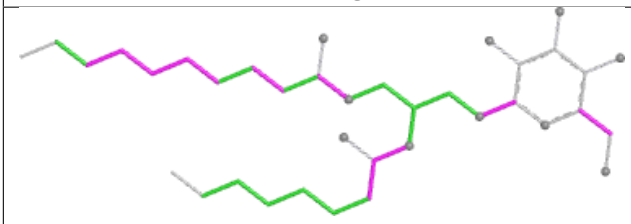
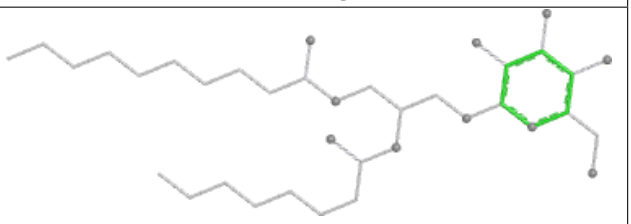


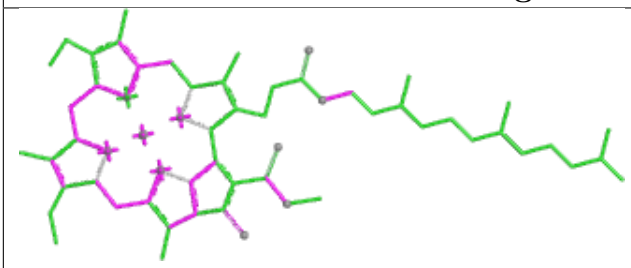
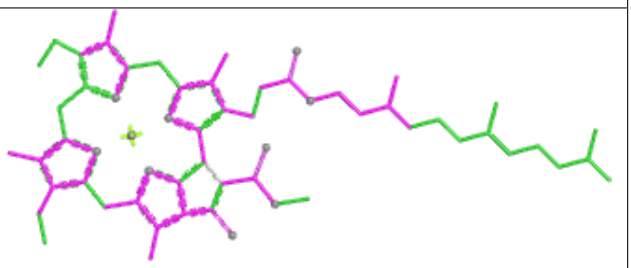
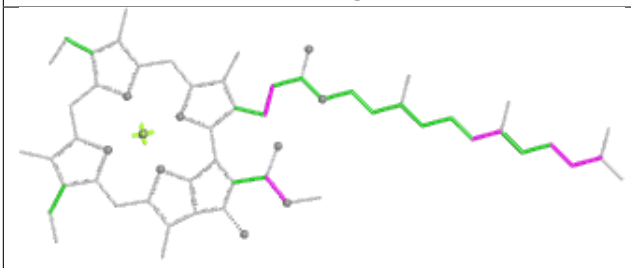
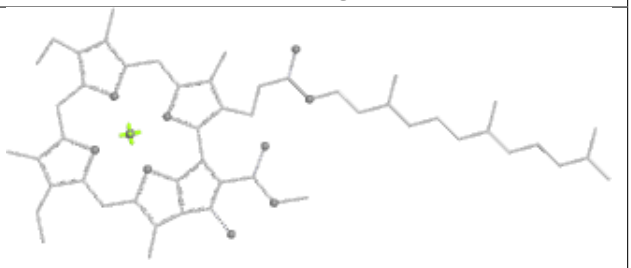
Bond angles



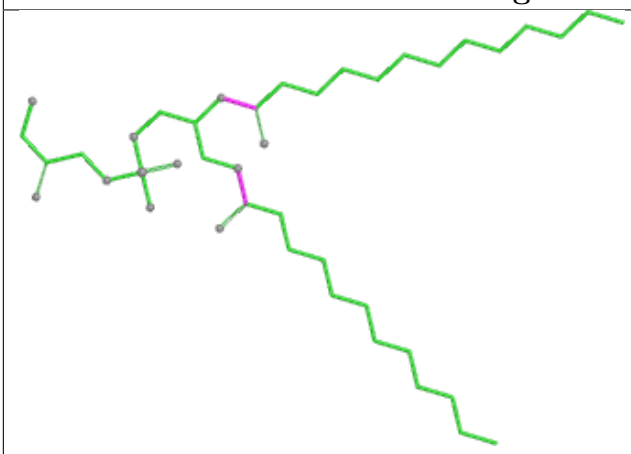
Torsions

Rings

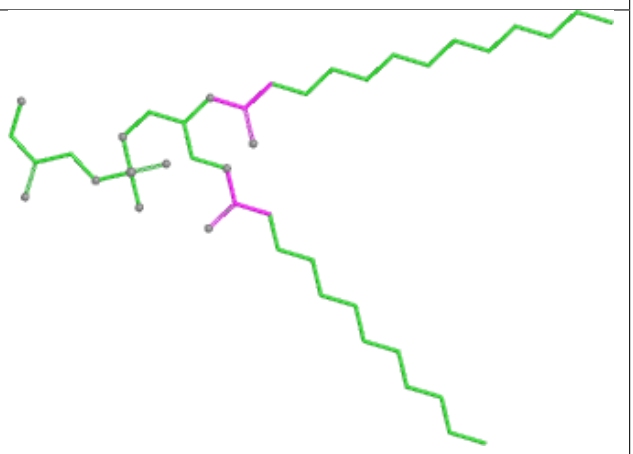
Ligand LMG i 5006	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1123	
 Bond lengths	 Bond angles
 Torsions	 Rings

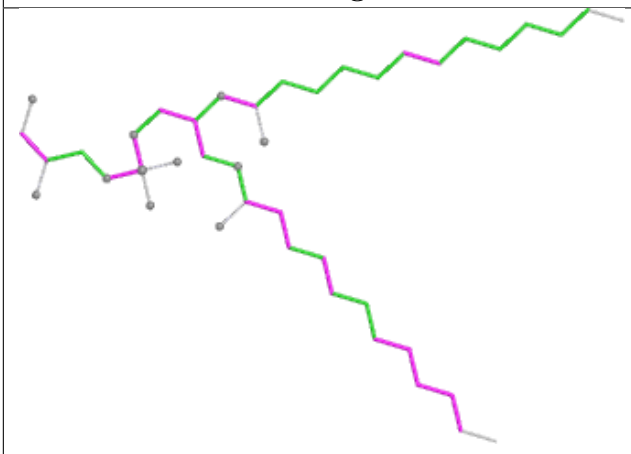
Ligand LHG A 5001



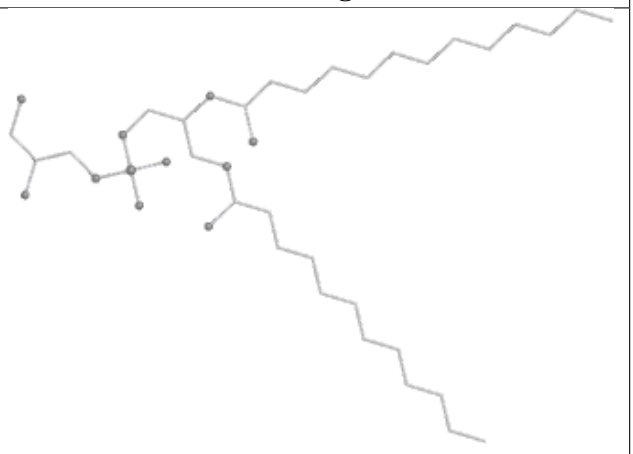
Bond lengths



Bond angles

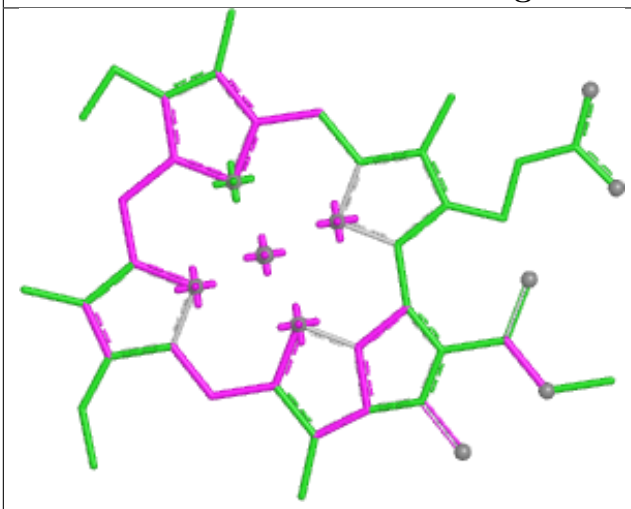


Torsions



Rings

Ligand CLA H 1236



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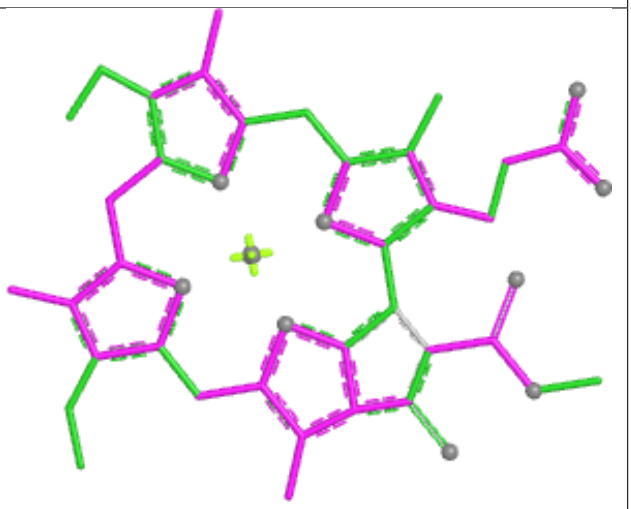
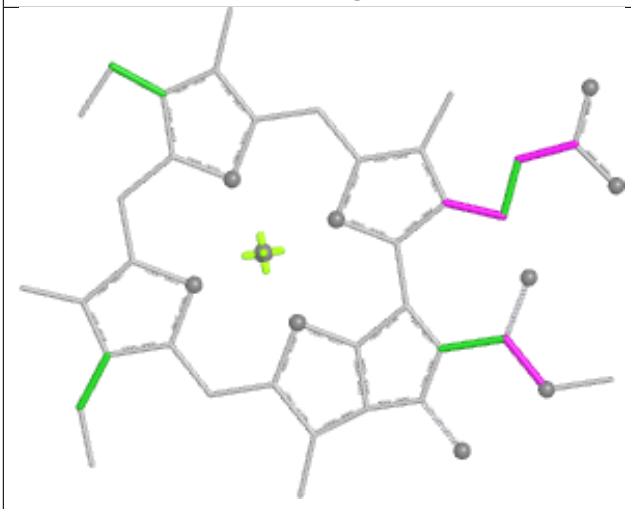


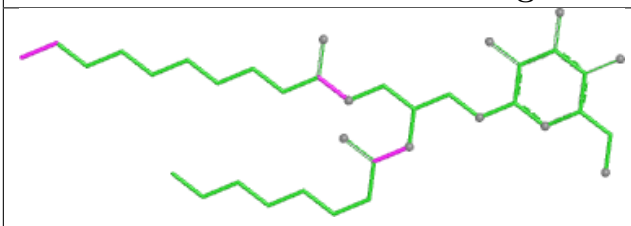
Bond angles



Torsions

Rings

Ligand LMG I 5006



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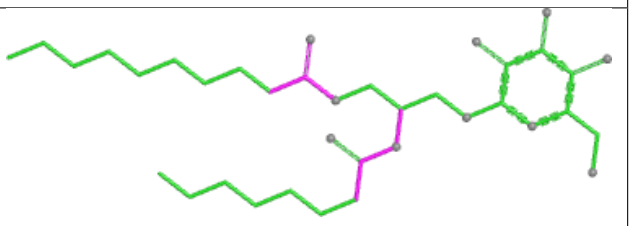
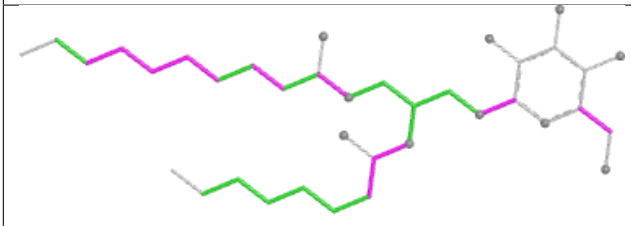


Bond angles



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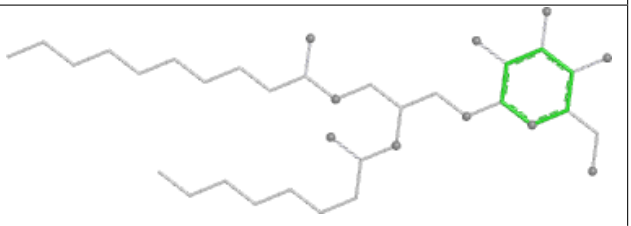
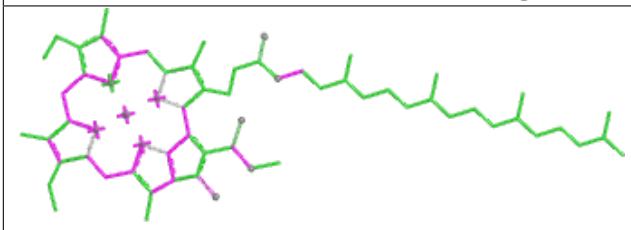


Rings

Ligand CLA B 1223



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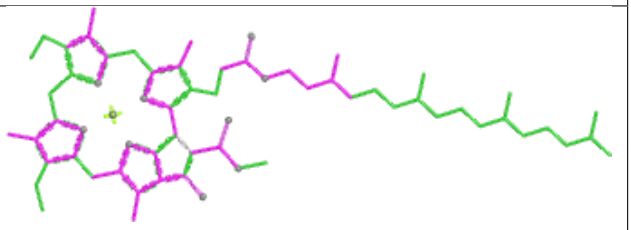

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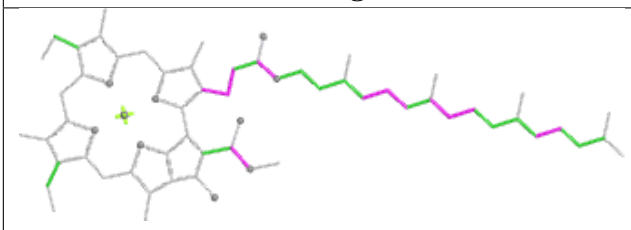

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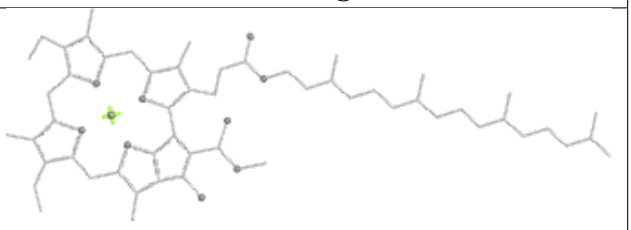
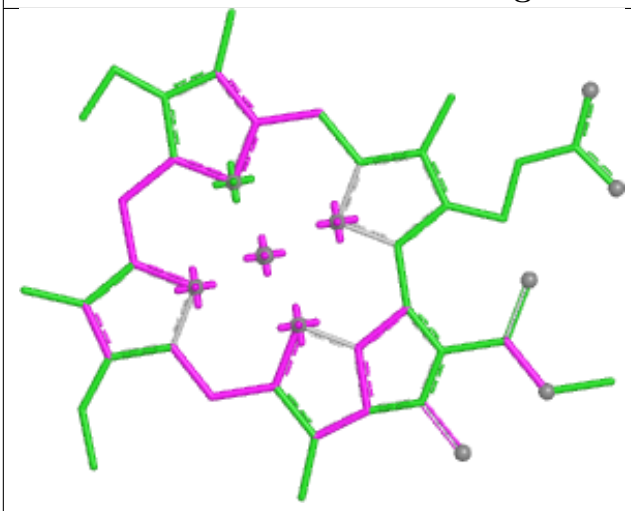


Rings

Ligand CLA G 1101



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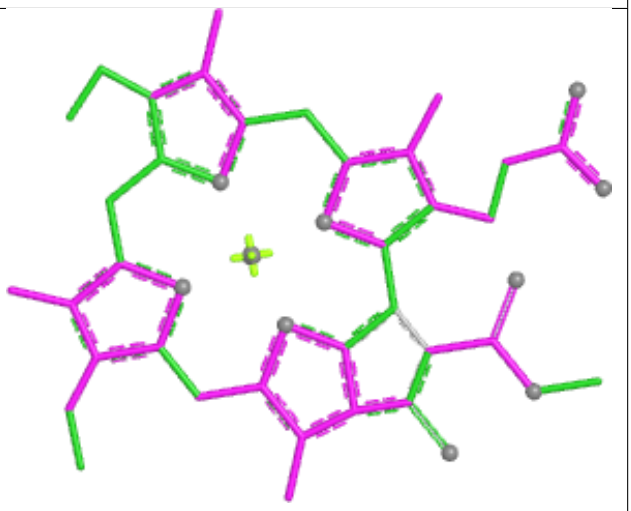
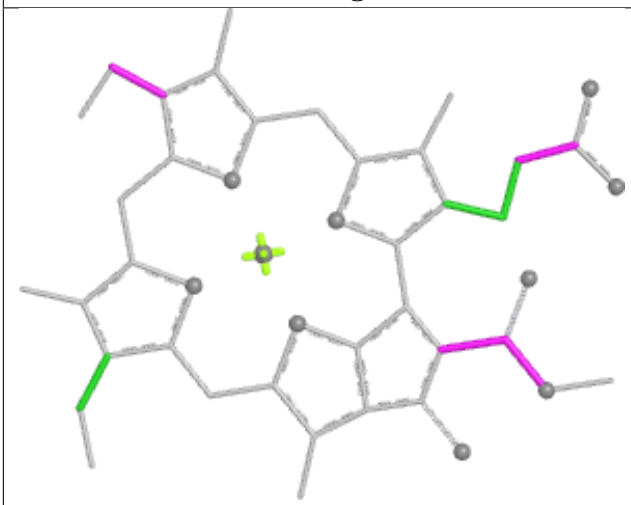


Bond angles



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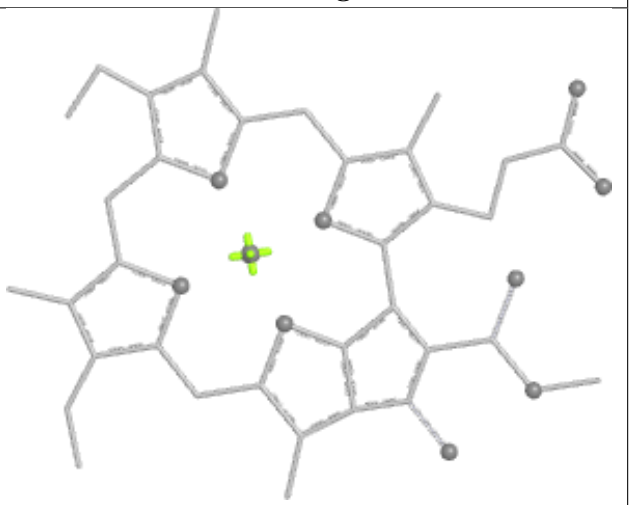
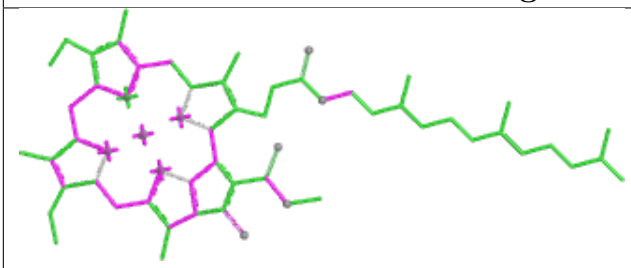
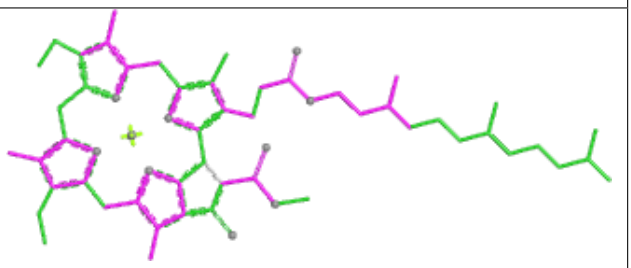
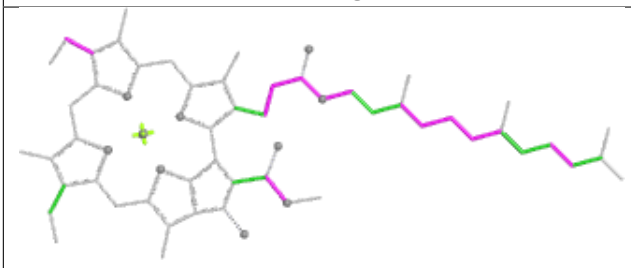
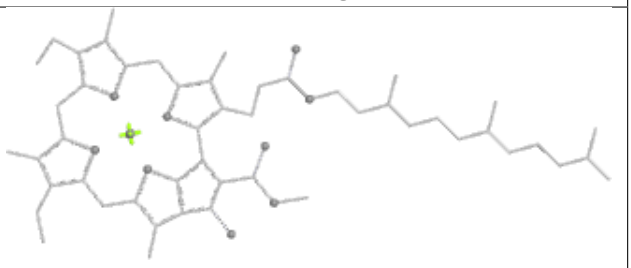
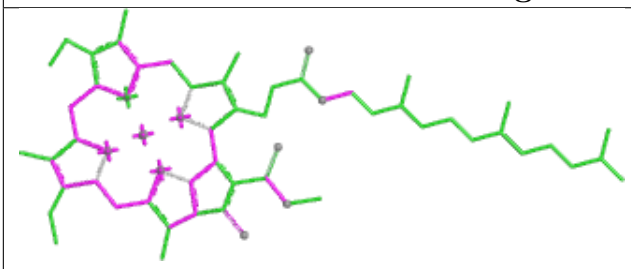
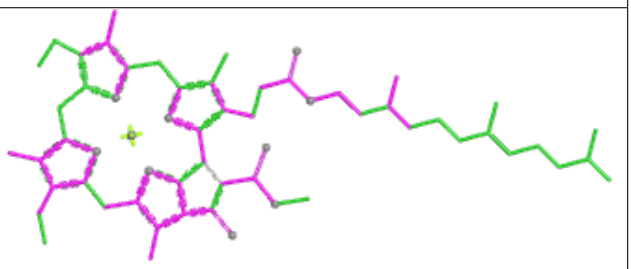
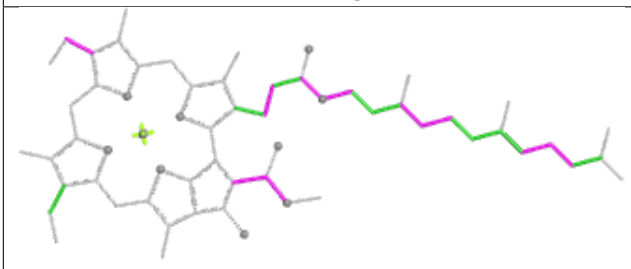
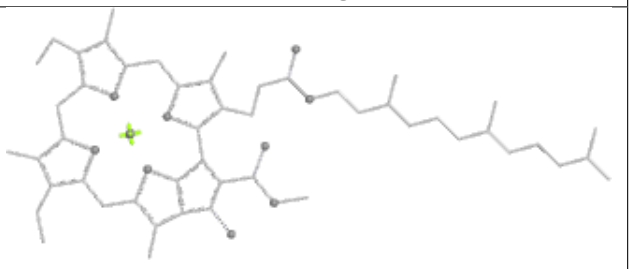
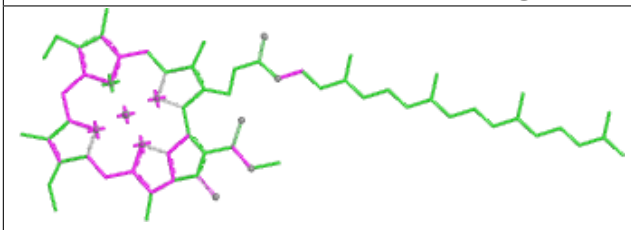


Rings

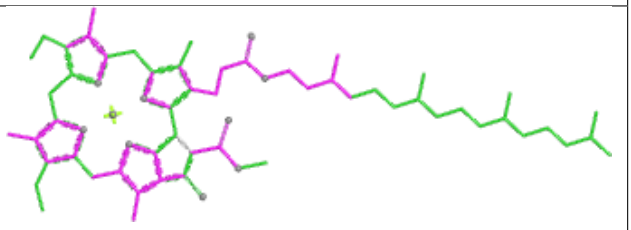
Ligand CLA a 1131	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1111	
	
Bond lengths	Bond angles
	
Torsions	Rings

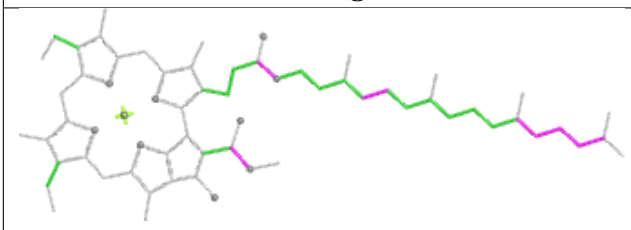
Ligand CLA B 1208



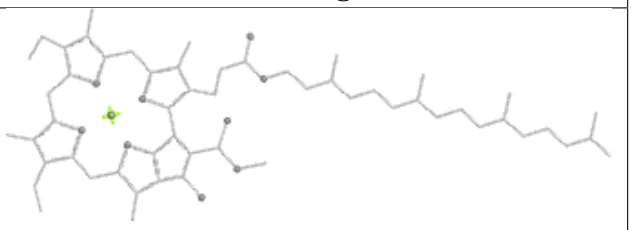
Bond lengths



Bond angles

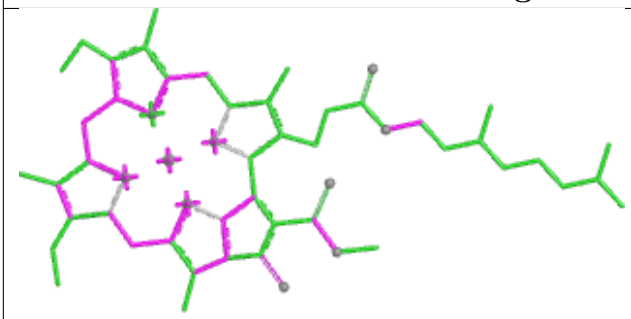


Torsions



Rings

Ligand CLA H 1231



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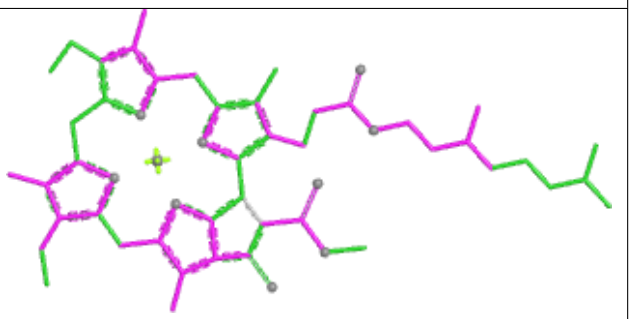
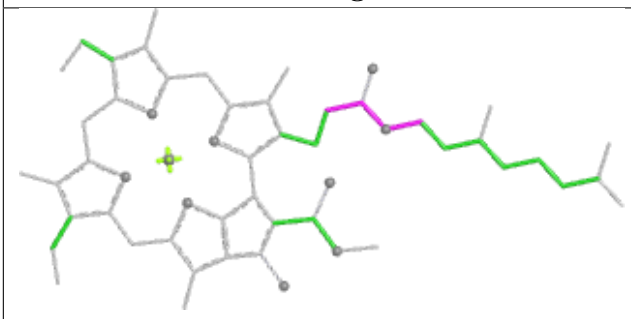
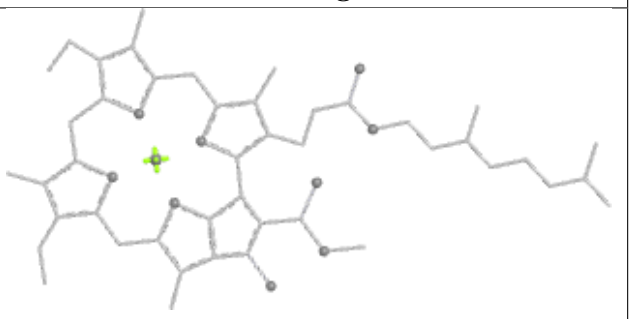


Bond angles

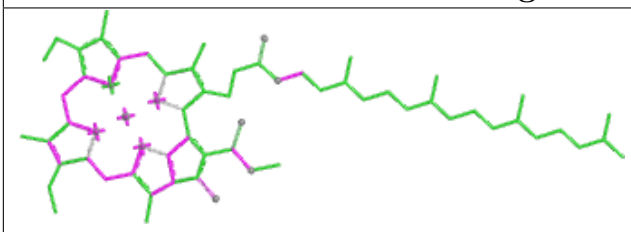


Torsions

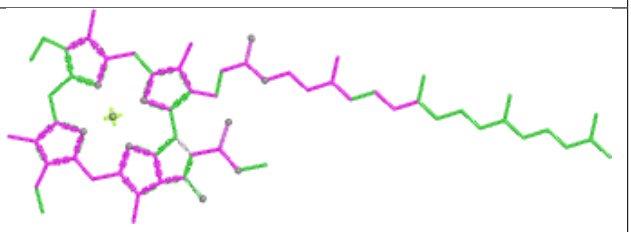


Rings

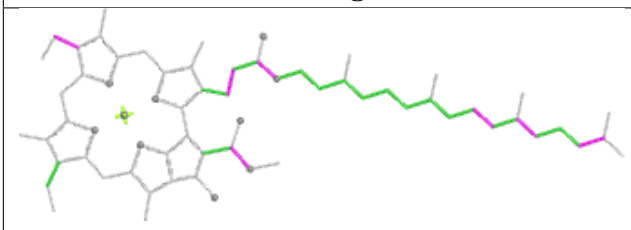
Ligand CLA b 1224



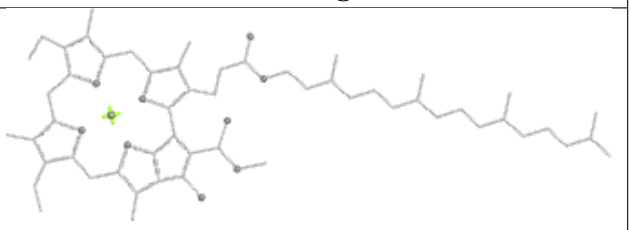
Bond lengths



Bond angles

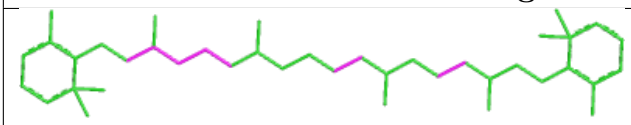


Torsions



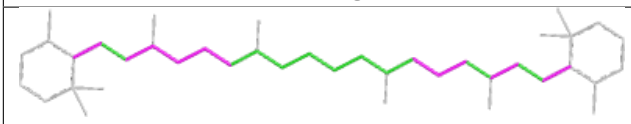
Rings

Ligand BCR a 4003

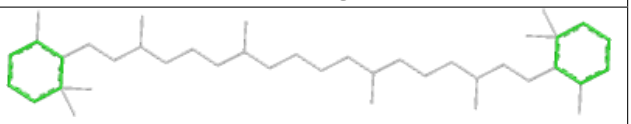


Bond lengths

Bond angles

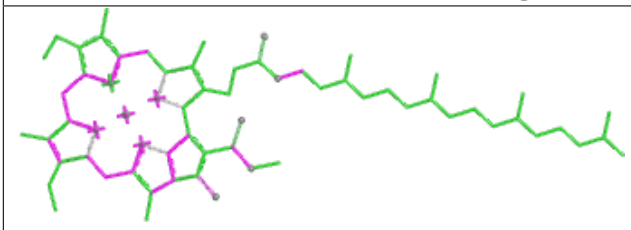


Torsions

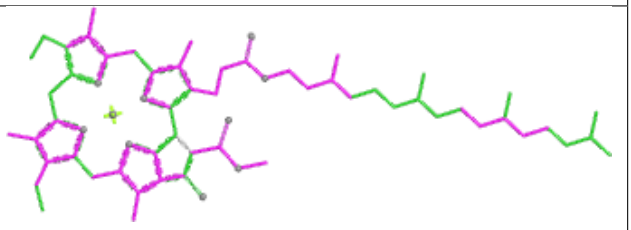


Rings

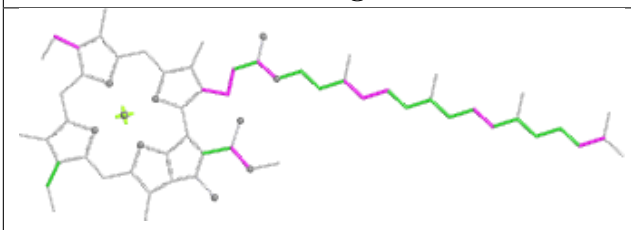
Ligand CLA B 1238



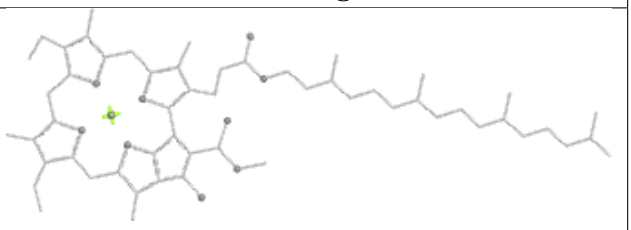
Bond lengths



Bond angles

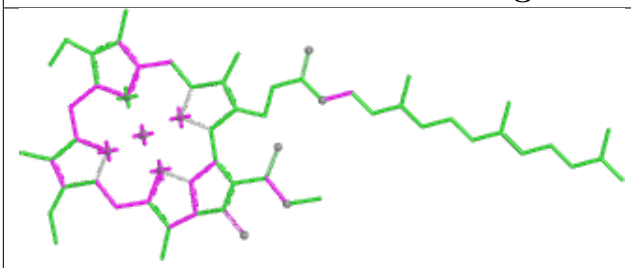


Torsions



Rings

Ligand CLA G 1102



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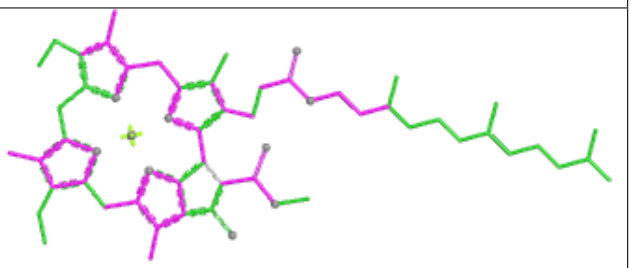
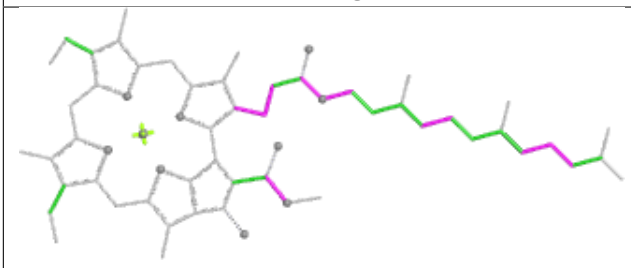
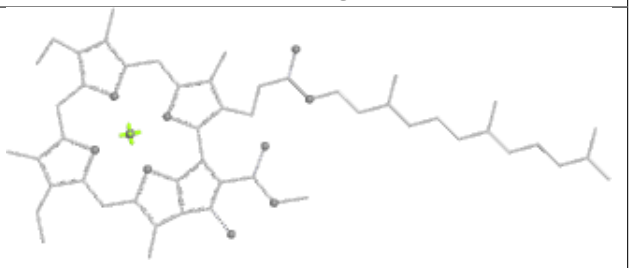


Bond angles

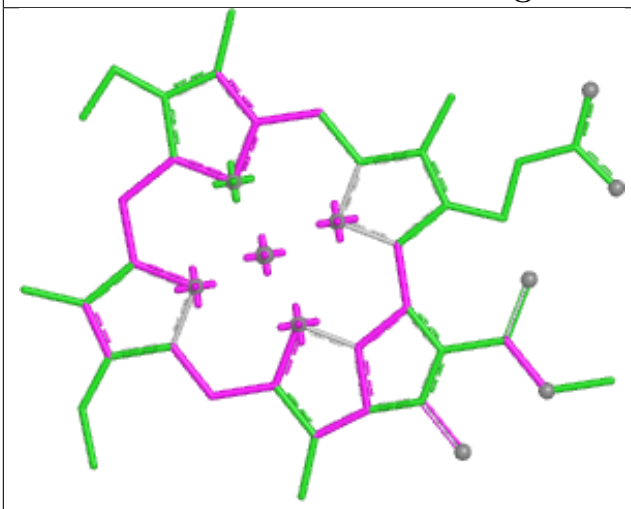


Torsions



Rings

Ligand CLA H 1212



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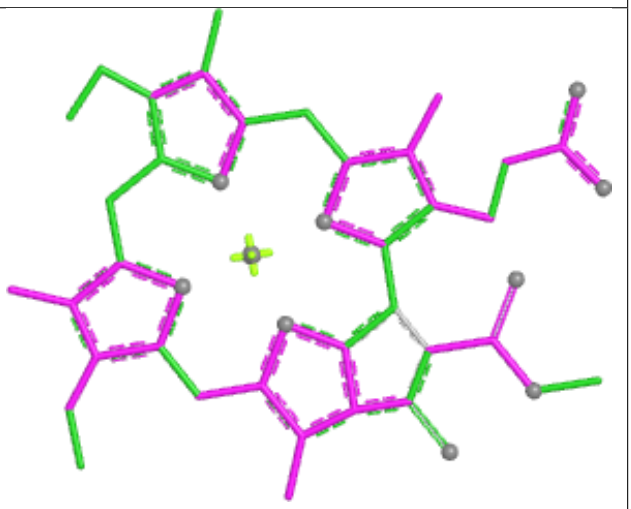
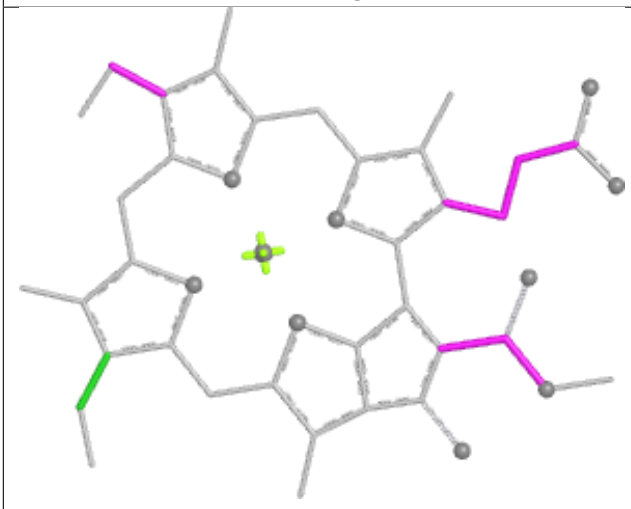


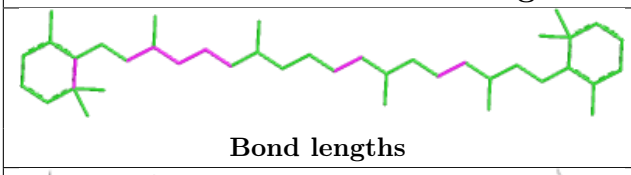
Bond angles



Torsions

Rings

Ligand BCR a 4011



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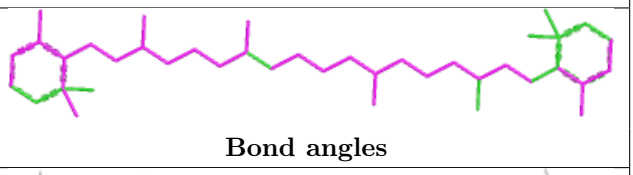
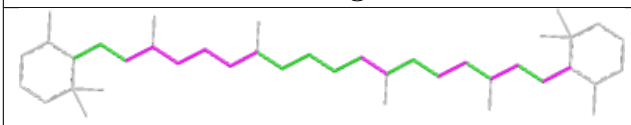
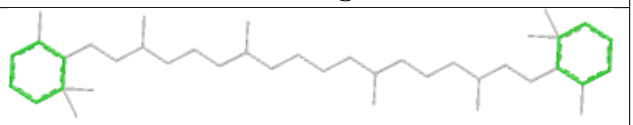


Bond angles

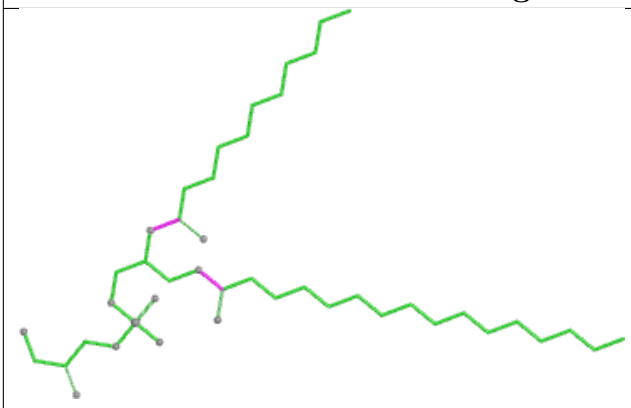


Torsions

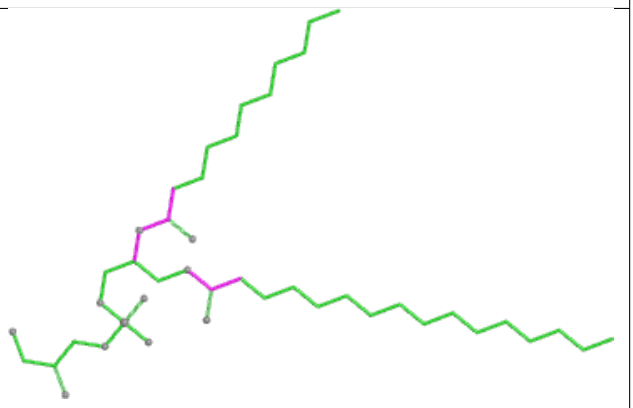


Rings

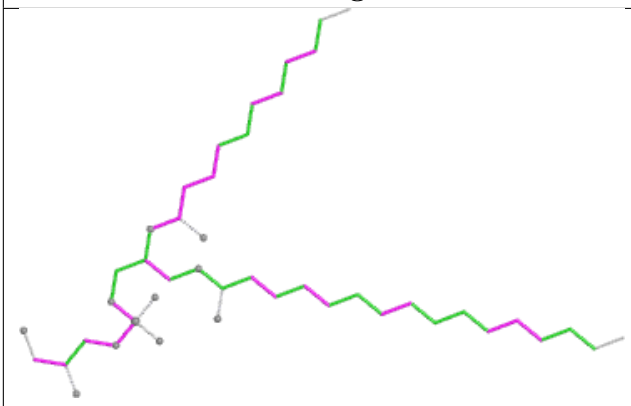
Ligand LHG H 5004



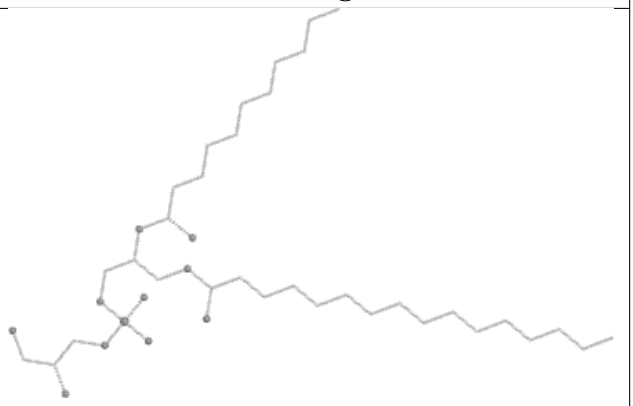
Bond lengths



Bond angles

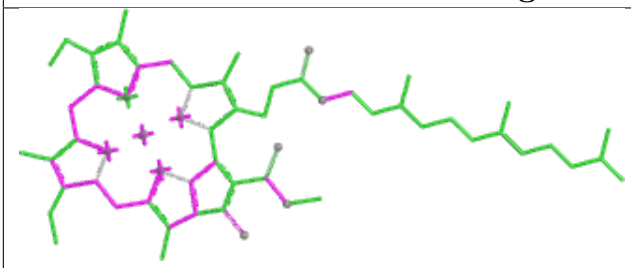


Torsions



Rings

Ligand CLA b 1214



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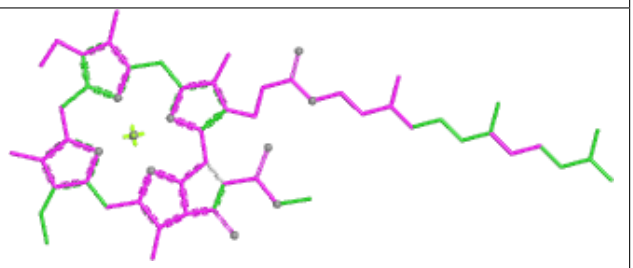
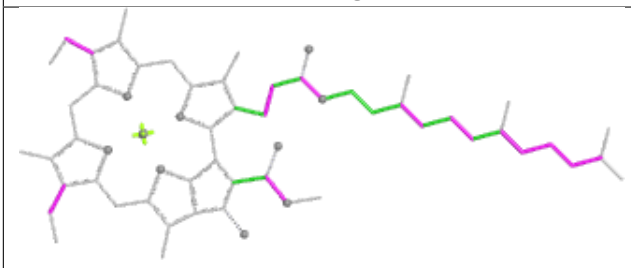
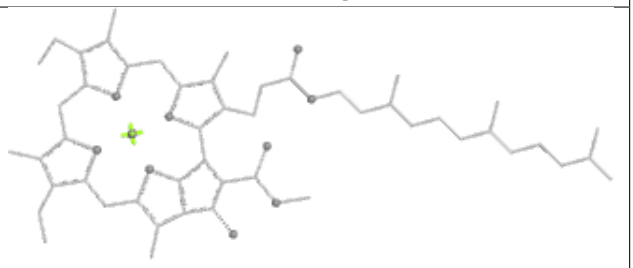


Bond angles

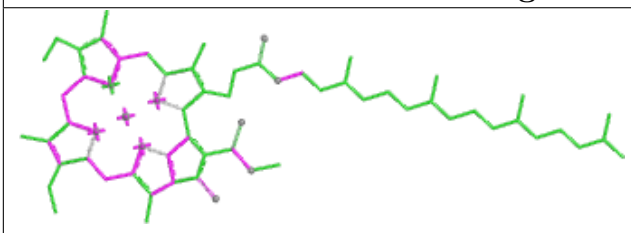


Torsions

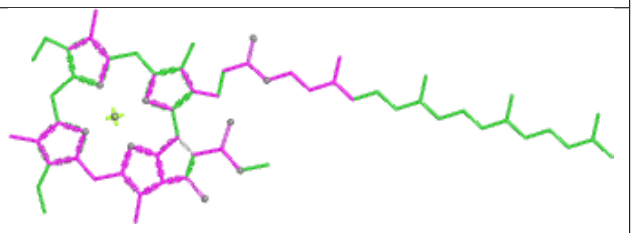


Rings

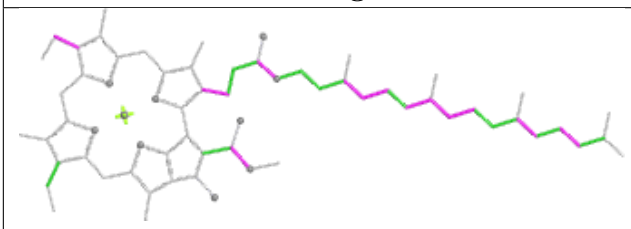
Ligand CLA b 1203



Bond lengths



Bond angles



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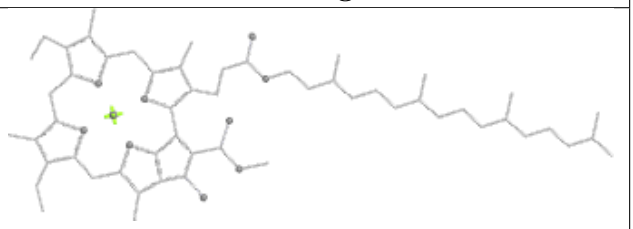
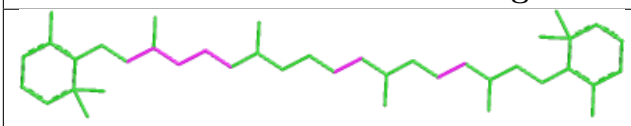


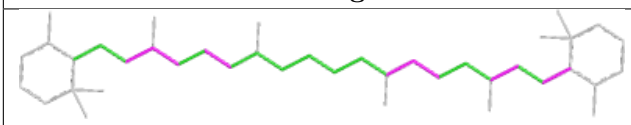
Rings

Ligand BCR m 4021



Bond lengths

Bond angles



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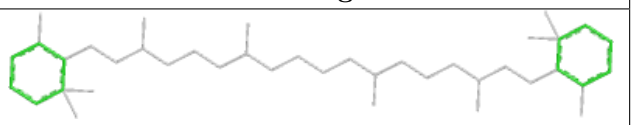
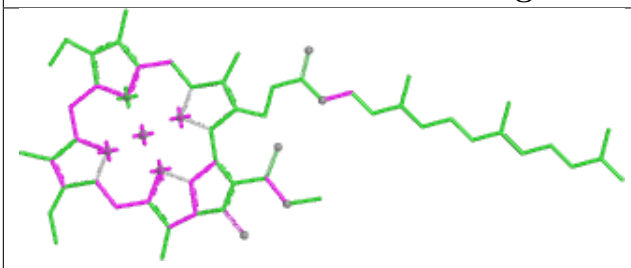
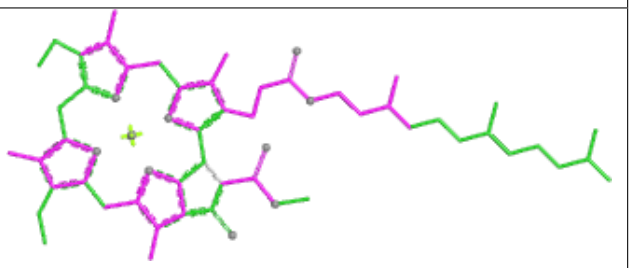
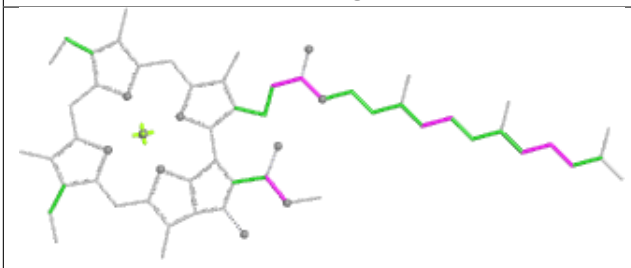
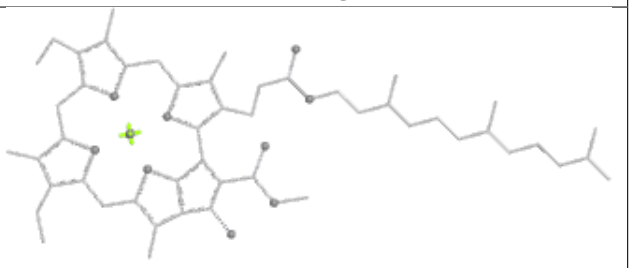
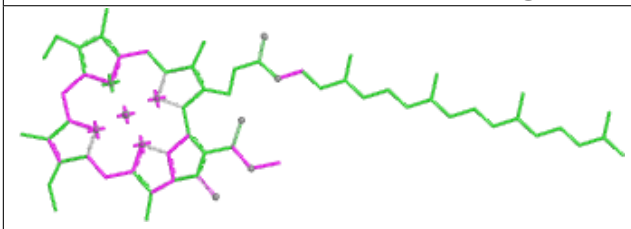
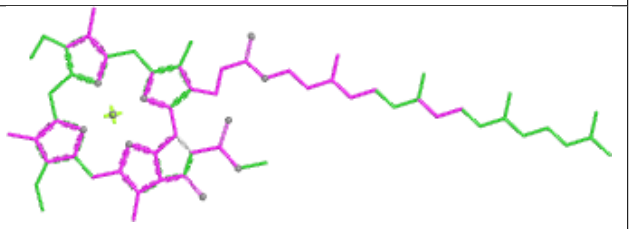
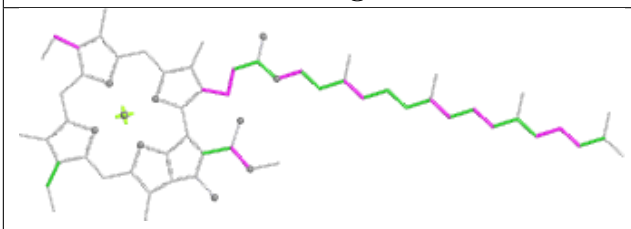
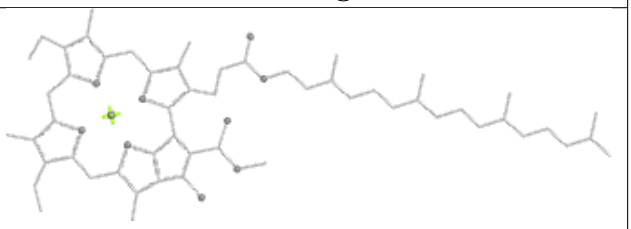
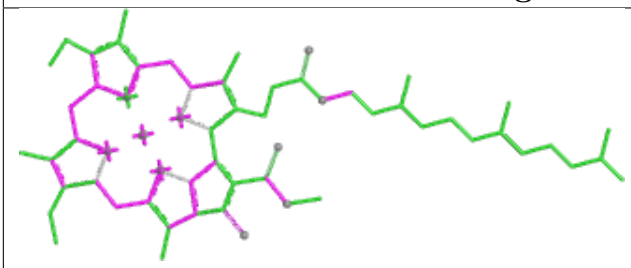
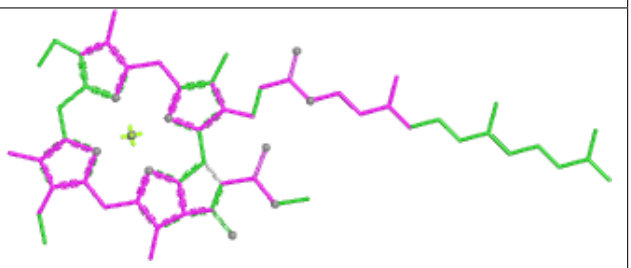
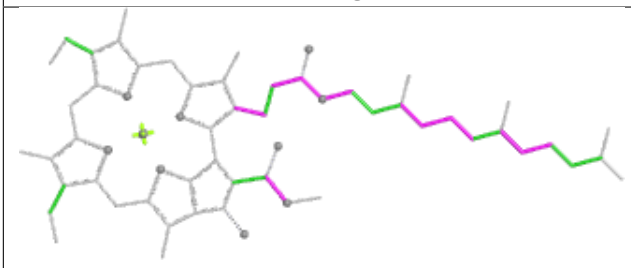
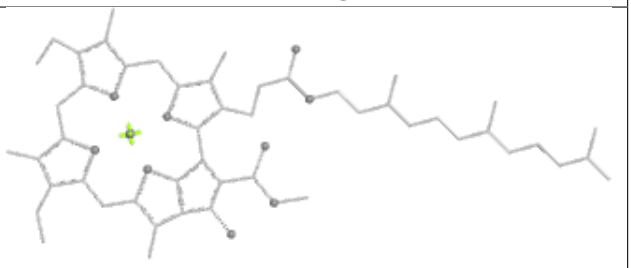
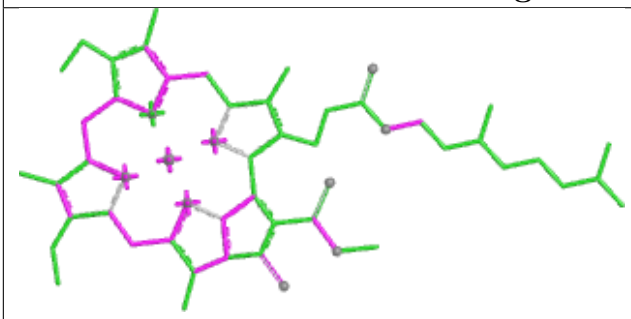
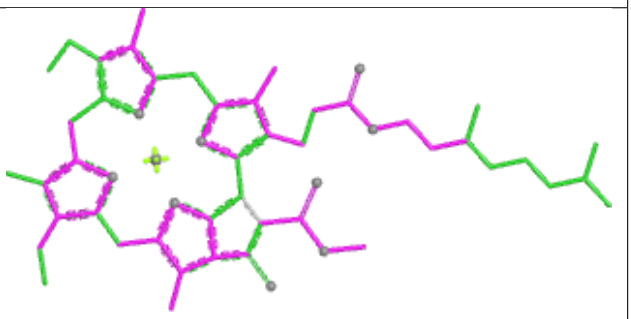
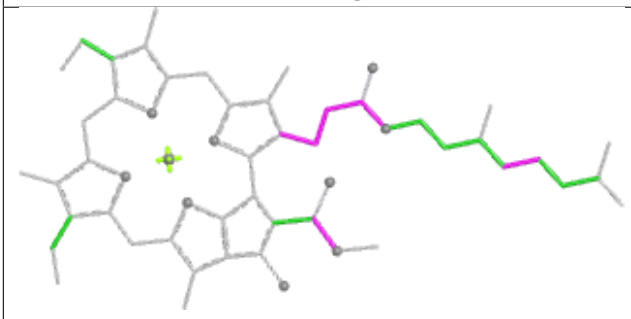
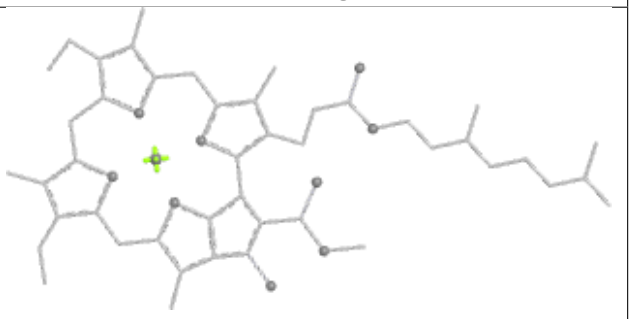


Rings

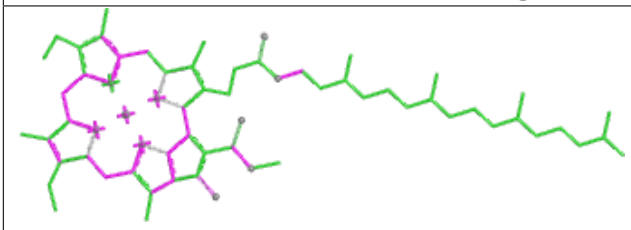
Ligand CLA B 1235	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 1012	
	
Bond lengths	Bond angles
	
Torsions	Rings

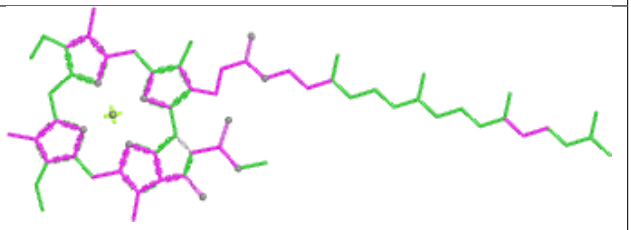
Ligand CLA A 1013	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1220	
	
Bond lengths	Bond angles
	
Torsions	Rings

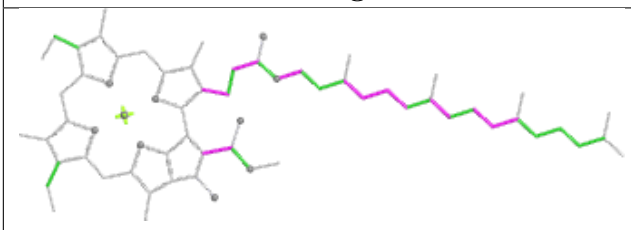
Ligand CLA H 1205



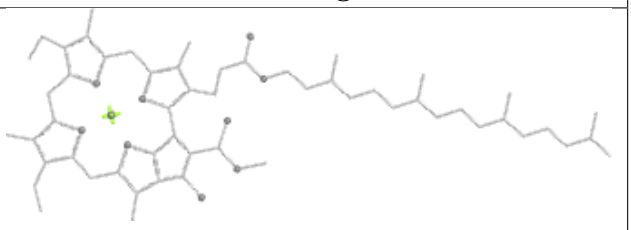
Bond lengths



Bond angles

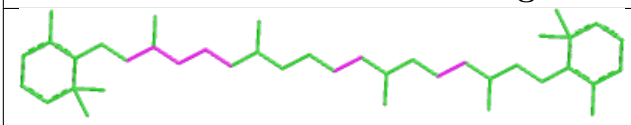


Torsions



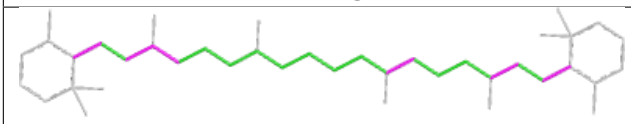
Rings

Ligand BCR a 4001

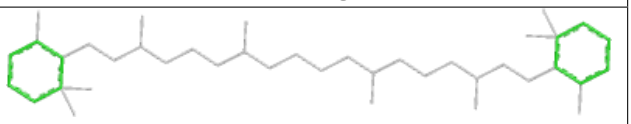


Bond lengths

Bond angles

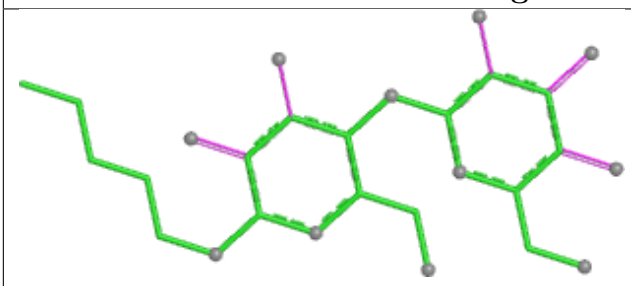


Torsions



Rings

Ligand LMT G 6002



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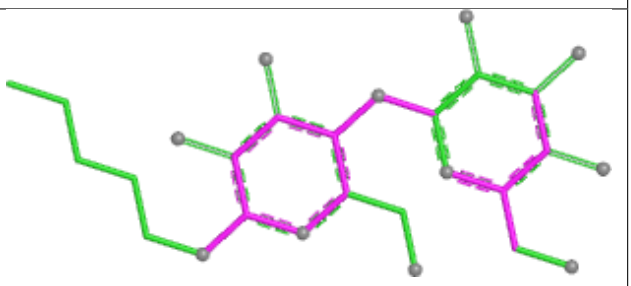
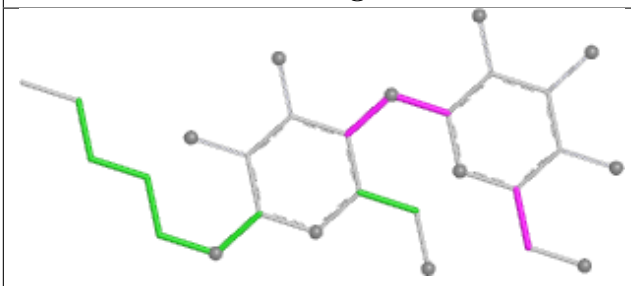


Bond angles



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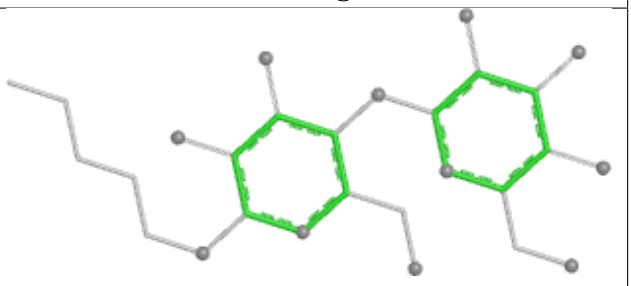
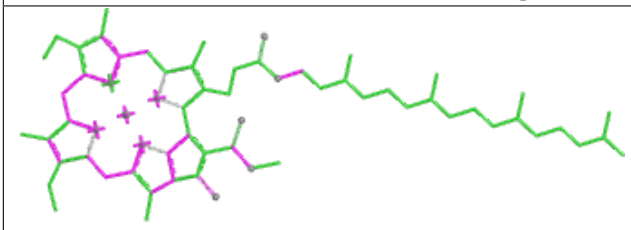
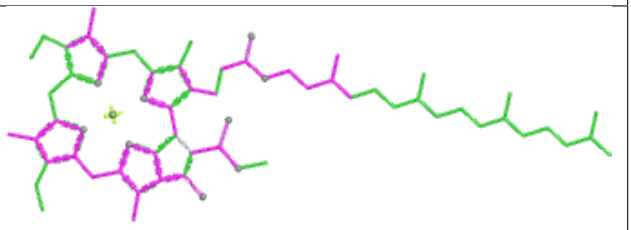


Rings

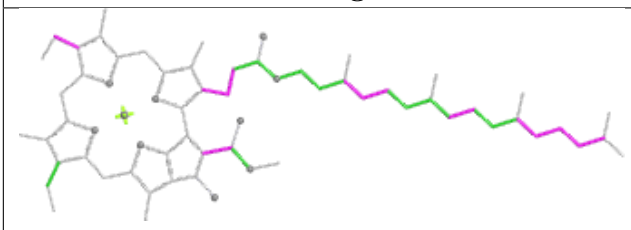
Ligand CLA H 1012



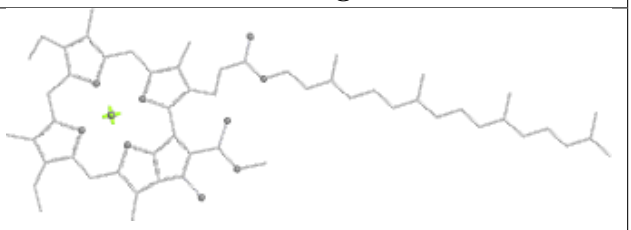
Bond lengths



Bond angles

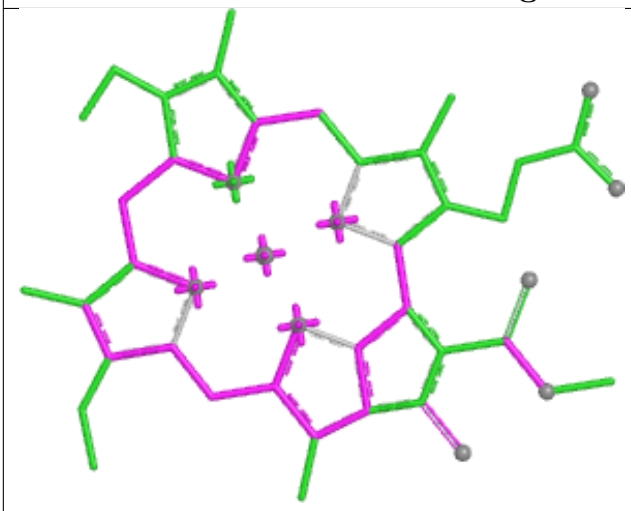


Torsions



Rings

Ligand CLA a 1114



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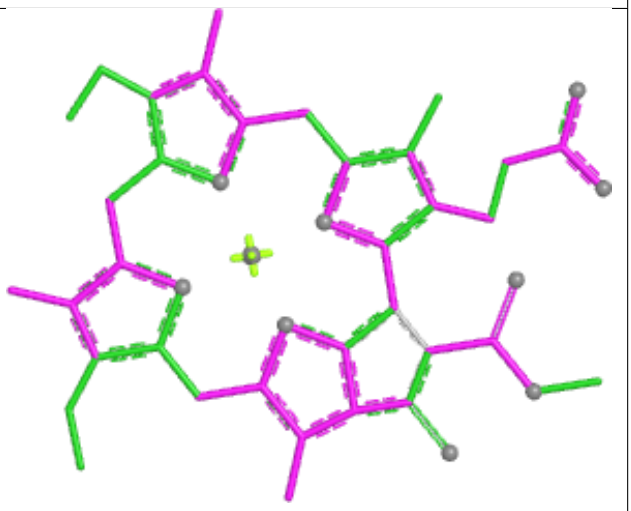

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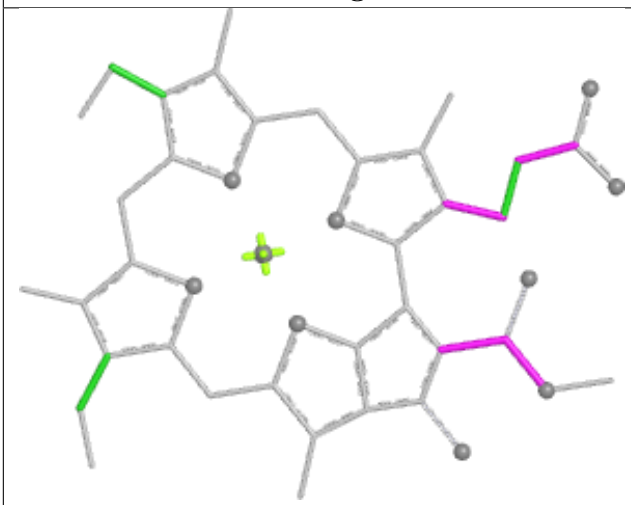

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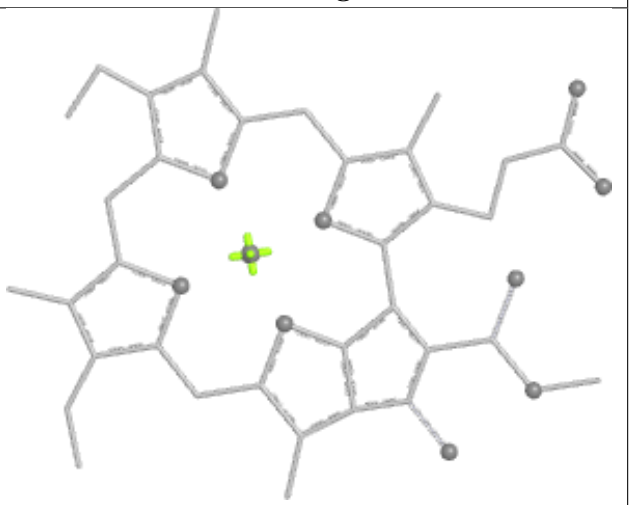
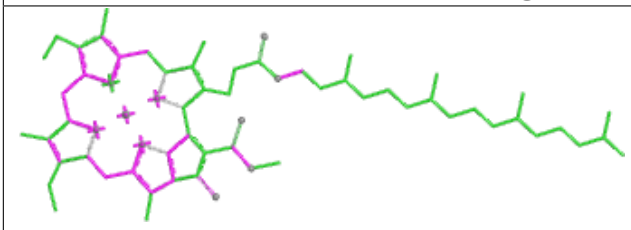


Rings

Ligand CLA b 1208



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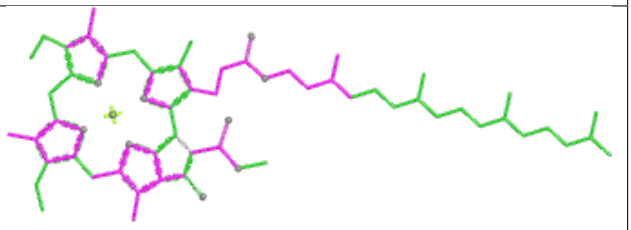

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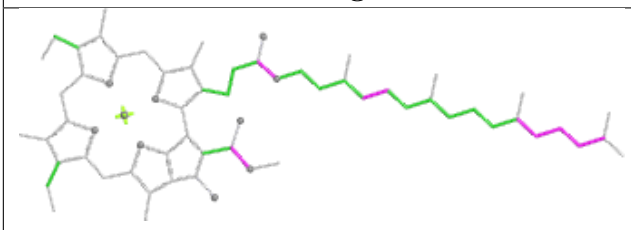

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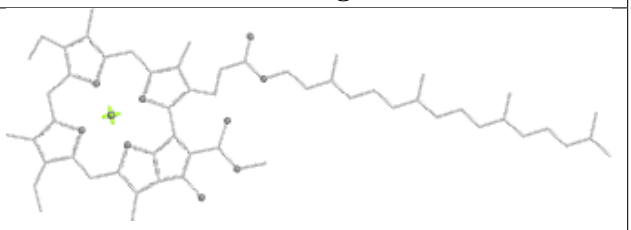
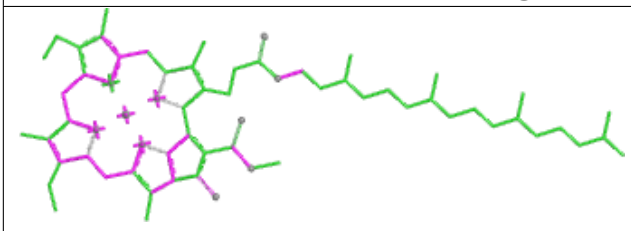


Rings

Ligand CLA B 1210



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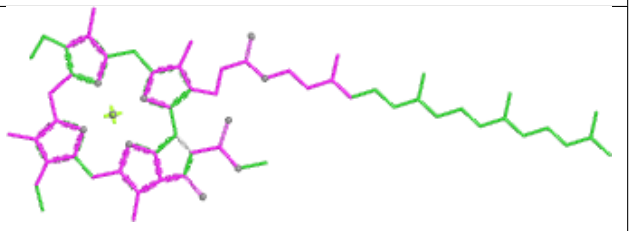
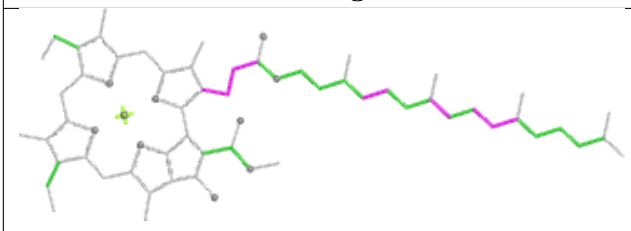


Bond angles



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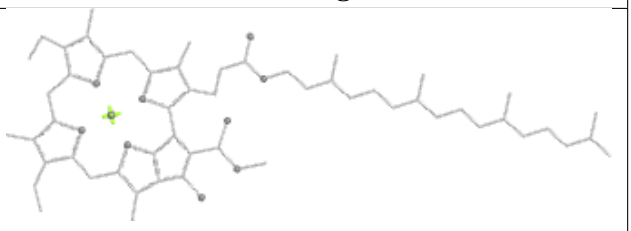
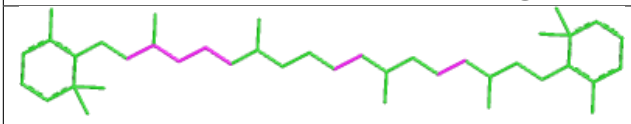


Rings

Ligand BCR b 4009



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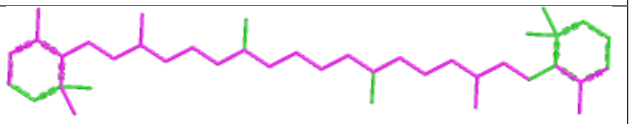
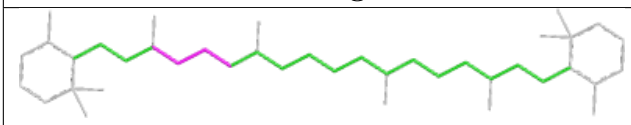


Bond angles



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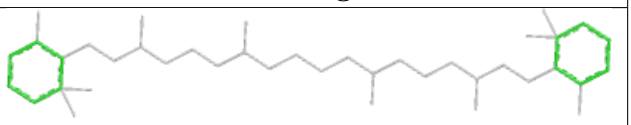
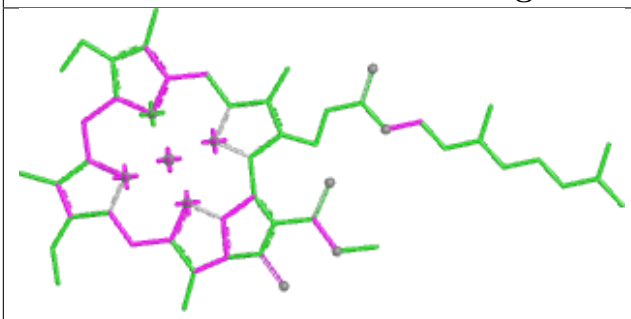


Rings

Ligand CLA B 1234



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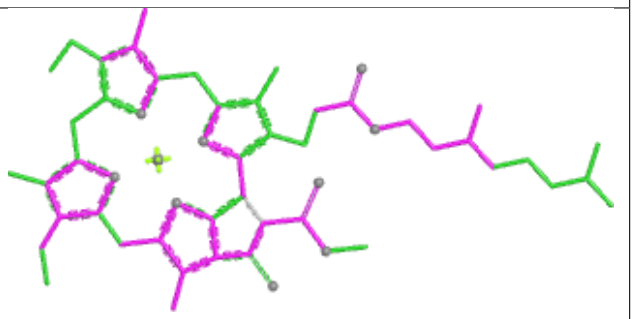
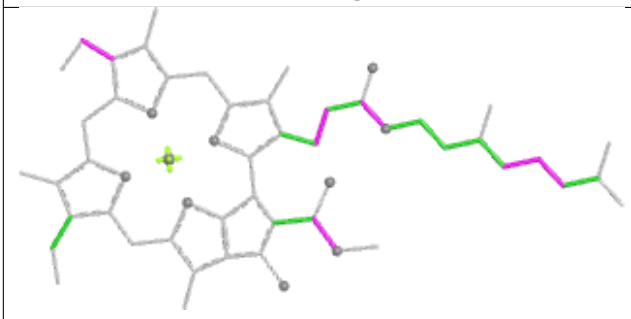


Bond angles



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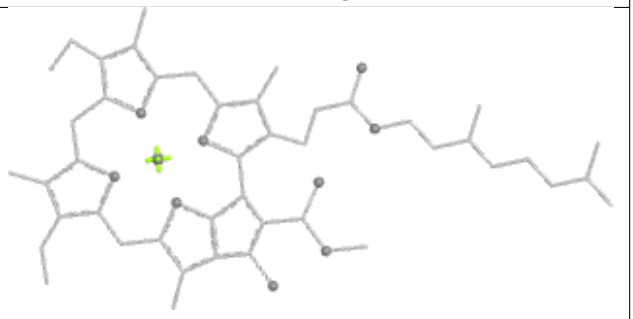
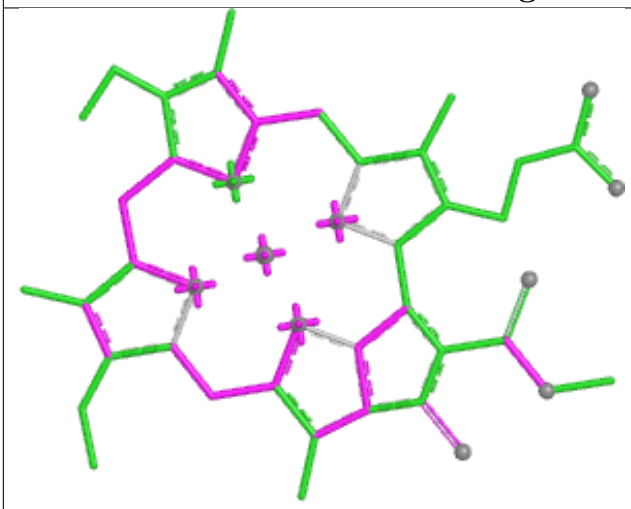


Rings

Ligand CLA x 1701



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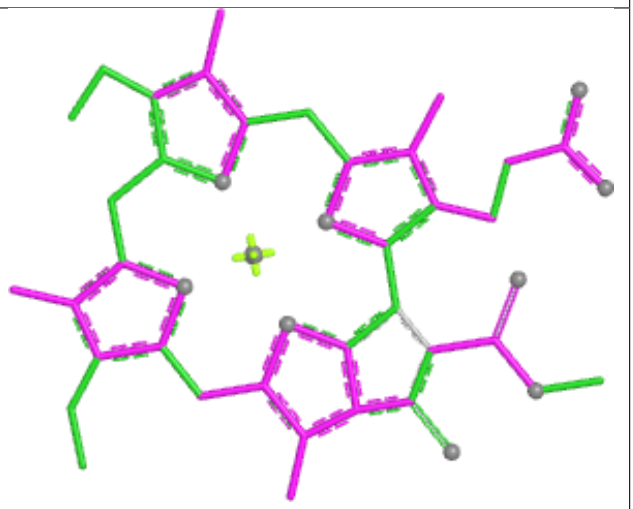
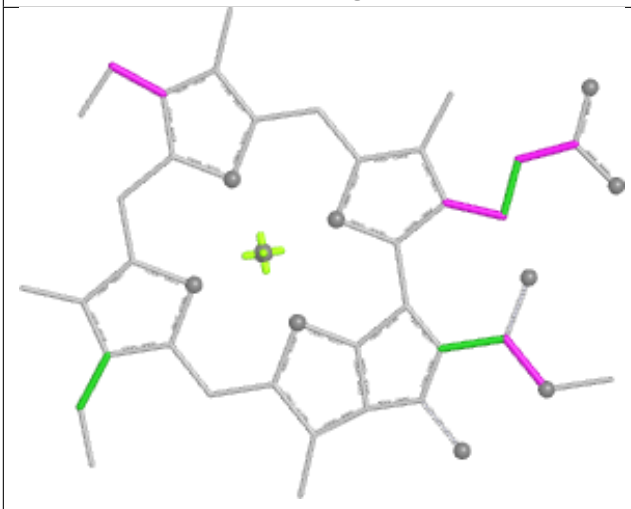


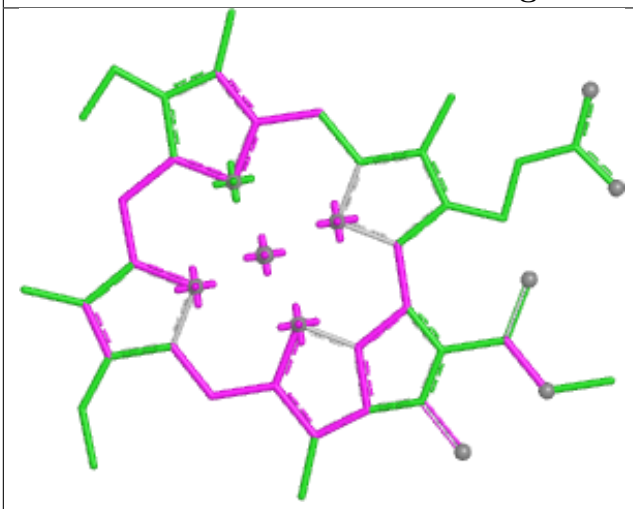
Bond angles



Torsions

Rings

Ligand CLA a 1109



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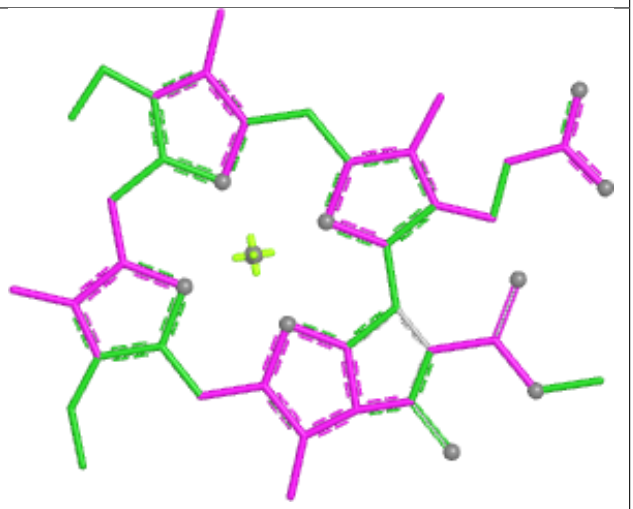
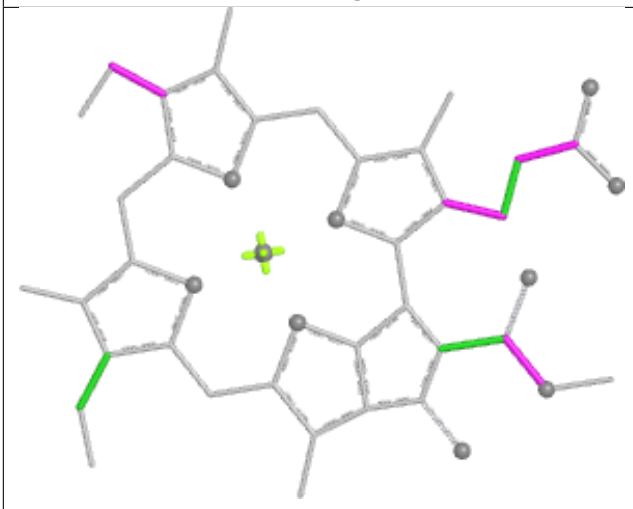


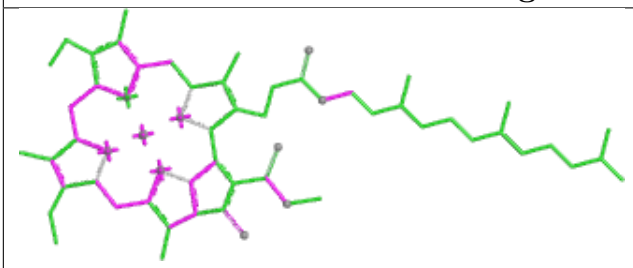
Bond angles



Torsions

Rings

Ligand CLA b 1202



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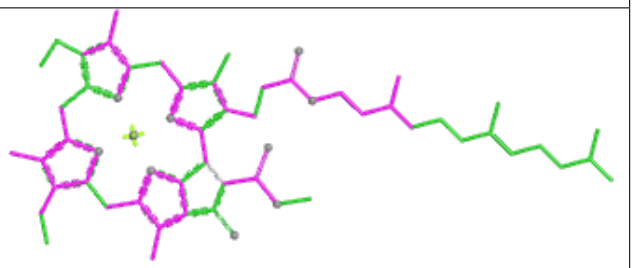
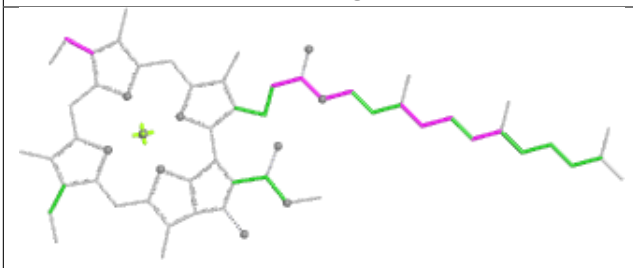
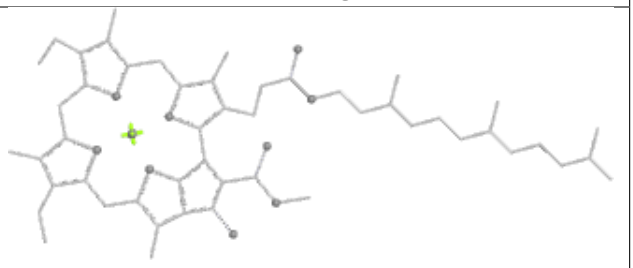


Bond angles

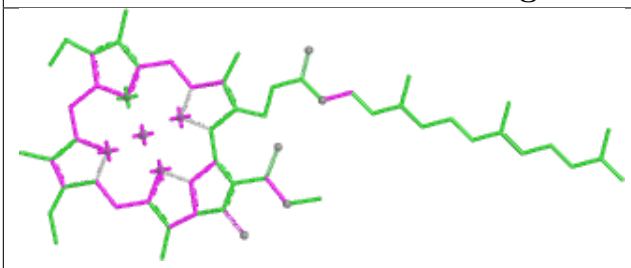


Torsions



Rings

Ligand CLA a 1013



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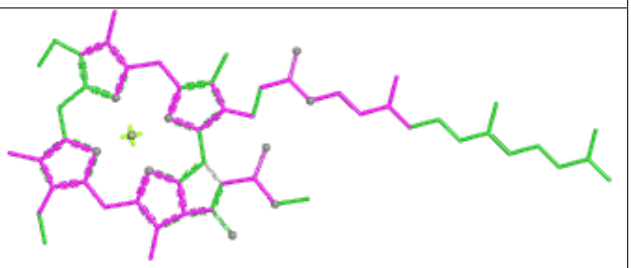
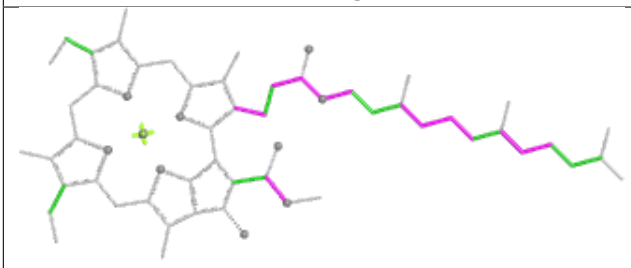


Bond angles



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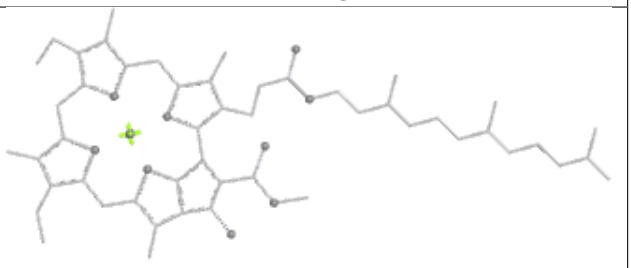
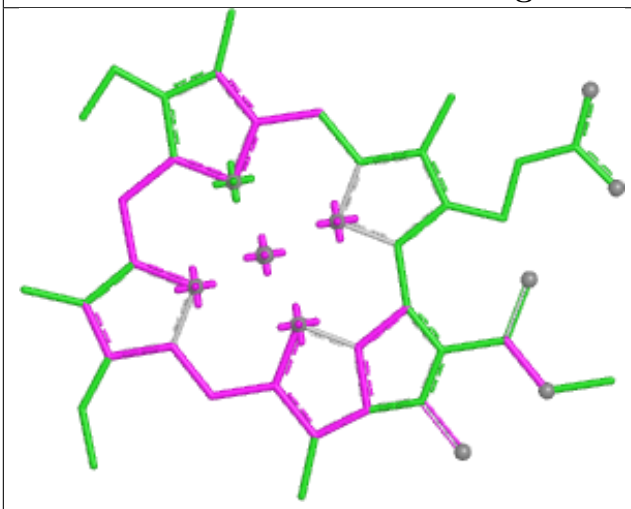


Rings

Ligand CLA B 1233



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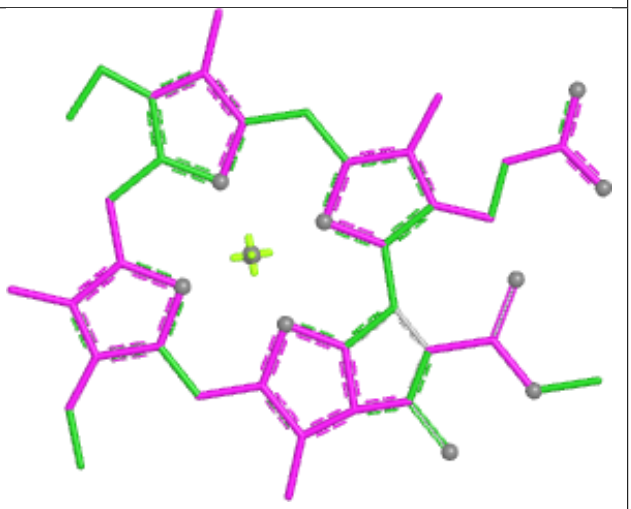
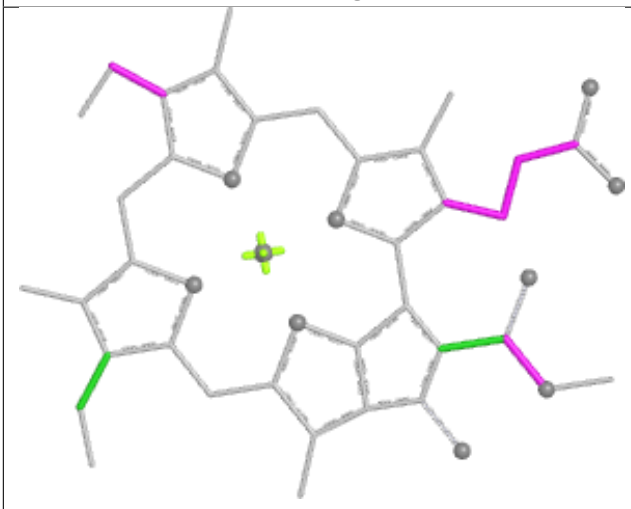


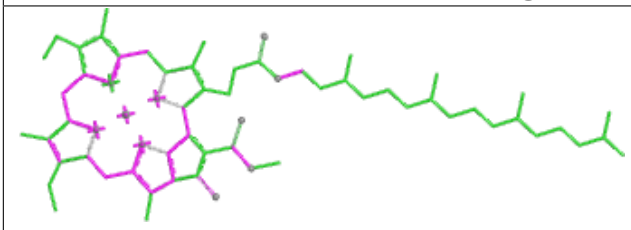
Bond angles



Torsions

Rings

Ligand CLA a 1117



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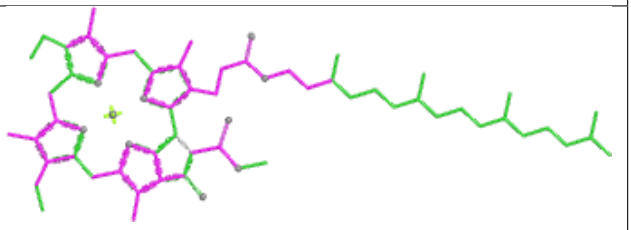
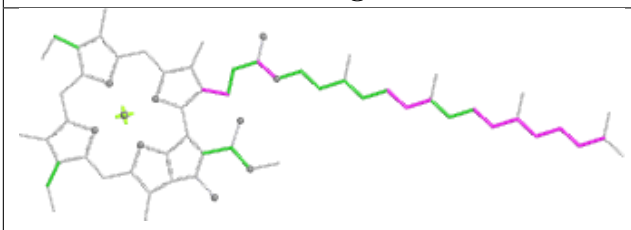
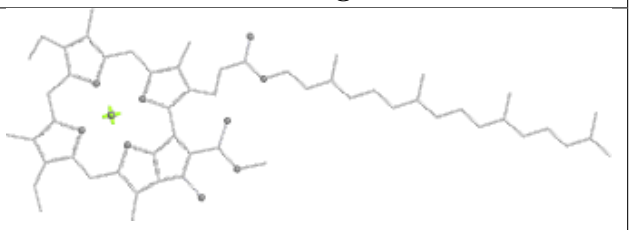


Bond angles

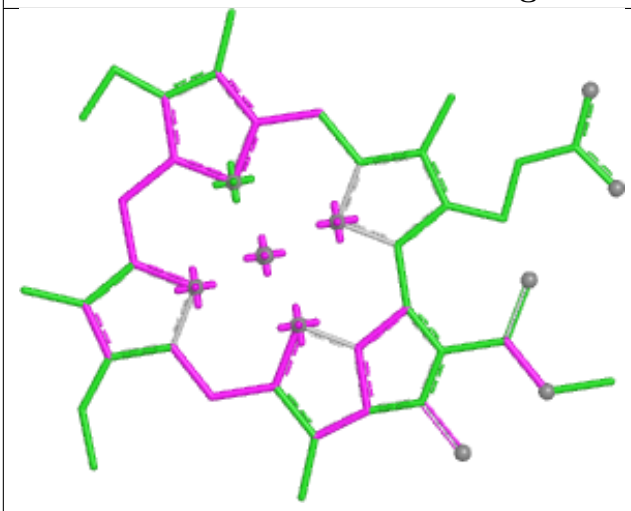


Torsions

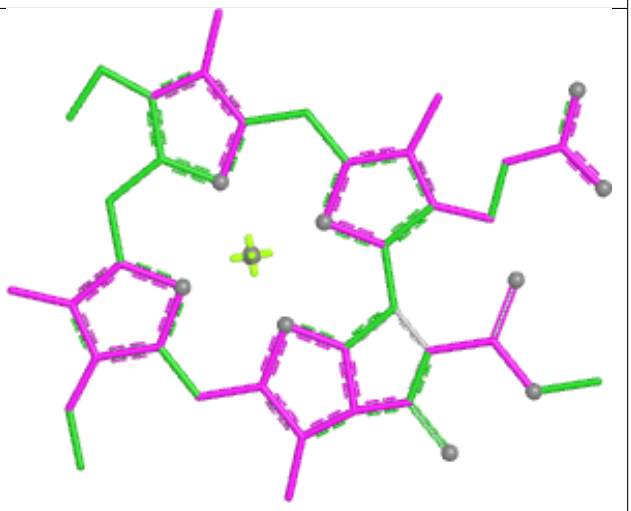


Rings

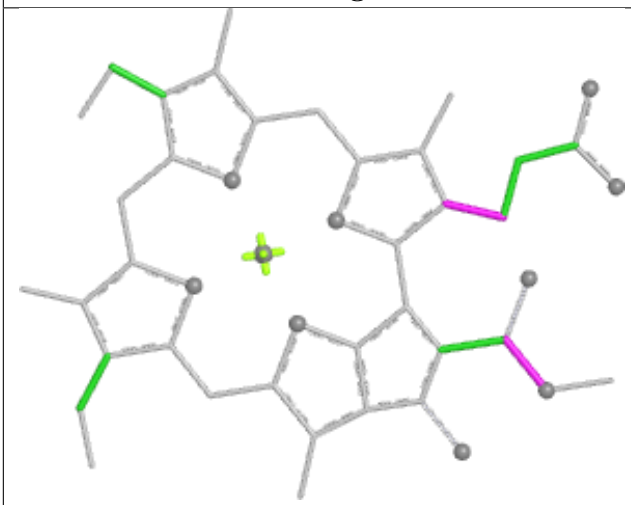
Ligand CLA a 1139



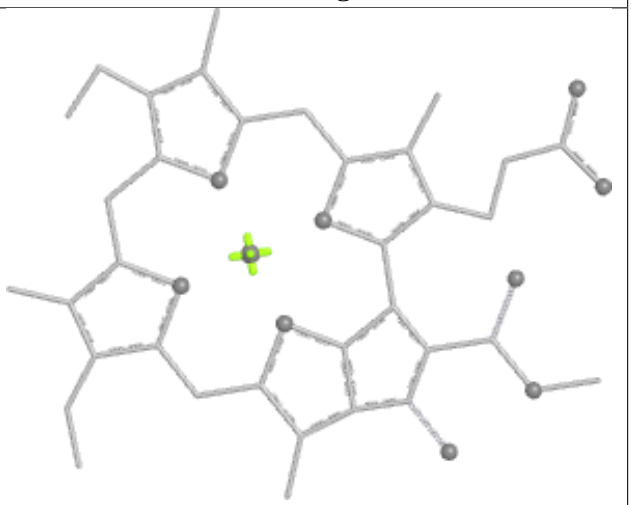
Bond lengths



Bond angles

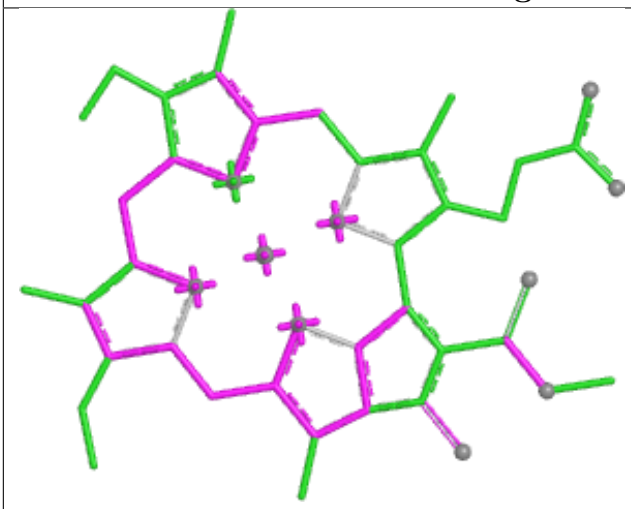


Torsions

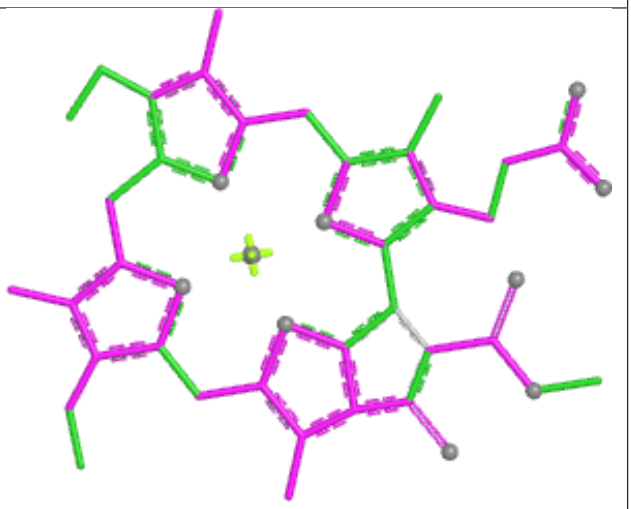


Rings

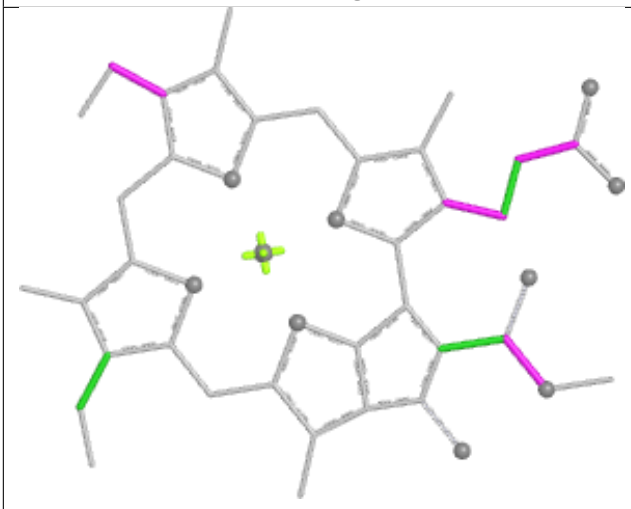
Ligand CLA H 1228



Bond lengths



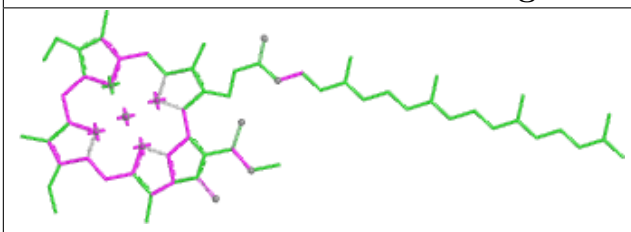
Bond angles



Torsions

Rings

Ligand CLA b 1239



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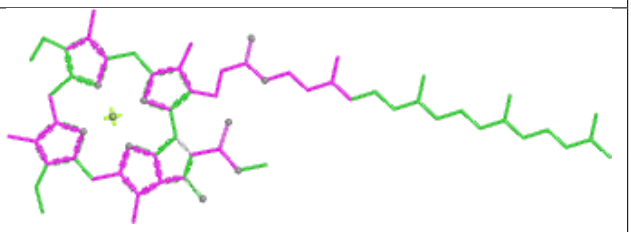
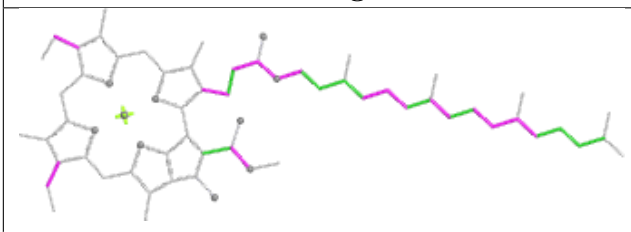
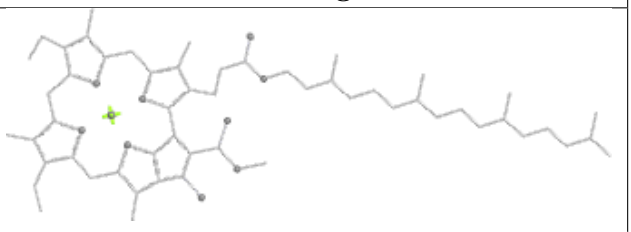


Bond angles

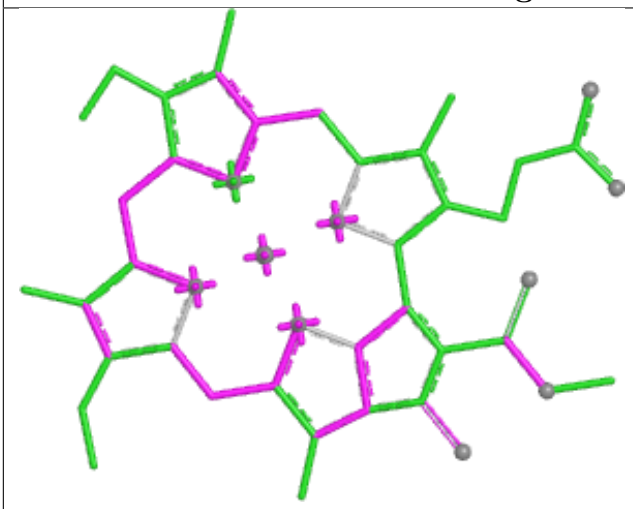


Torsions



Rings

Ligand CLA B 1227



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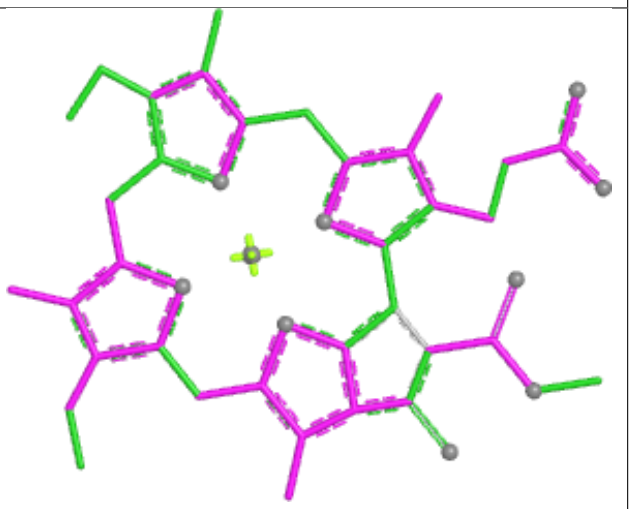
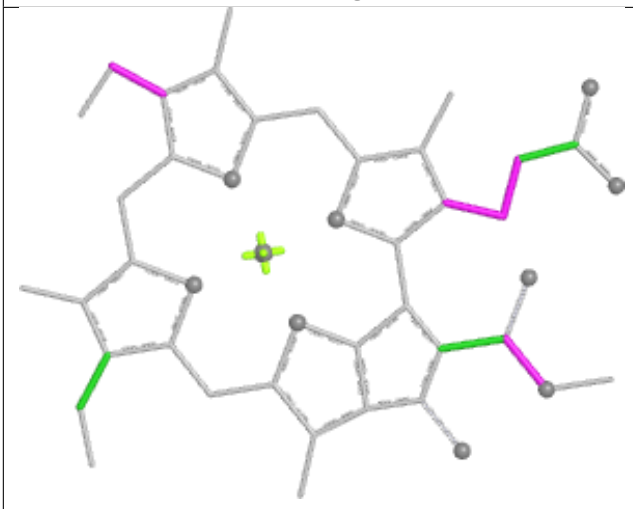


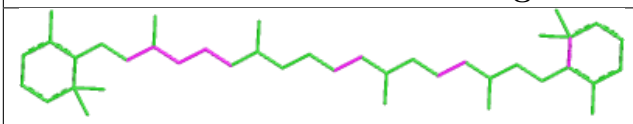
Bond angles



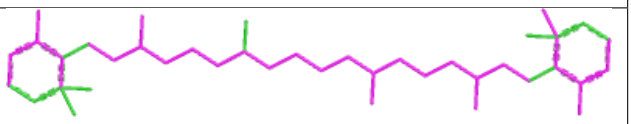
Torsions

Rings

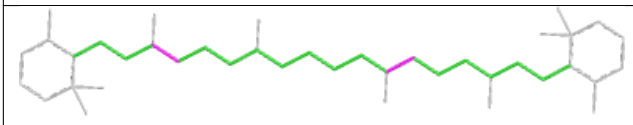
Ligand BCR B 4005



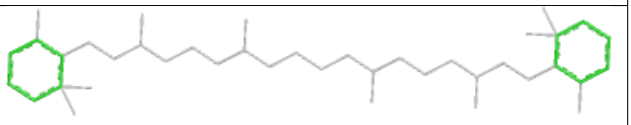
Bond lengths



Bond angles

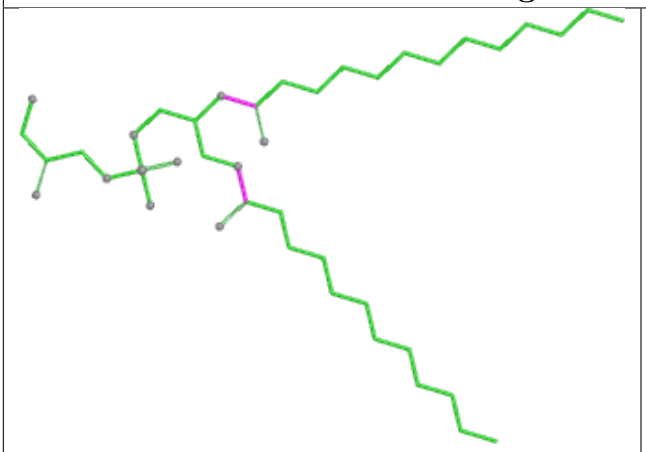


Torsions

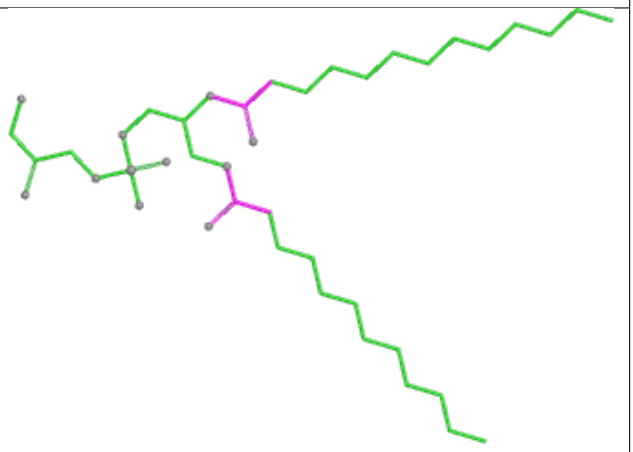


Rings

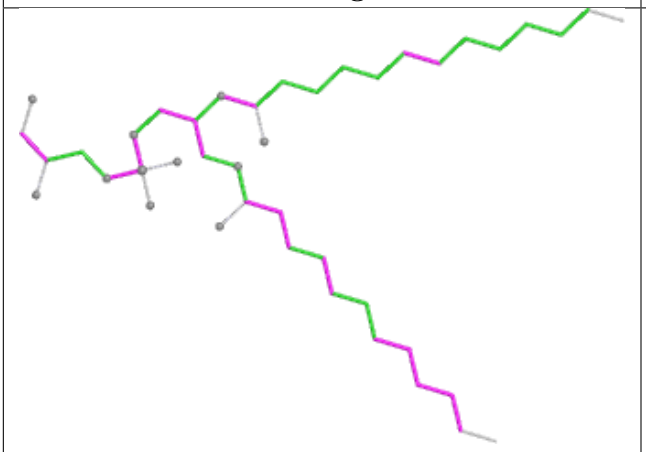
Ligand LHG a 5001



Bond lengths



Bond angles



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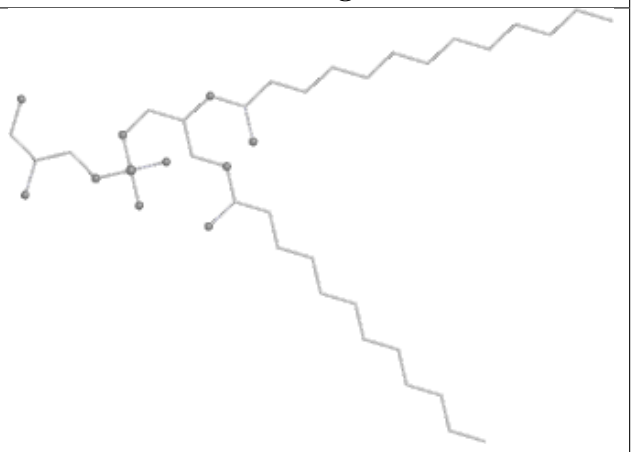
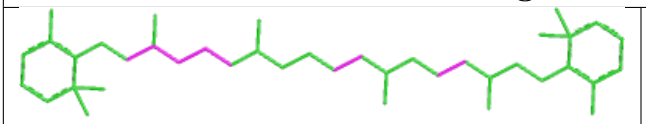


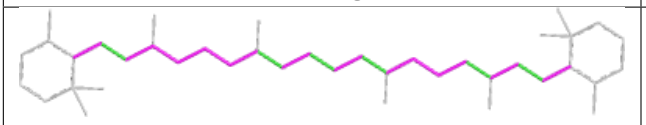
Rings

Ligand BCR b 4013



Bond lengths

Bond angles



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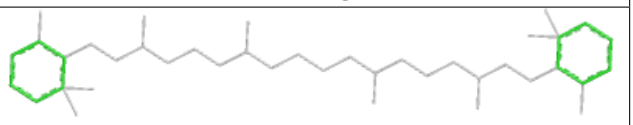
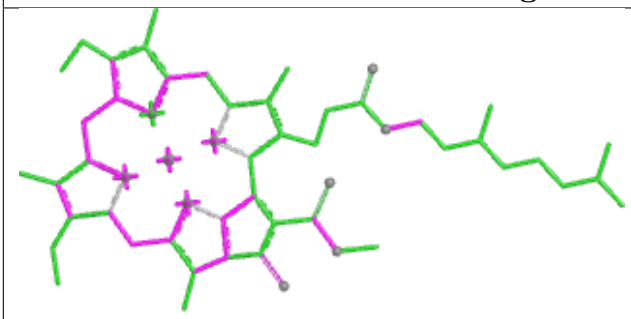


Rings

Ligand CLA a 1124



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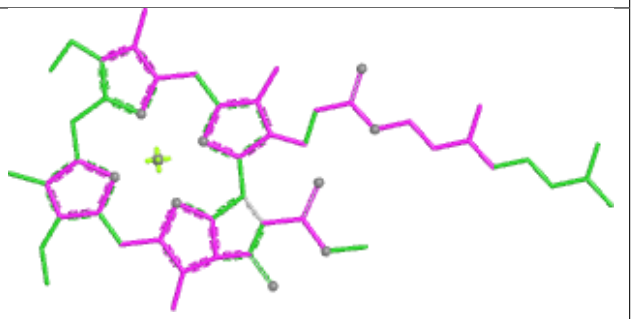
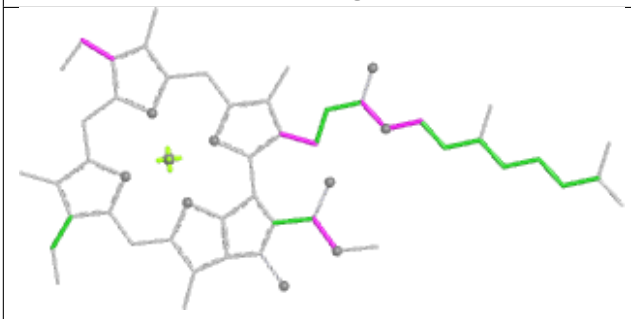
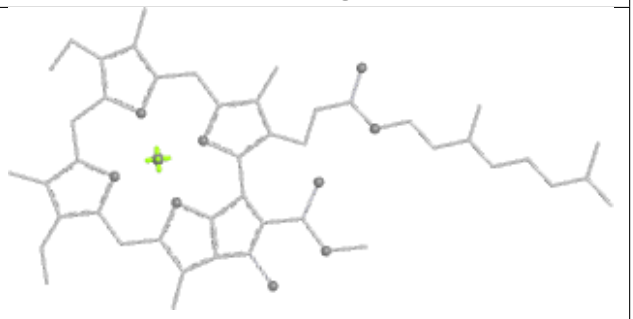


Bond angles

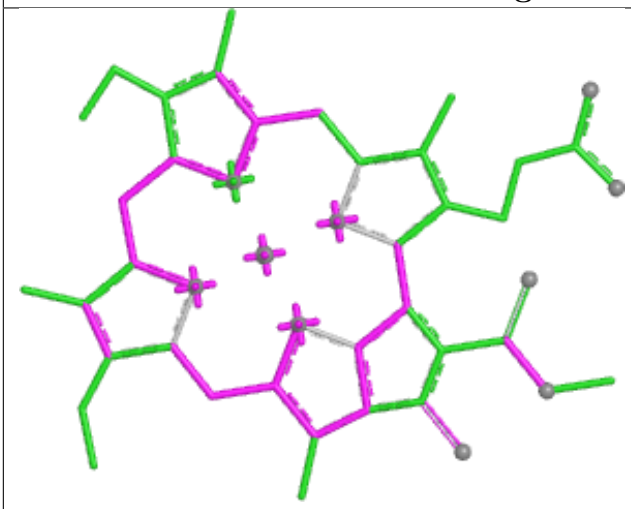


Torsions



Rings

Ligand CLA A 1109



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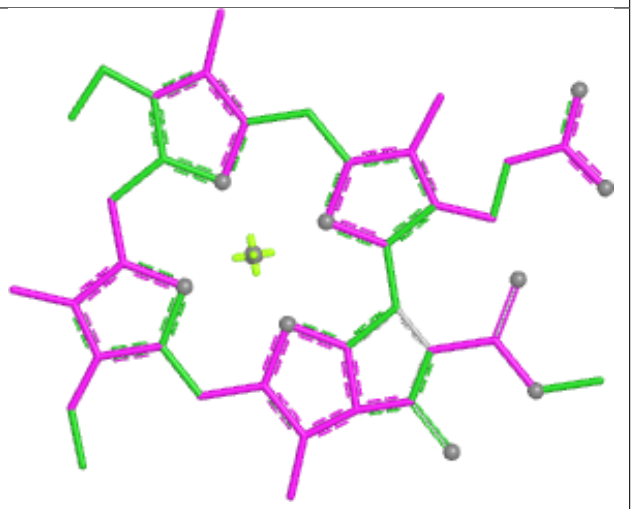
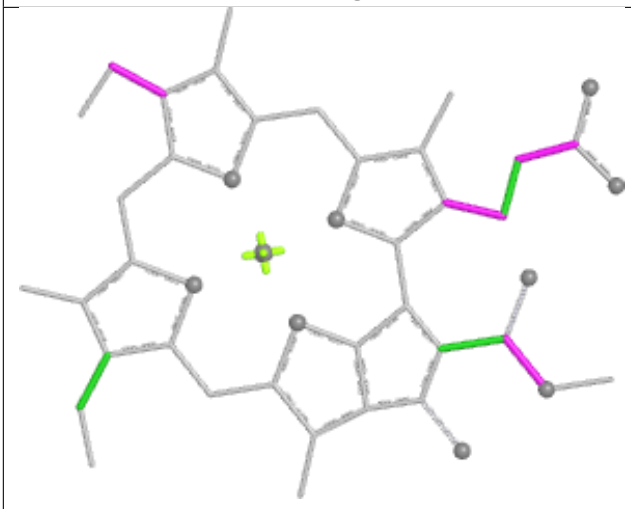


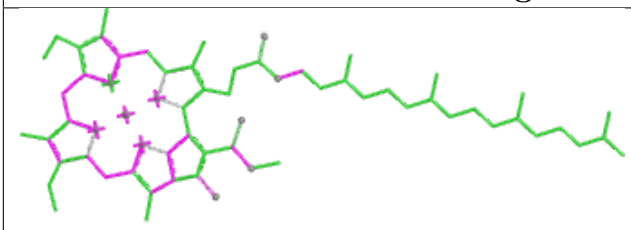
Bond angles



Torsions

Rings

Ligand CLA A 1104



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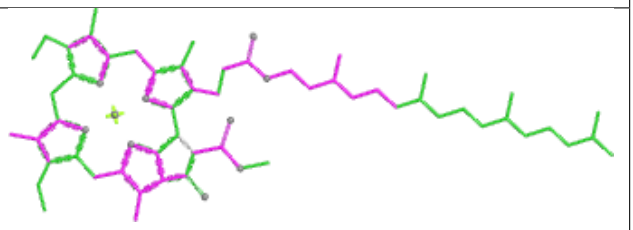
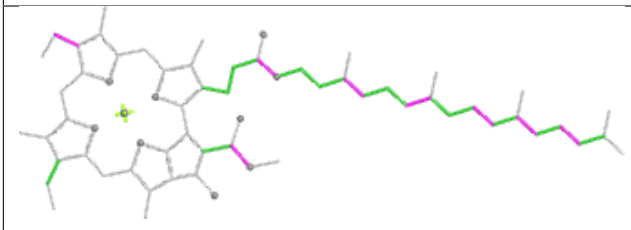
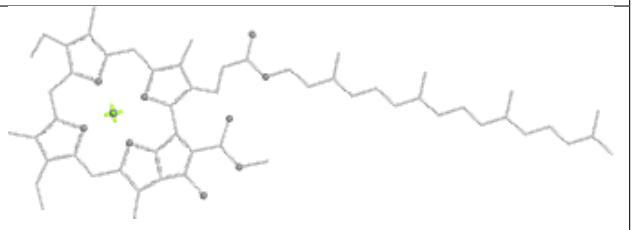


Bond angles

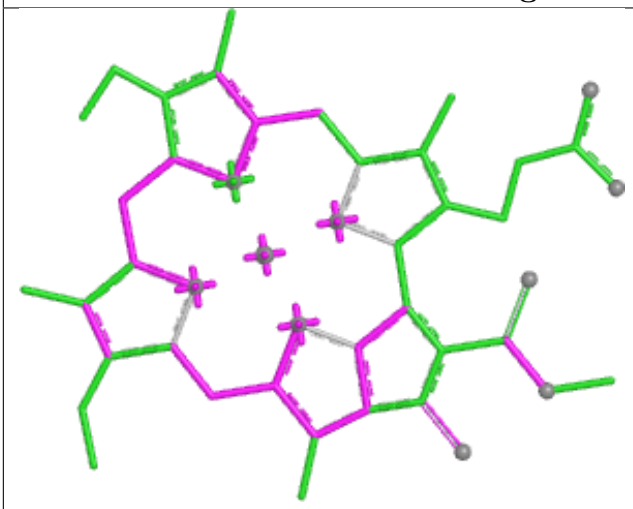


Torsions

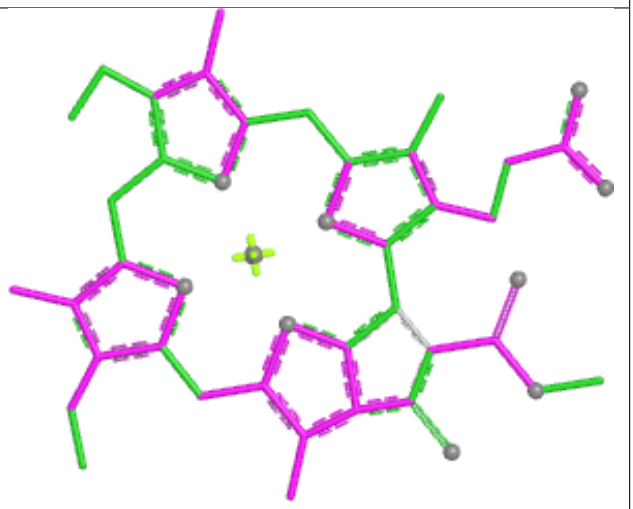


Rings

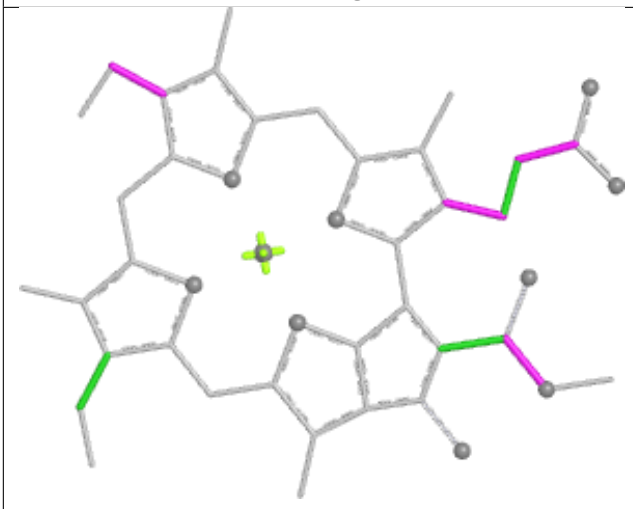
Ligand CLA a 1105



Bond lengths



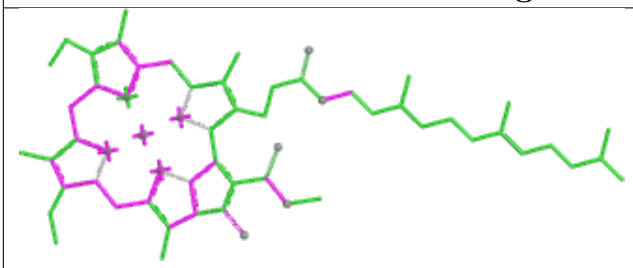
Bond angles



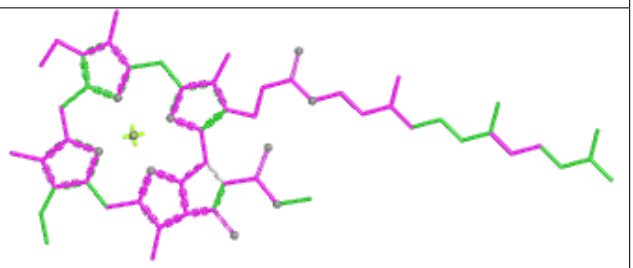
Torsions

Rings

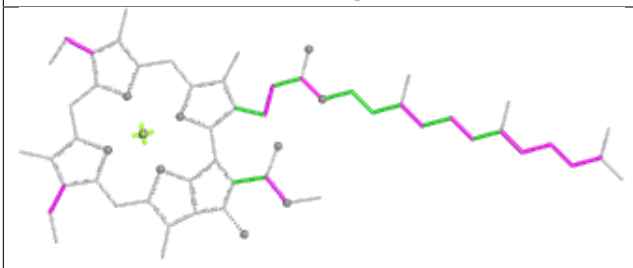
Ligand CLA B 1214



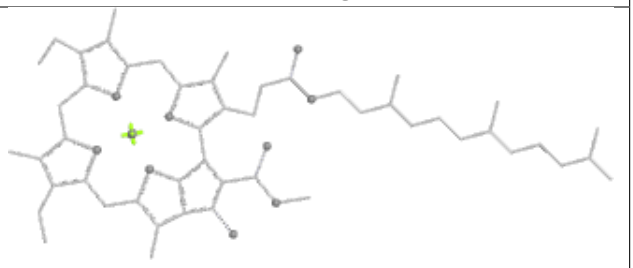
Bond lengths



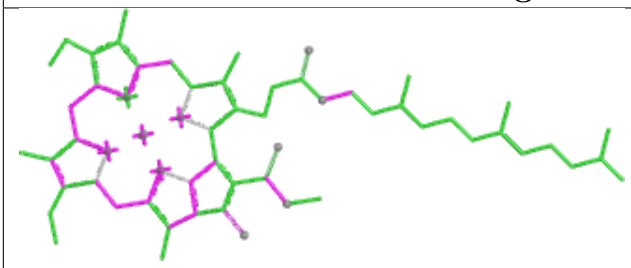
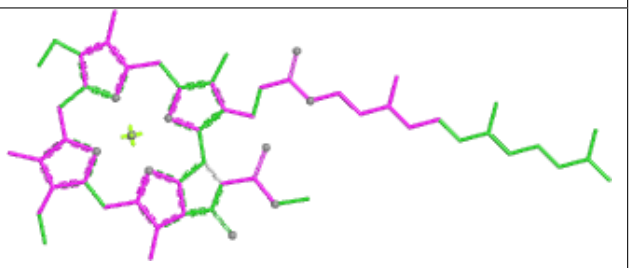
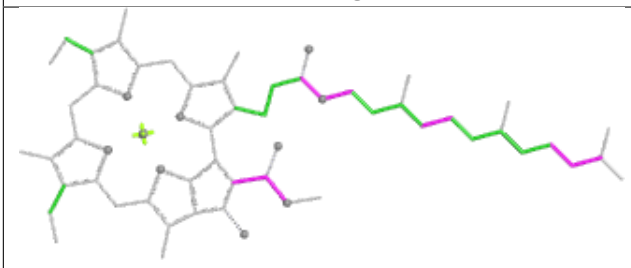
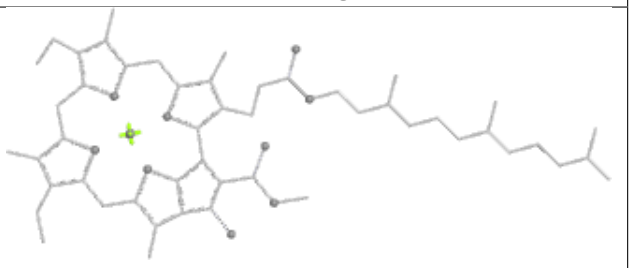
Bond angles

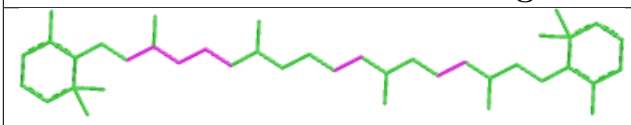
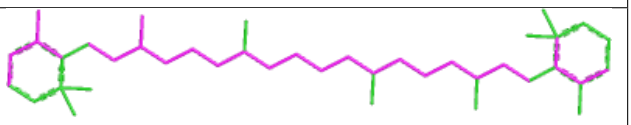
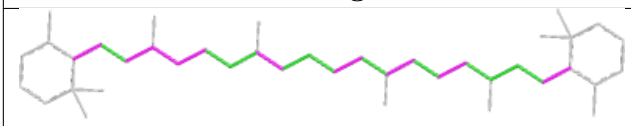
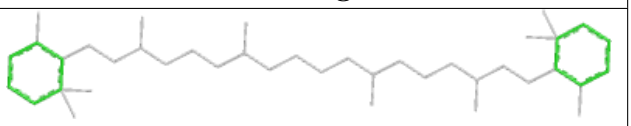


Torsions

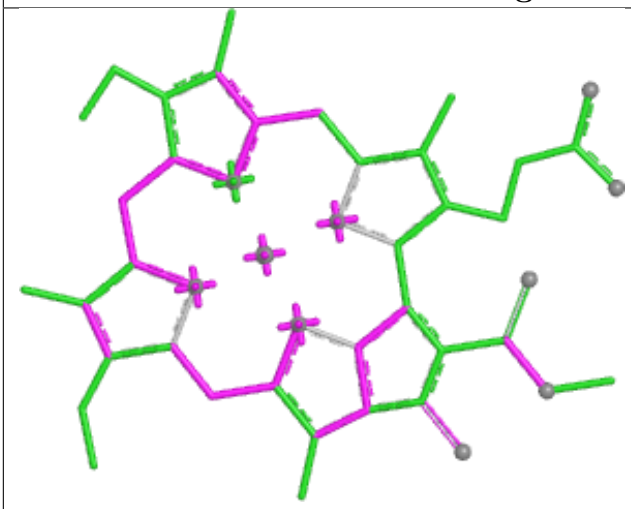


Rings

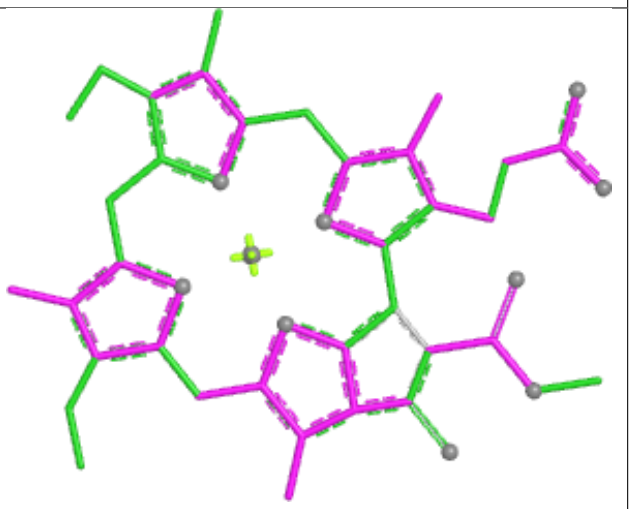
Ligand CLA A 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

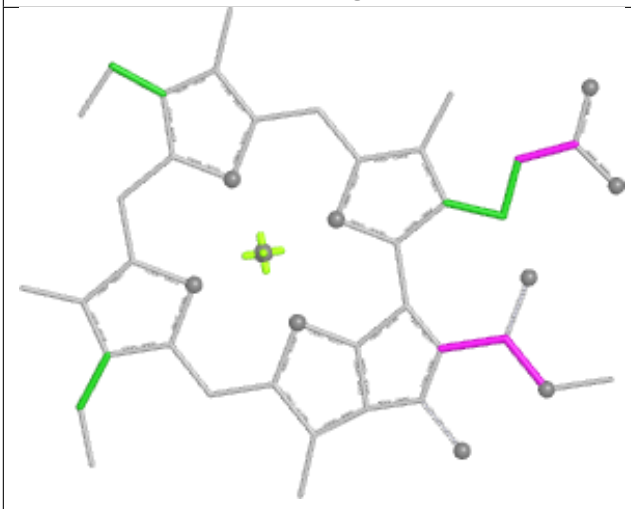
Ligand CLA B 1218



Bond lengths



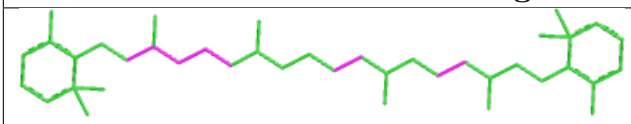
Bond angles



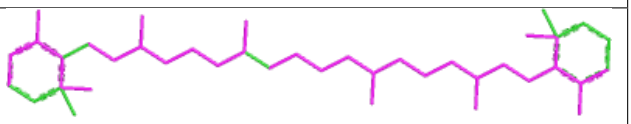
Torsions

Rings

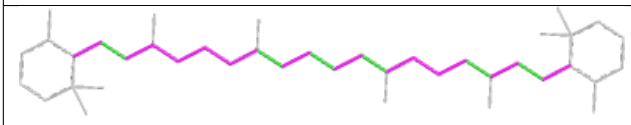
Ligand BCR B 4012



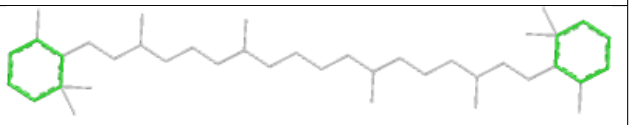
Bond lengths



Bond angles

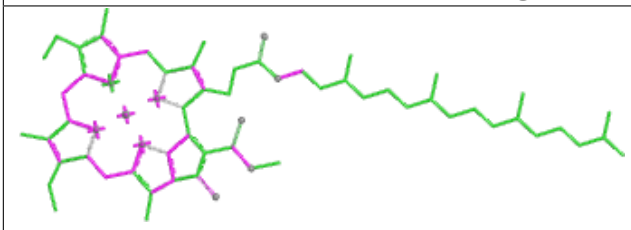


Torsions

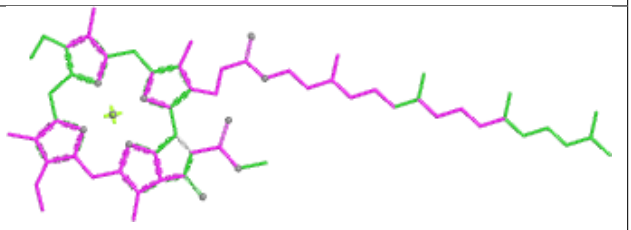


Rings

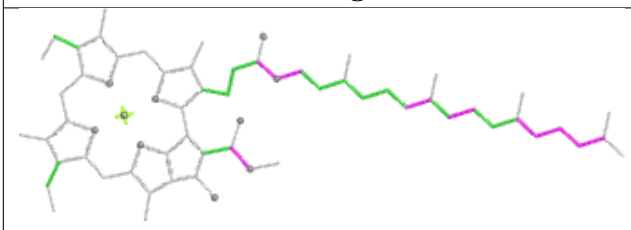
Ligand CLA H 1021



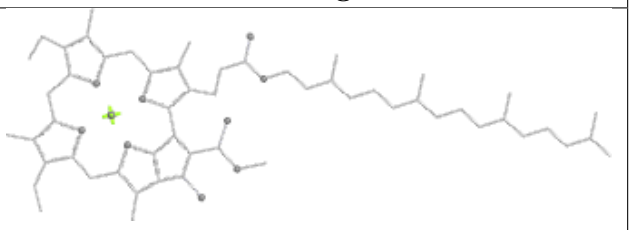
Bond lengths



Bond angles

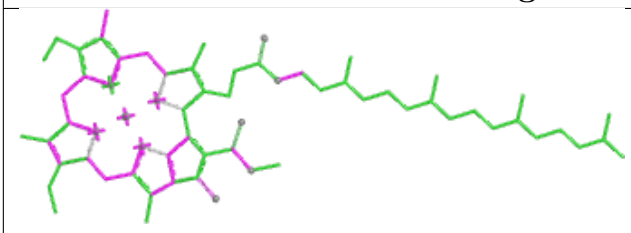


Torsions



Rings

Ligand CLA b 1226



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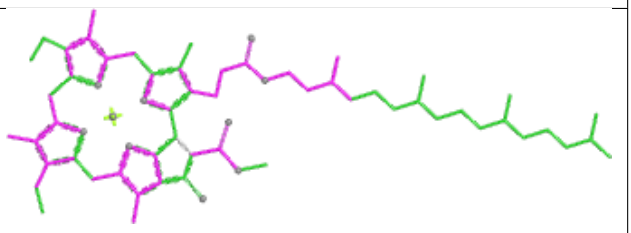
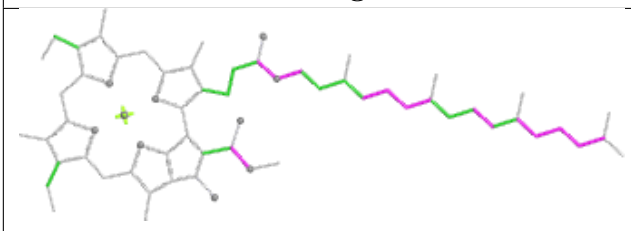


Bond angles



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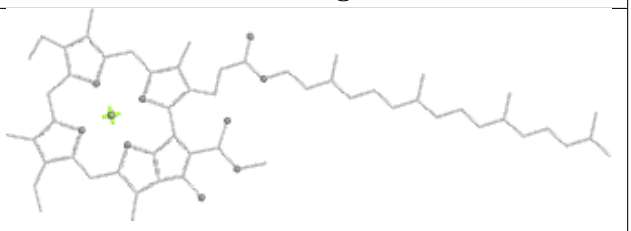
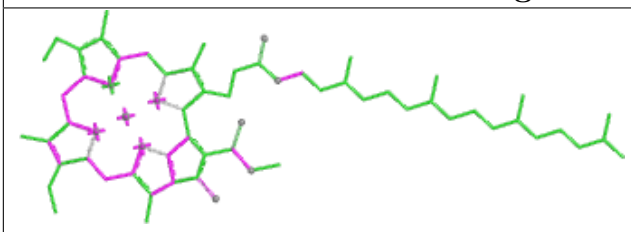
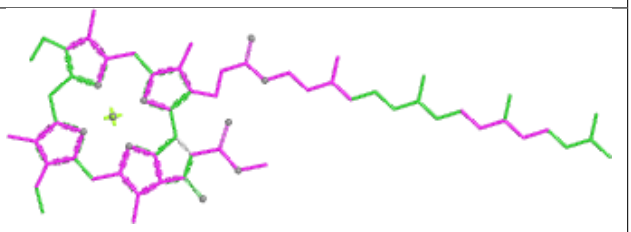


Rings

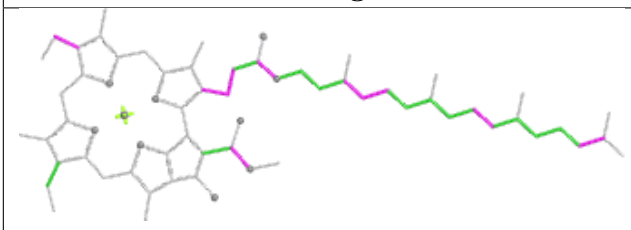
Ligand CLA H 1238



Bond lengths



Bond angles



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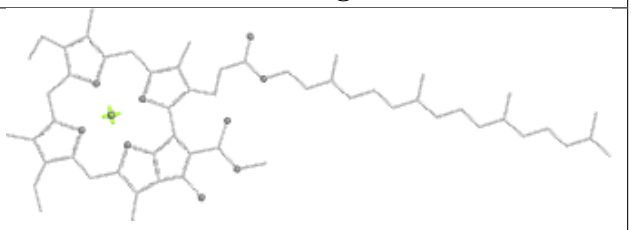
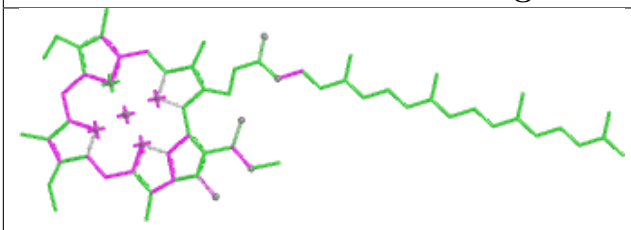
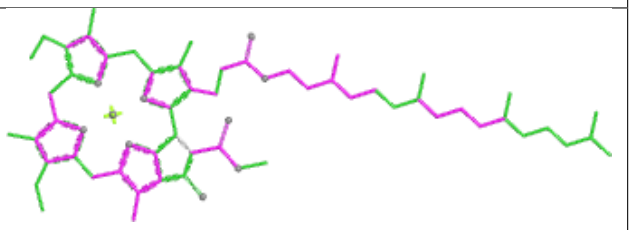
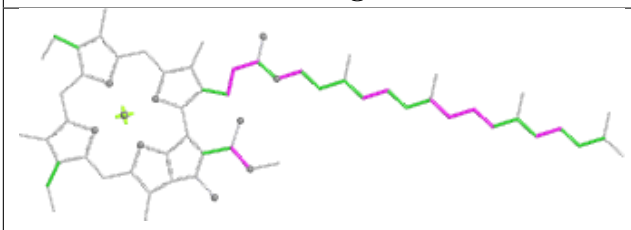
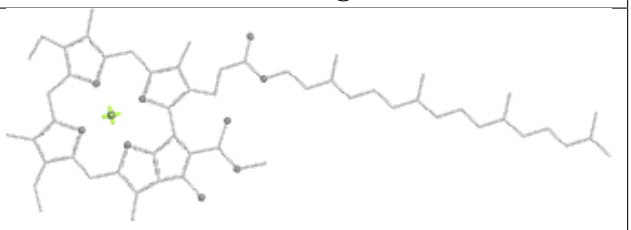
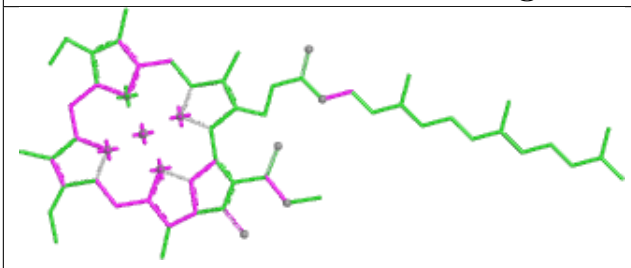
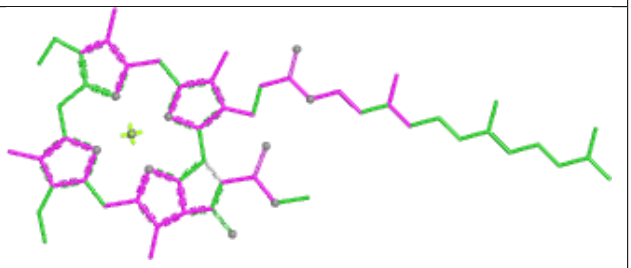
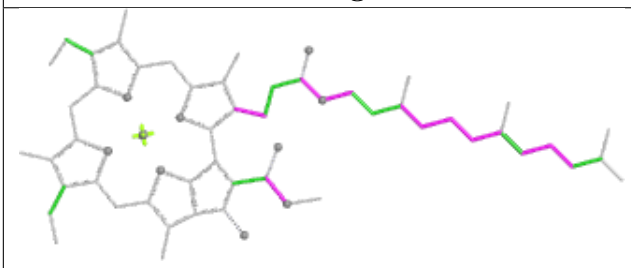
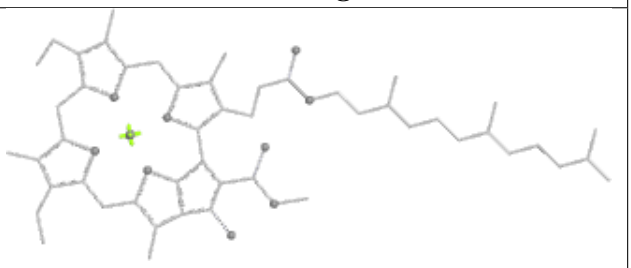
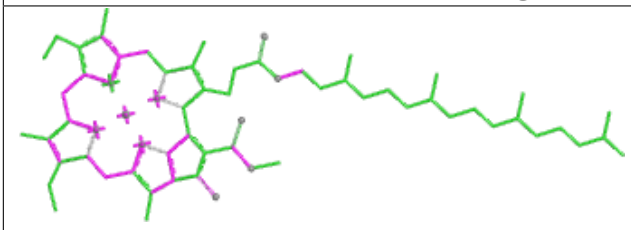


Rings

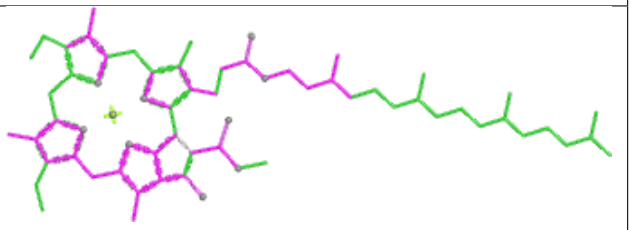
Ligand CLA U 1503	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1229	
	
Bond lengths	Bond angles
	
Torsions	Rings

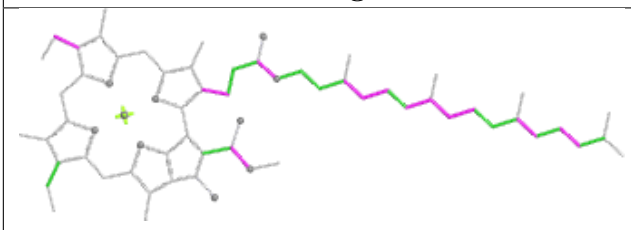
Ligand CLA H 1203



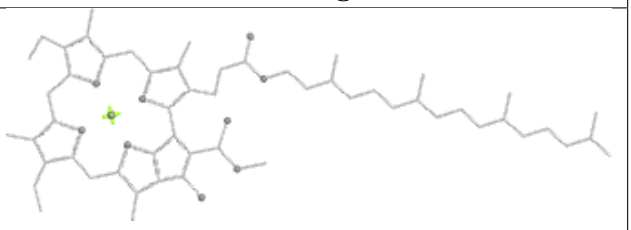
Bond lengths



Bond angles

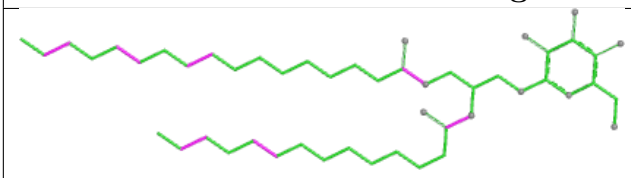


Torsions



Rings

Ligand LMG U 5007



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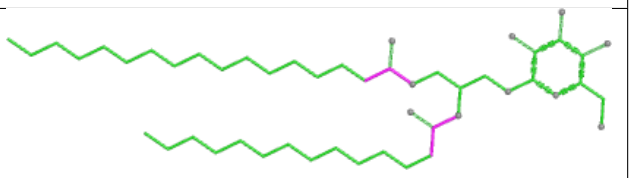
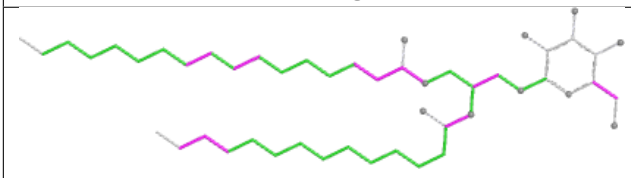


Bond angles



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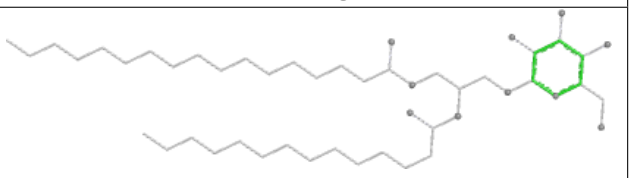
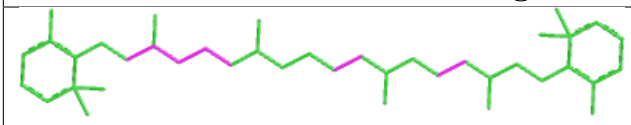


Rings

Ligand BCR G 4003



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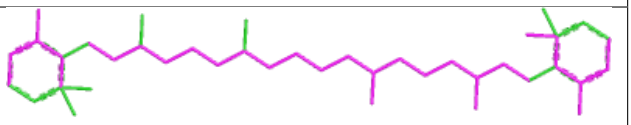
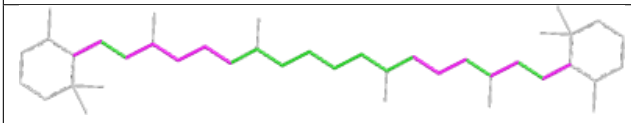
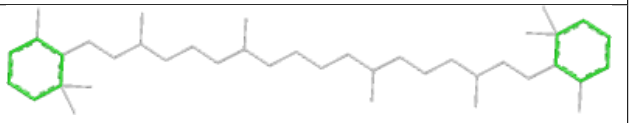


Bond angles

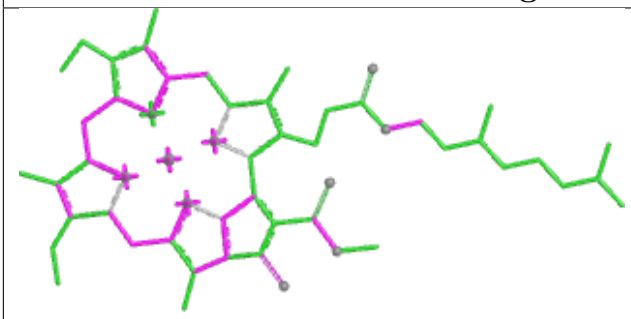


Torsions



Rings

Ligand CLA a 1116



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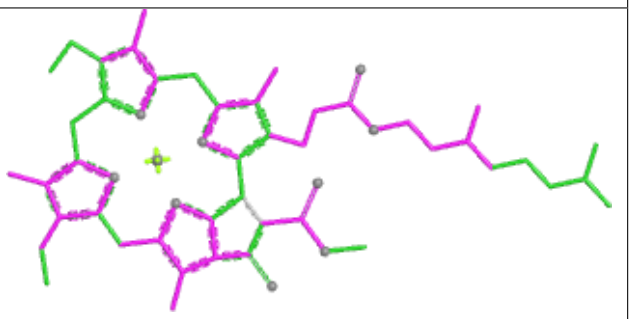
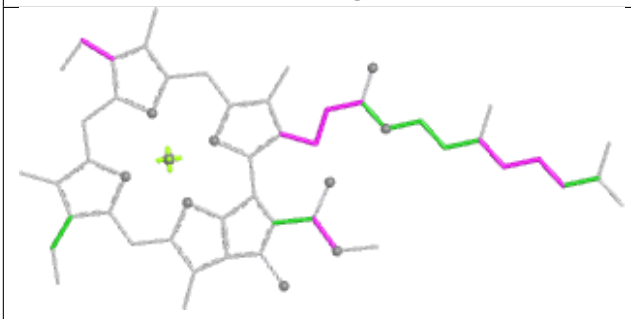


Bond angles



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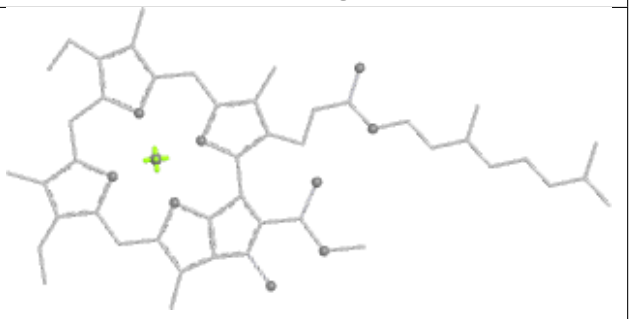
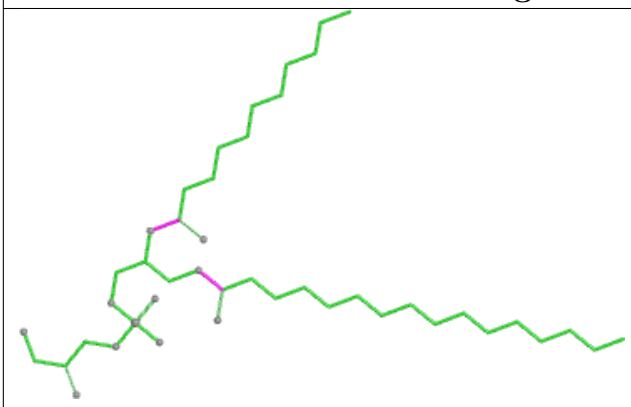


Rings

Ligand LHG B 5004



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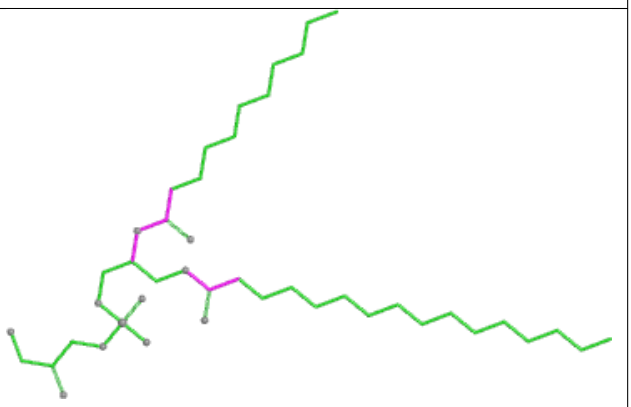
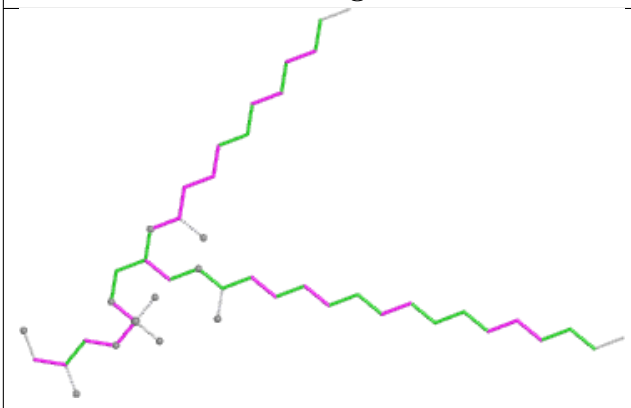
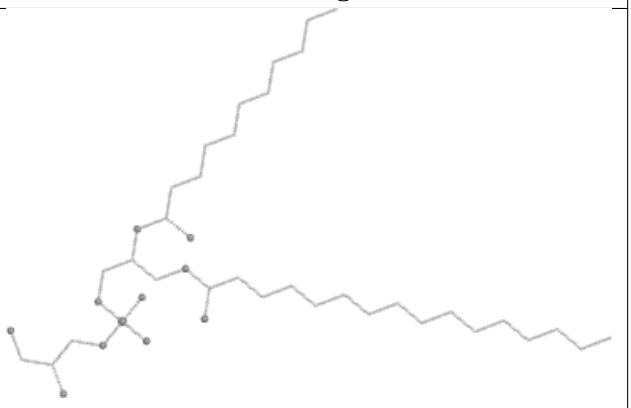


Bond angles

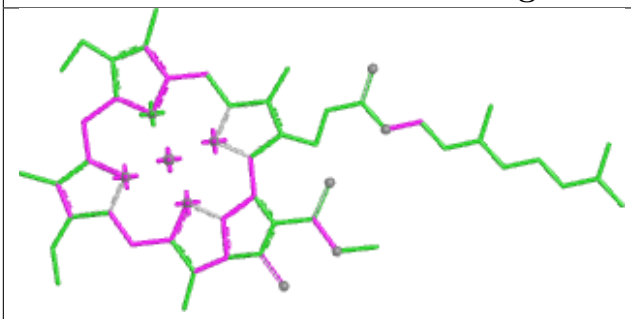


Torsions

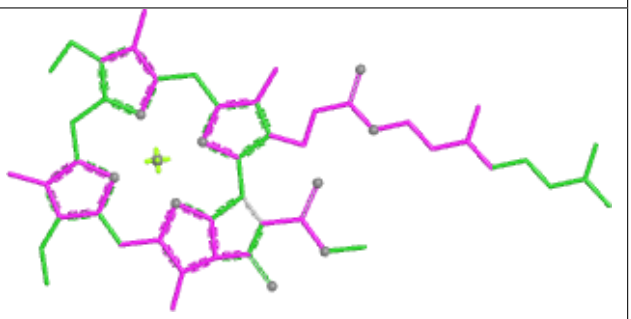


Rings

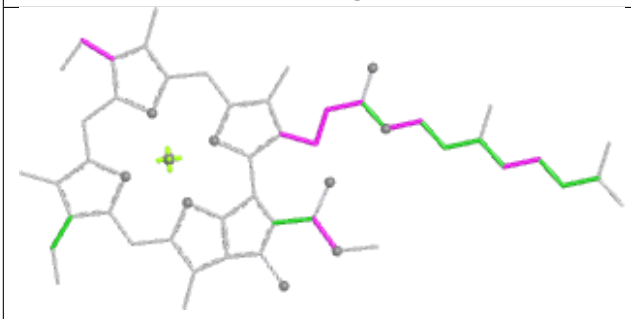
Ligand CLA b 1217



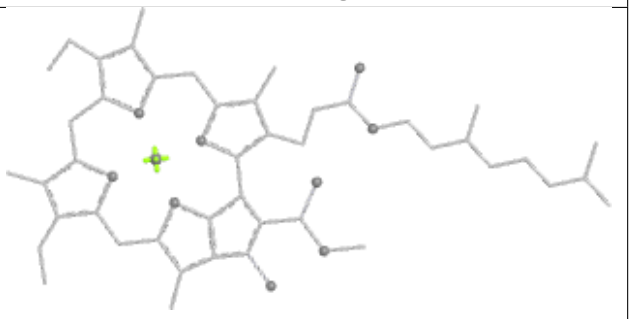
Bond lengths



Bond angles

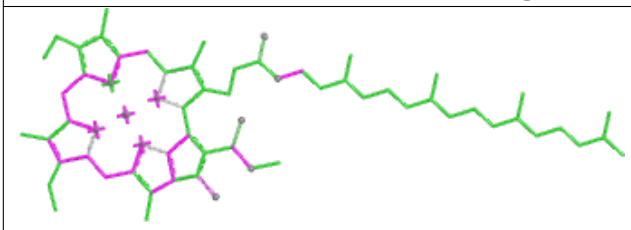


Torsions

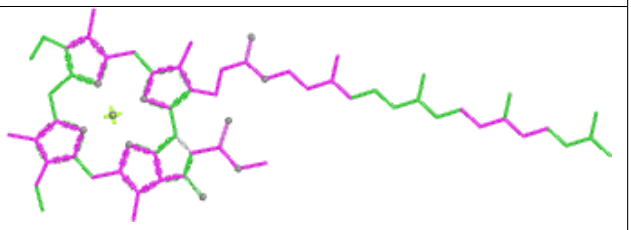


Rings

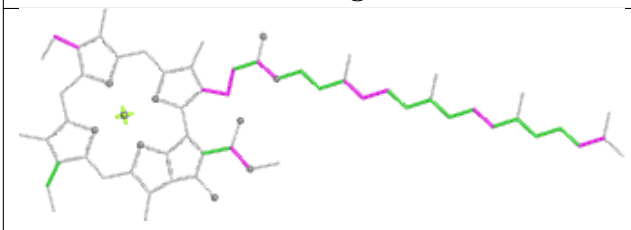
Ligand CLA b 1238



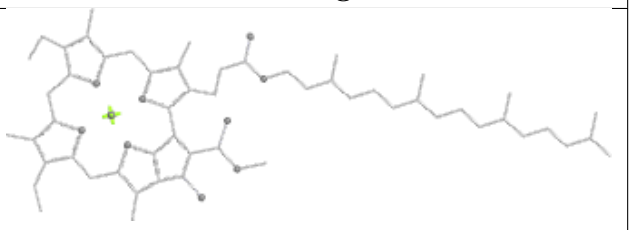
Bond lengths



Bond angles

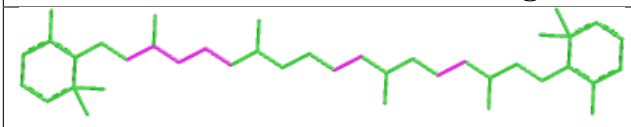


Torsions

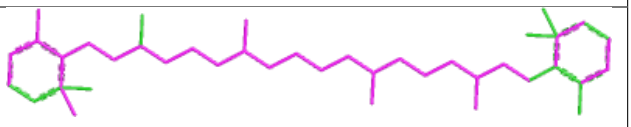


Rings

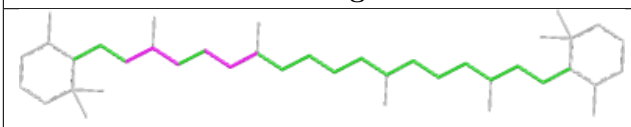
Ligand BCR l 4022



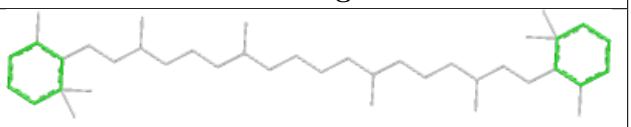
Bond lengths



Bond angles

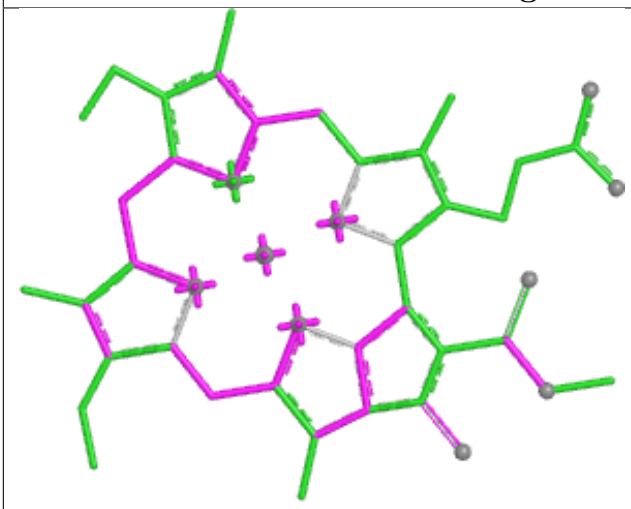


Torsions

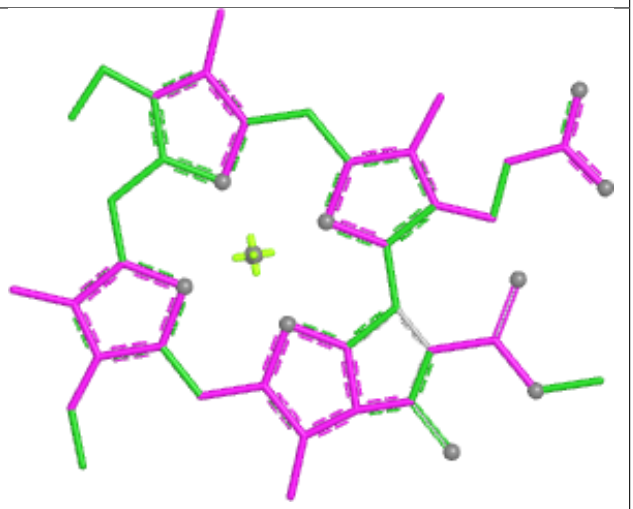


Rings

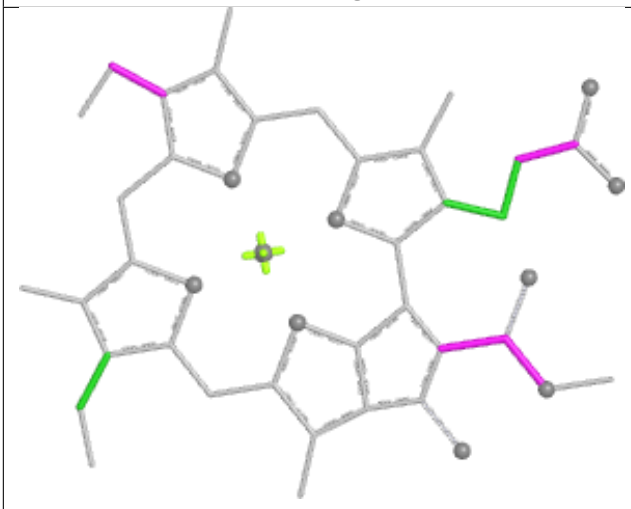
Ligand CLA a 1101



Bond lengths



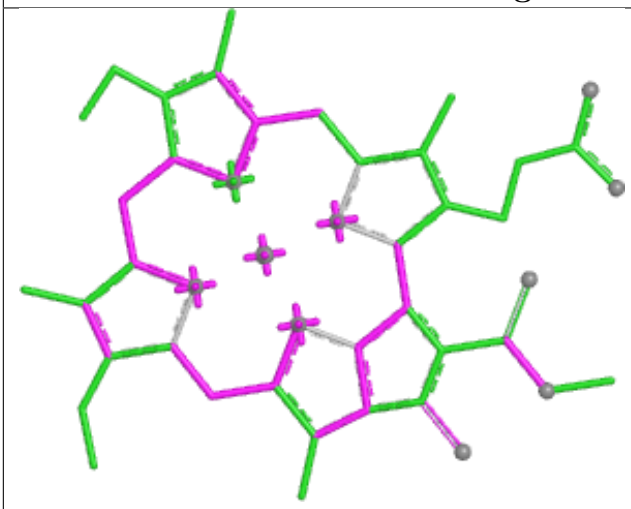
Bond angles



Torsions

Rings

Ligand CLA G 1110



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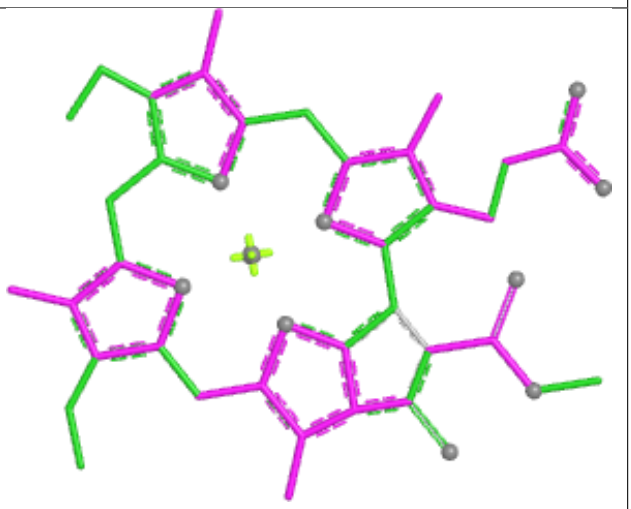
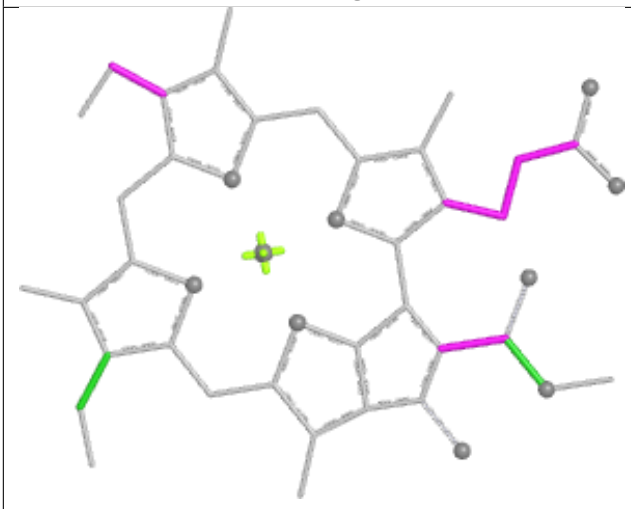


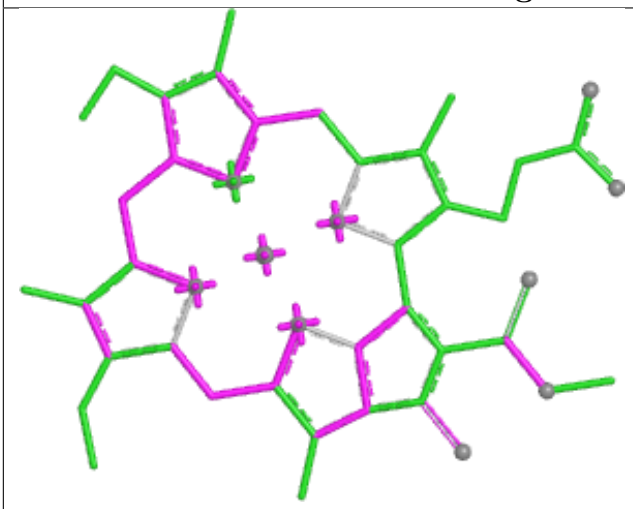
Bond angles



Torsions

Rings

Ligand CLA B 1236



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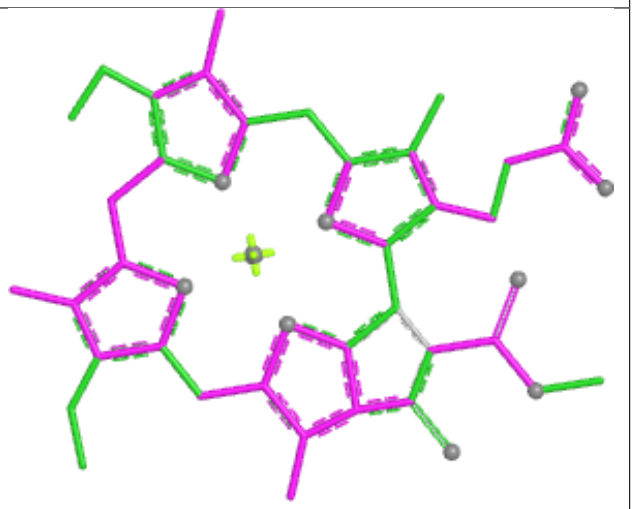
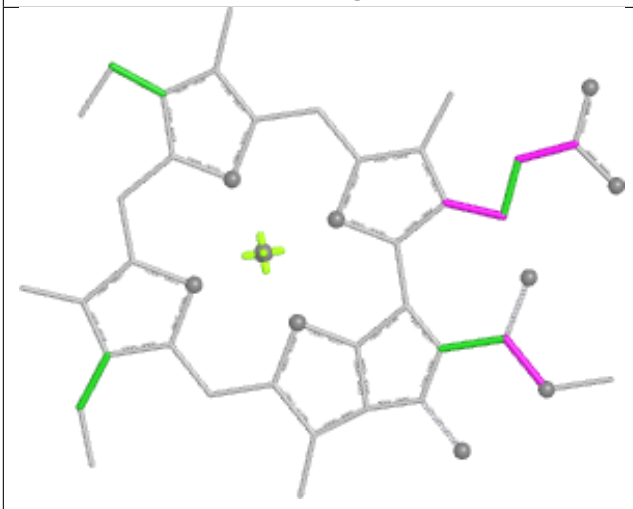


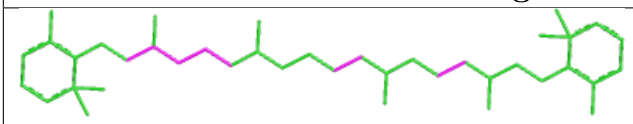
Bond angles



Torsions

Rings

Ligand BCR U 4022



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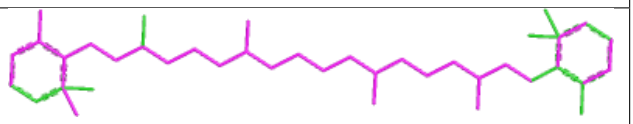
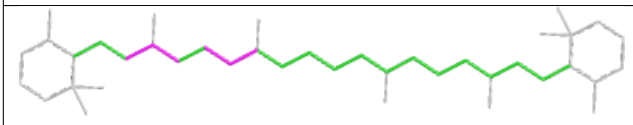
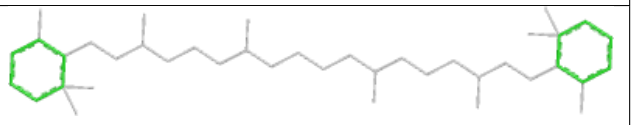


Bond angles

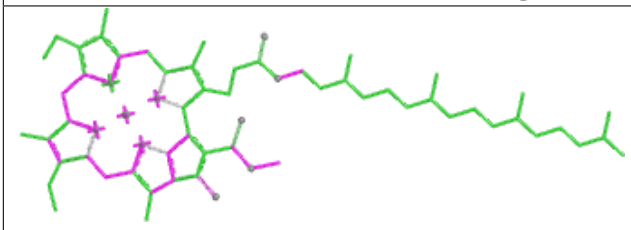


Torsions



Rings

Ligand CLA A 1012



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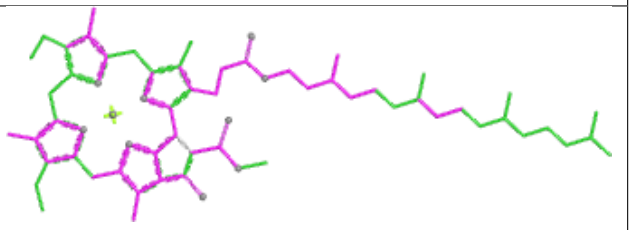
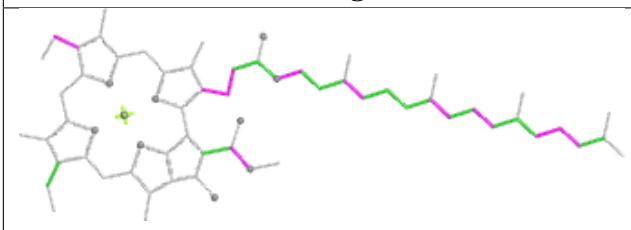
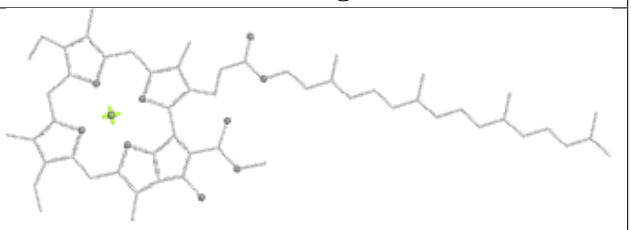


Bond angles

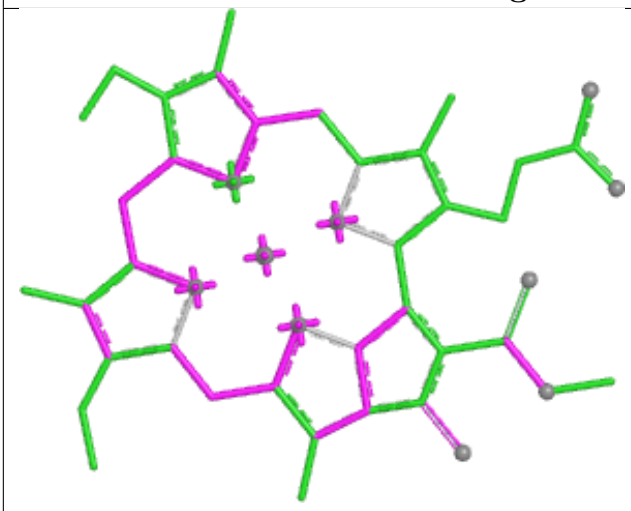


Torsions



Rings

Ligand CLA W 1701



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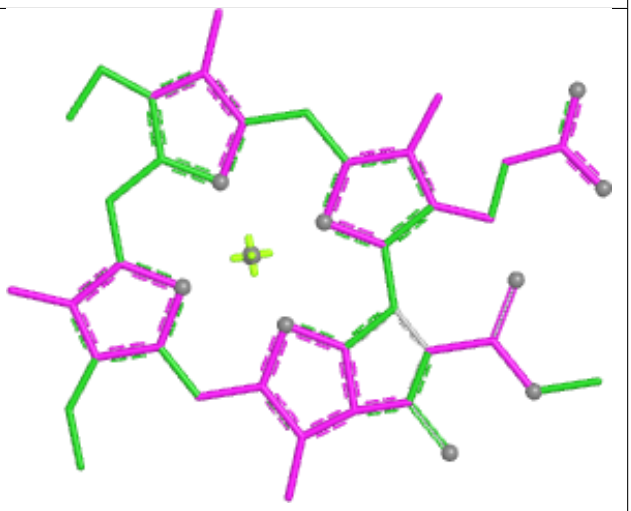
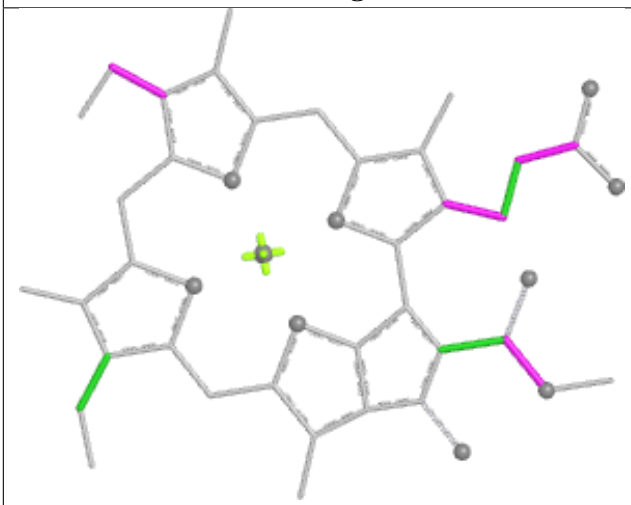


Bond angles



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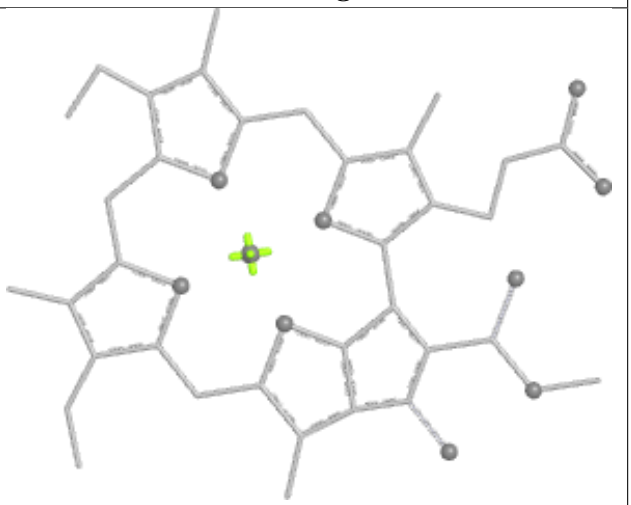
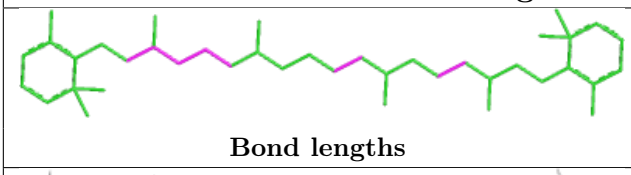


Rings

Ligand BCR b 4006



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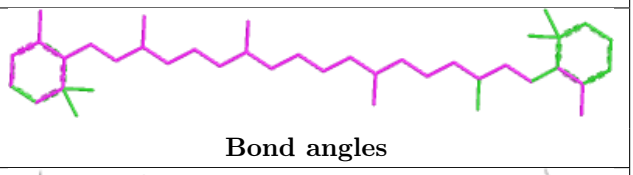
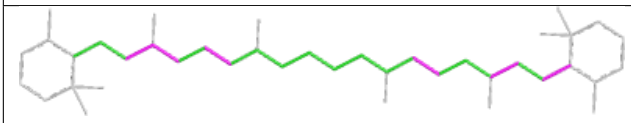
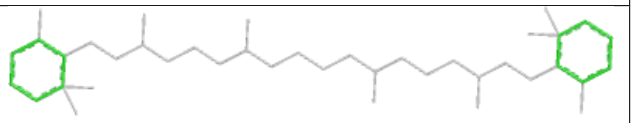


Bond angles

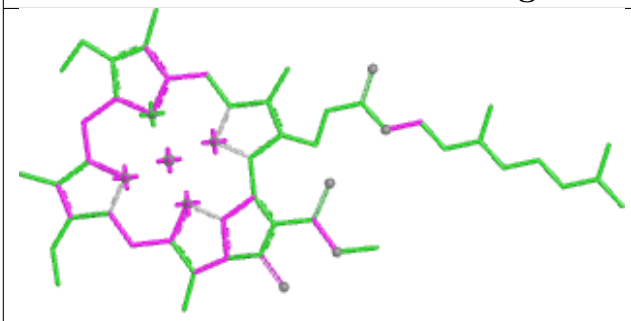


Torsions



Rings

Ligand CLA b 1220



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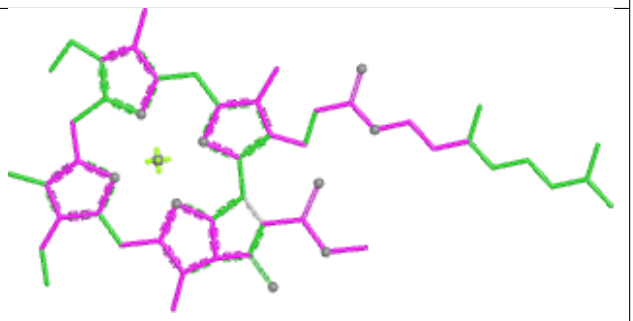
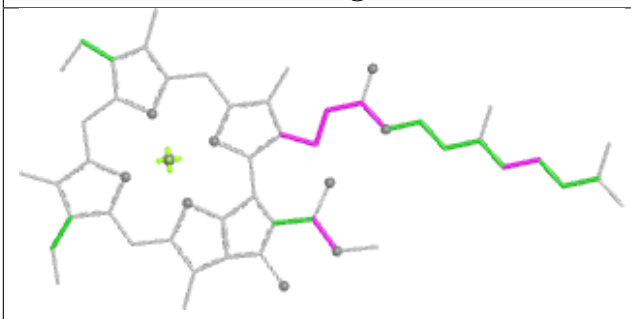


Bond angles



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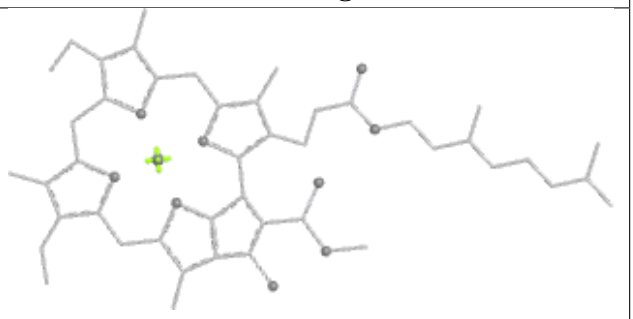
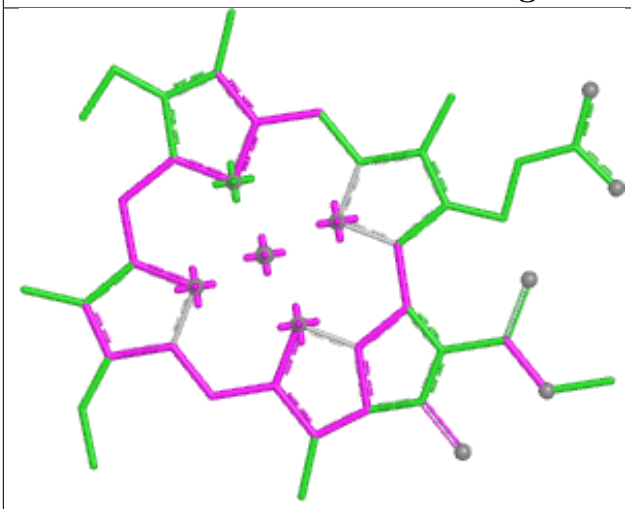


Rings

Ligand CLA k 1401



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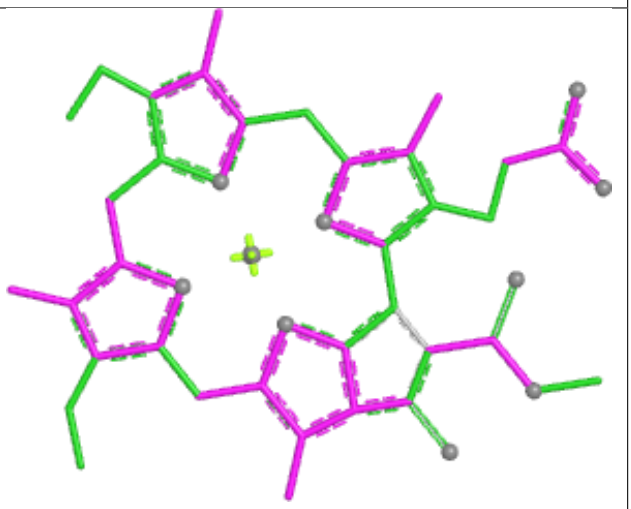
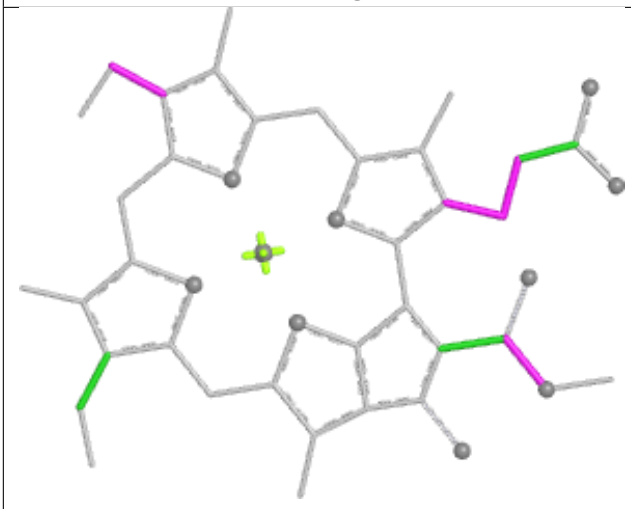


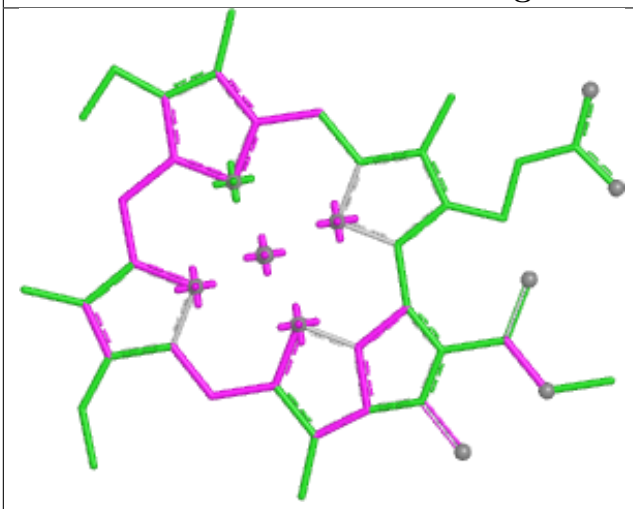
Bond angles



Torsions

Rings

Ligand CLA G 1139



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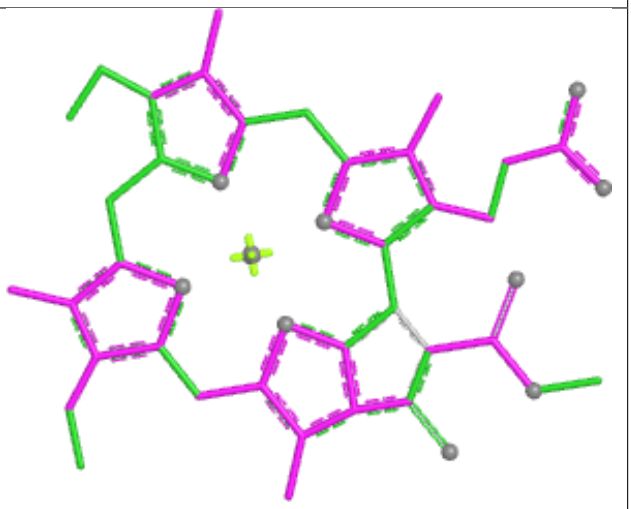
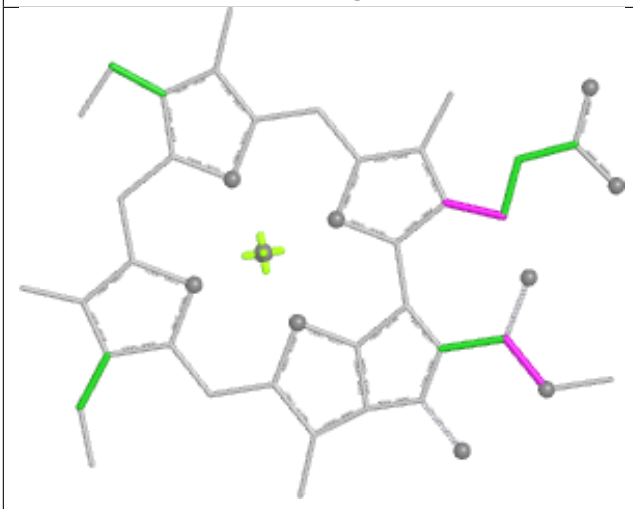


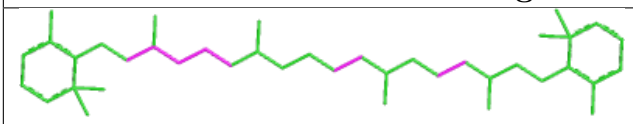
Bond angles



Torsions

Rings

Ligand BCR L 4019



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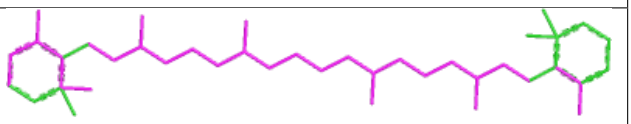
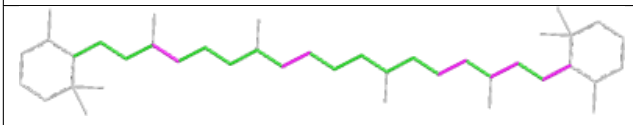
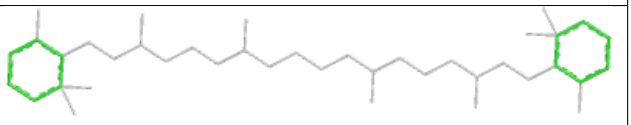


Bond angles

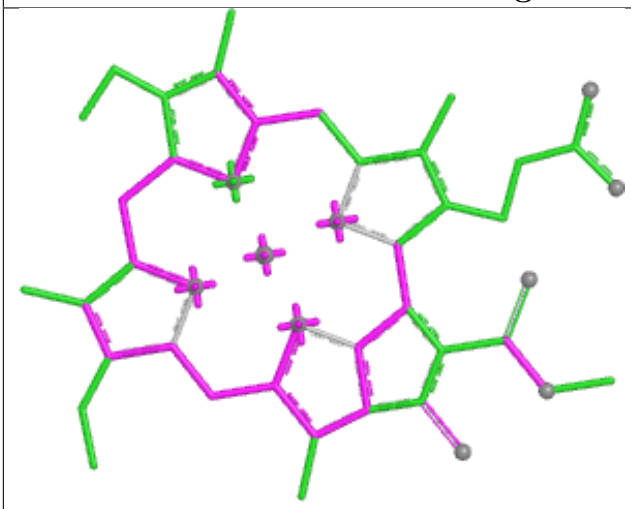


Torsions



Rings

Ligand CLA A 1114



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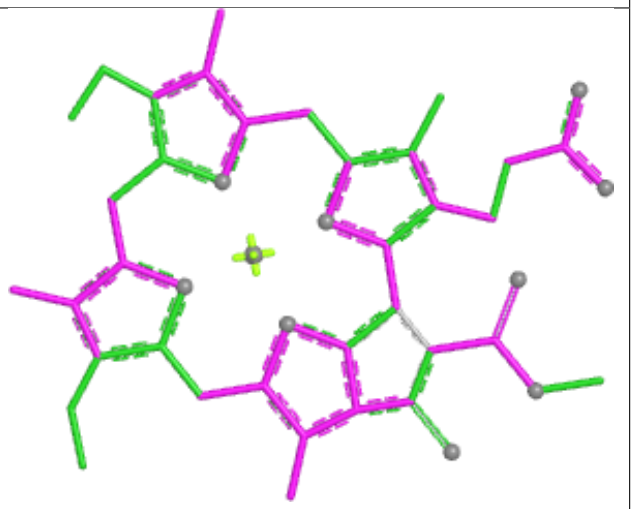
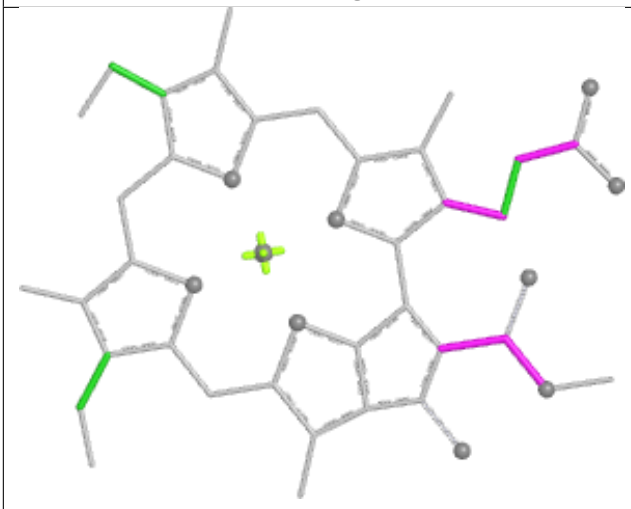


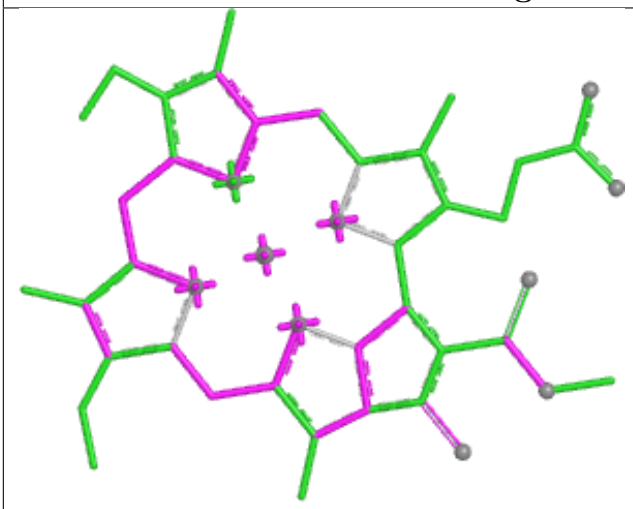
Bond angles



Torsions

Rings

Ligand CLA A 1113



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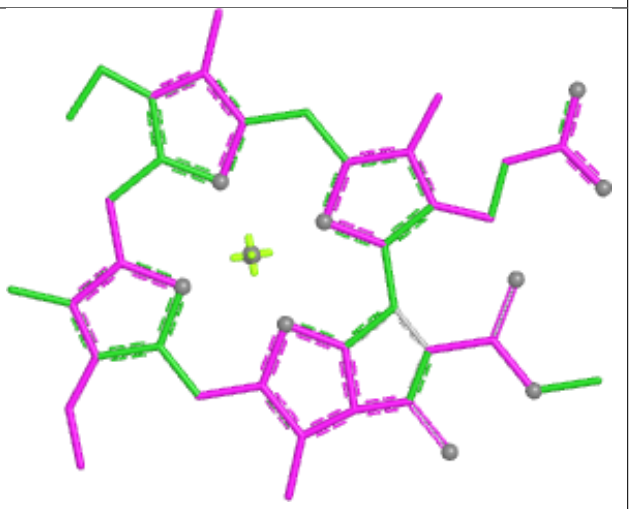
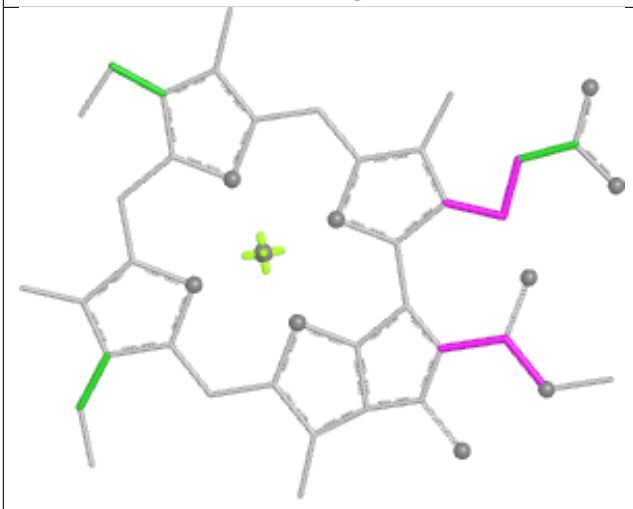


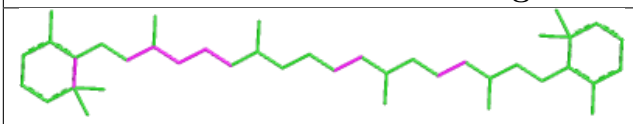
Bond angles



Torsions

Rings

Ligand BCR G 4011



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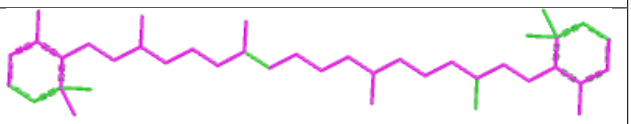
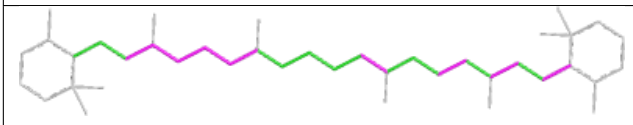
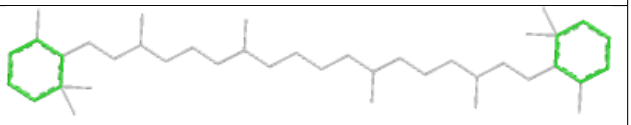


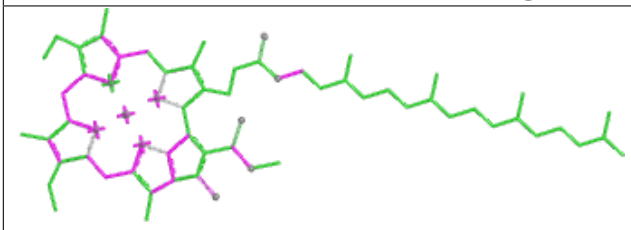
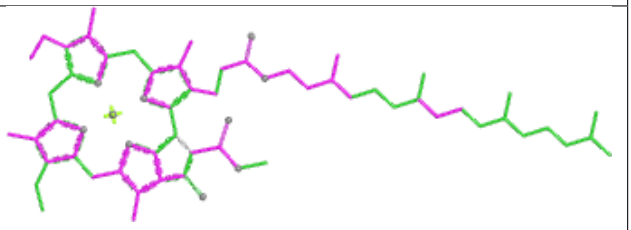
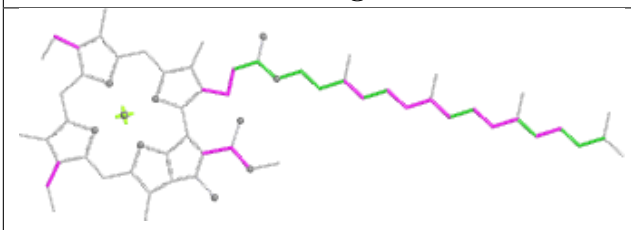
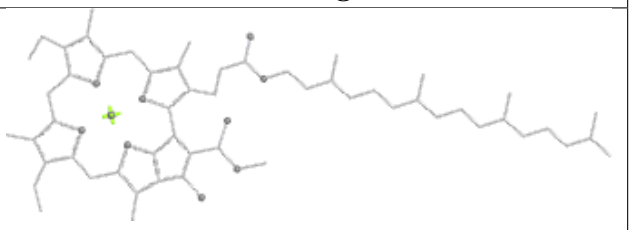
Bond angles



Torsions



Rings

Ligand CLA a 1132	
 Bond lengths	 Bond angles
 Torsions	 Rings

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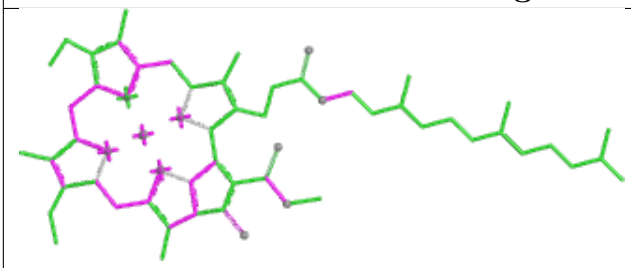
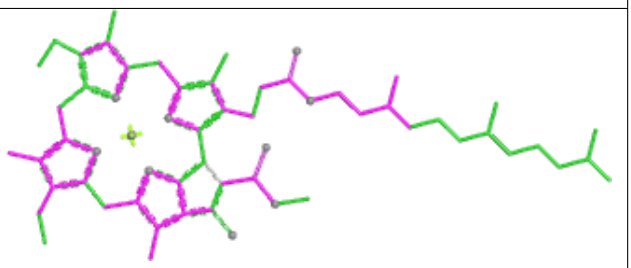
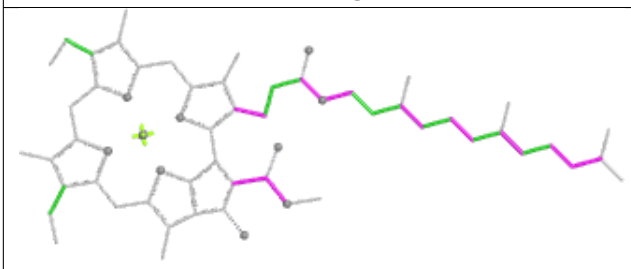
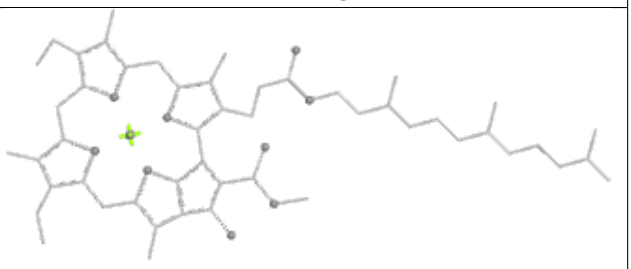
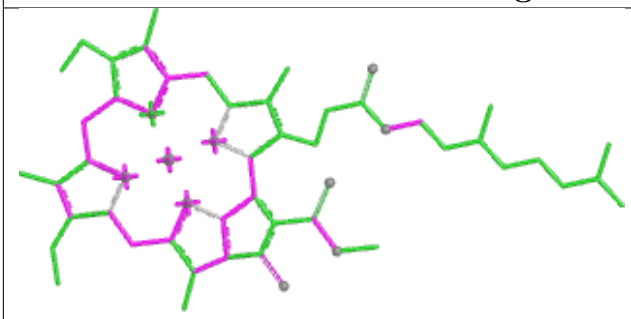
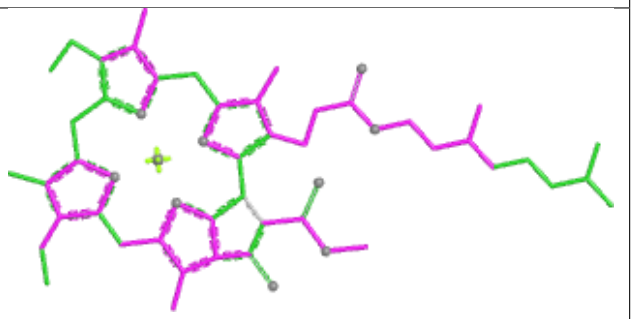
 Bond lengths	 Bond angles
 Torsions	 Rings

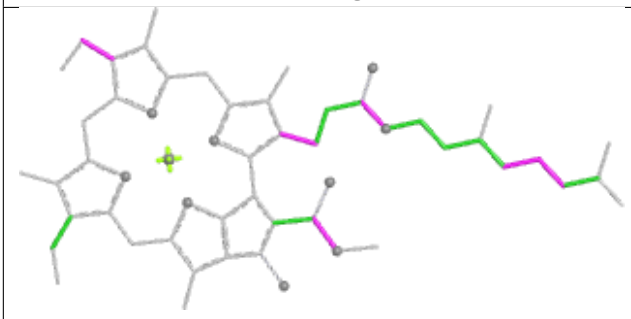
Ligand CLA A 1122



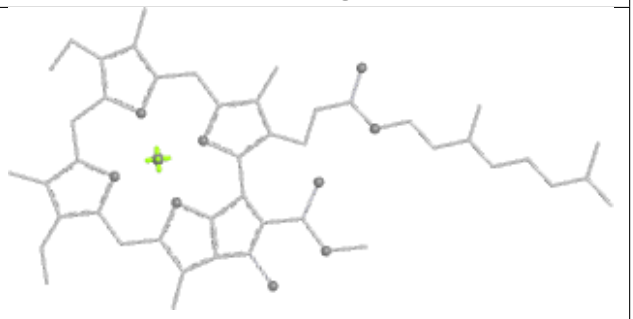
Bond lengths



Bond angles

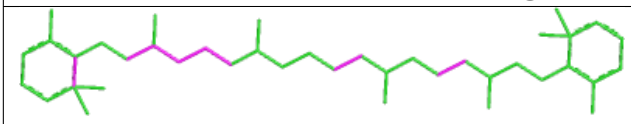


Torsions



Rings

Ligand BCR i 4018



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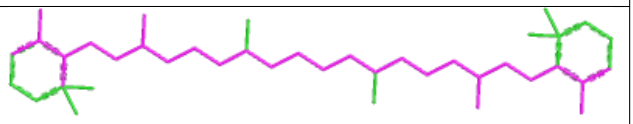
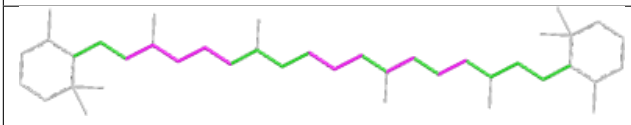
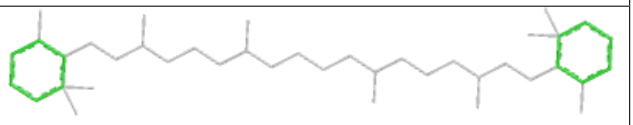


Bond angles

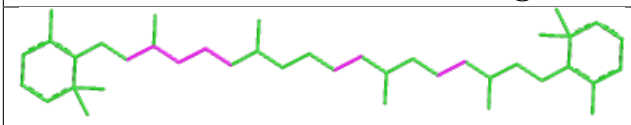


Torsions



Rings

Ligand BCR B 4013



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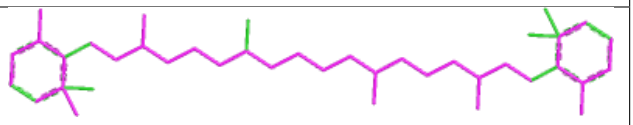
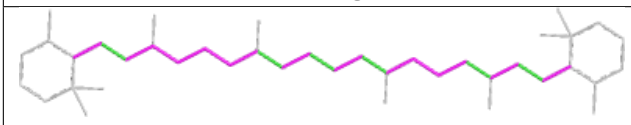


Bond angles



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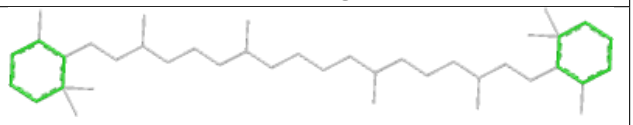
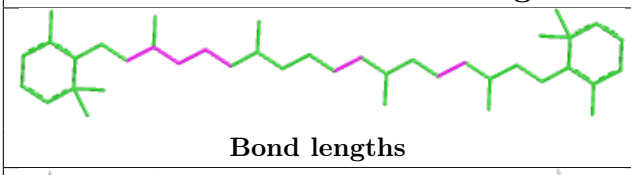


Rings

Ligand BCR B 4014



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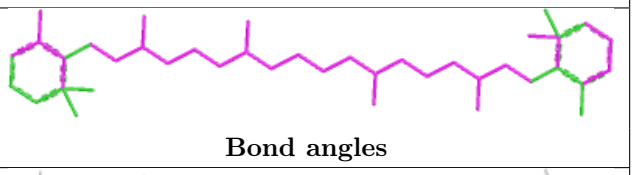
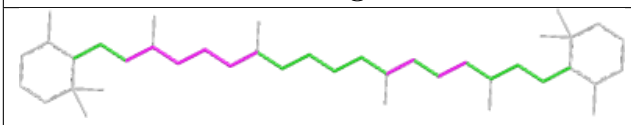


Bond angles



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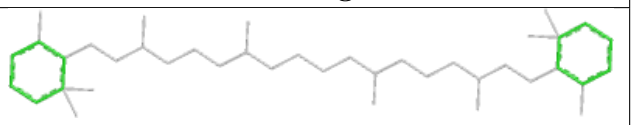
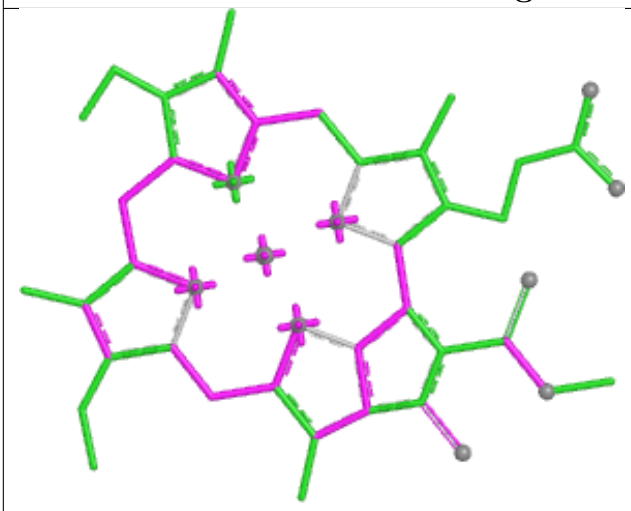


Rings

Ligand CLA B 1212



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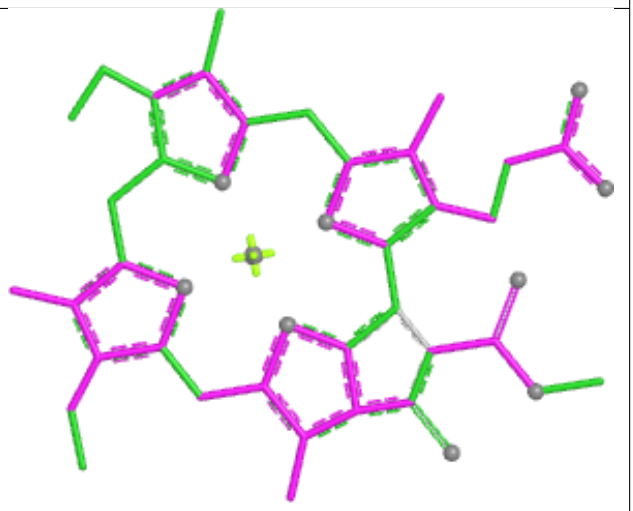
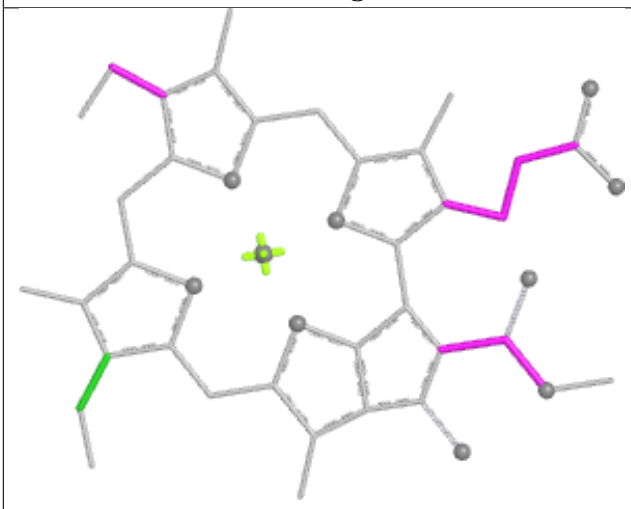


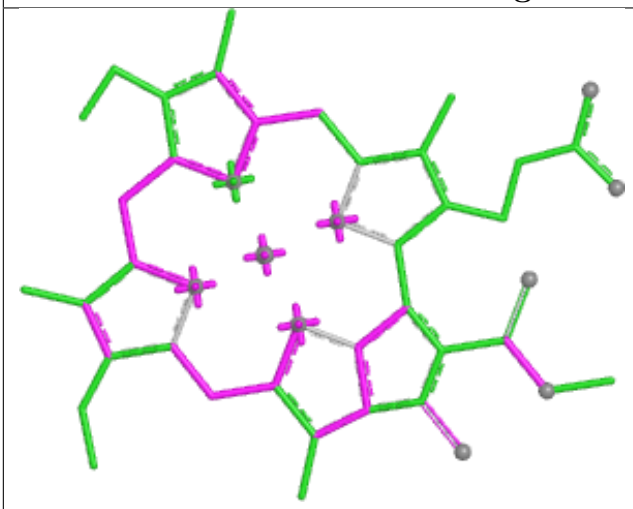
Bond angles



Torsions

Rings

Ligand CLA G 1113



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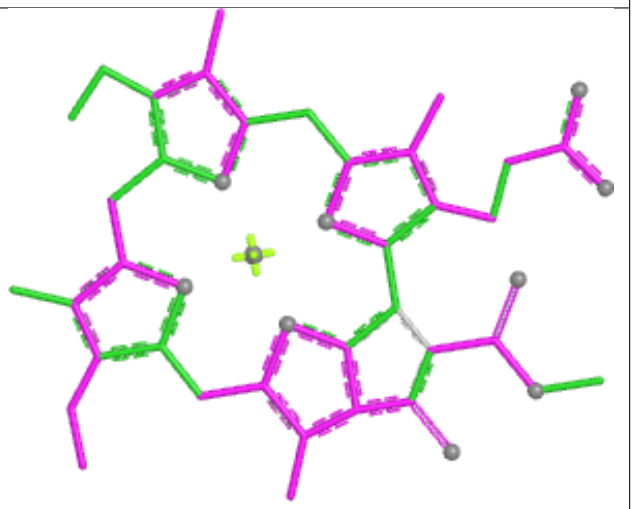

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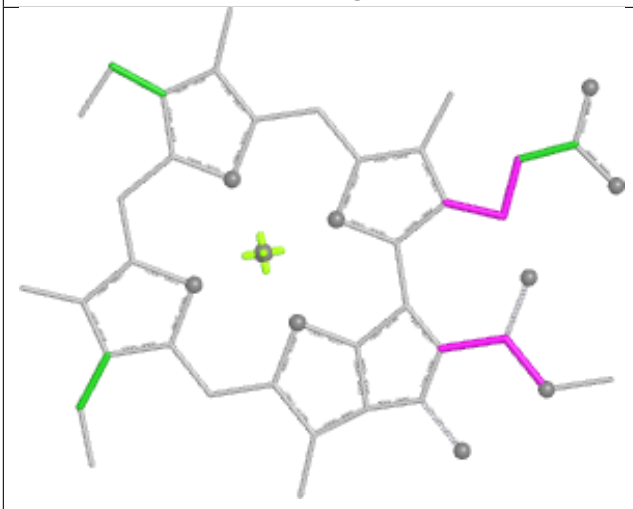
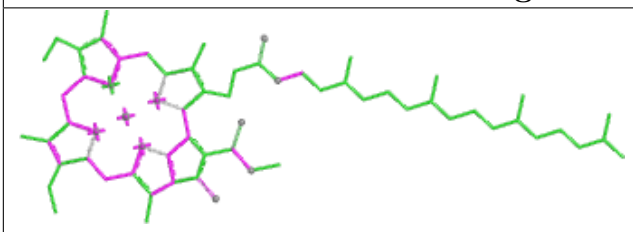


Torsions

Rings

Ligand CLA A 1127



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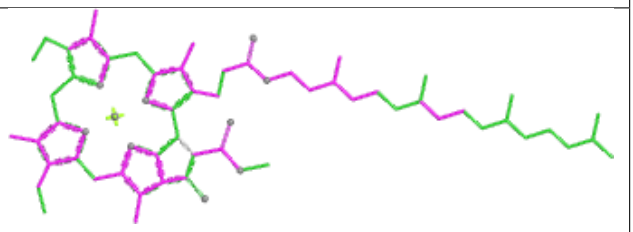

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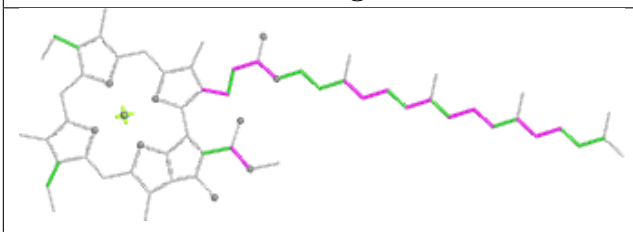

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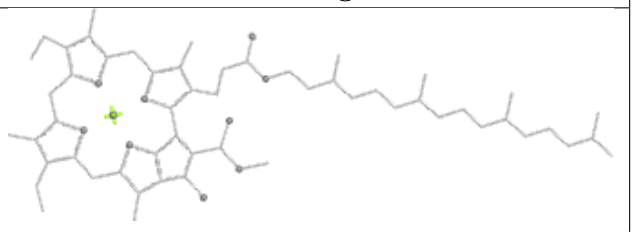
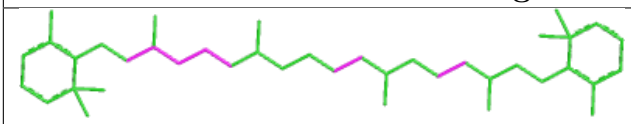


Rings

Ligand BCR A 4003



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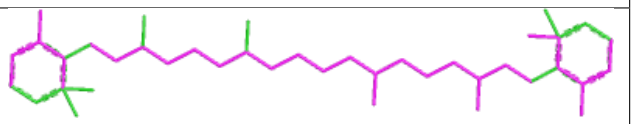

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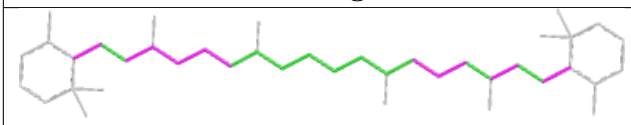

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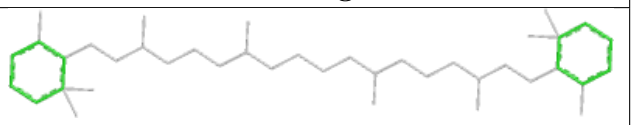
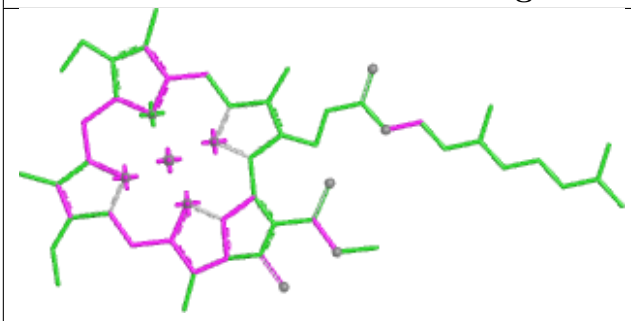


Rings

Ligand CLA B 1213



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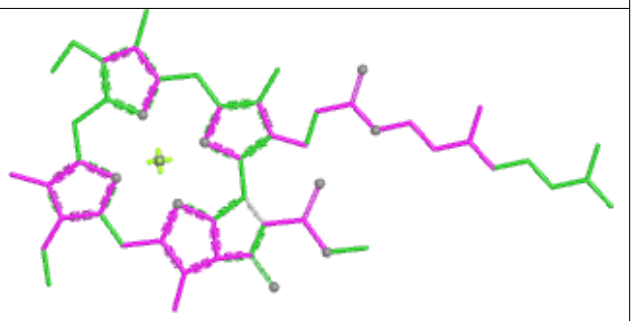

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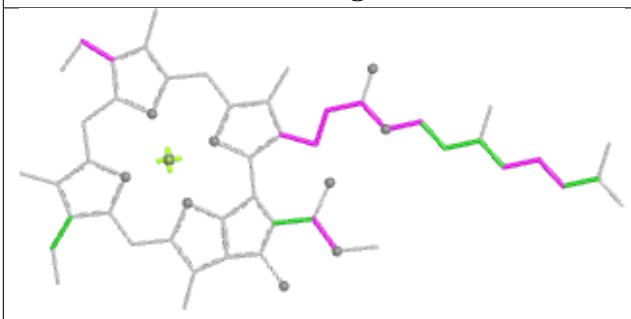

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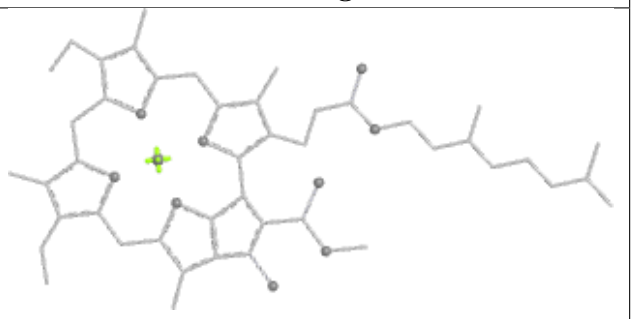
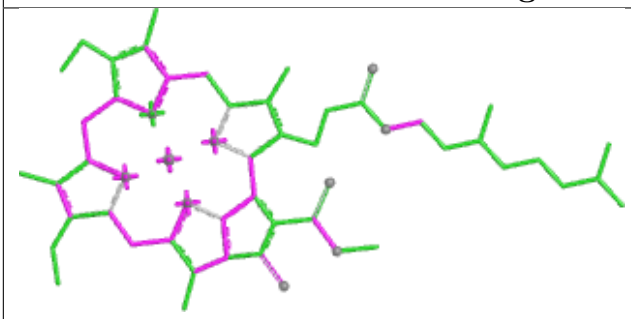


Rings

Ligand CLA b 1201



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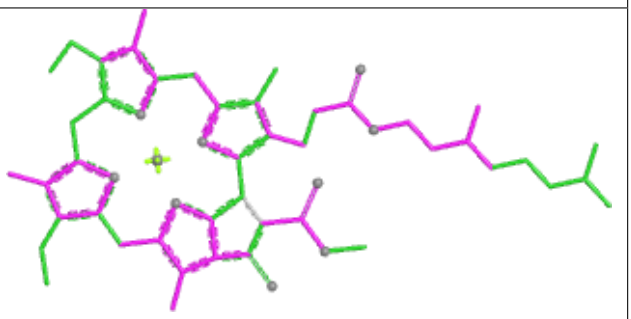
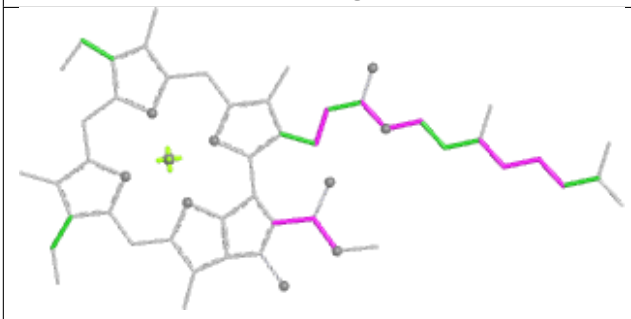


Bond angles



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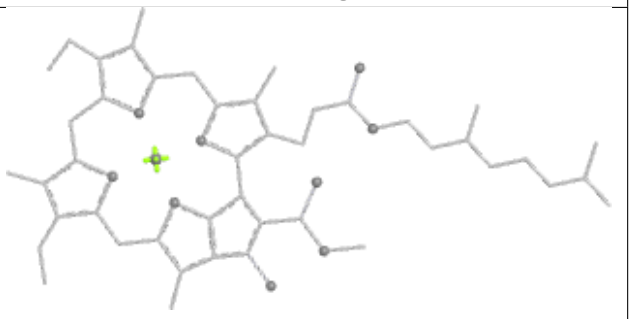
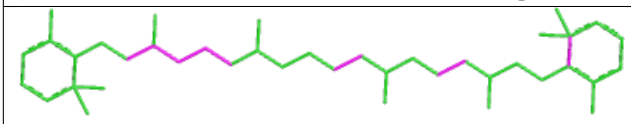


Rings

Ligand BCR A 4008



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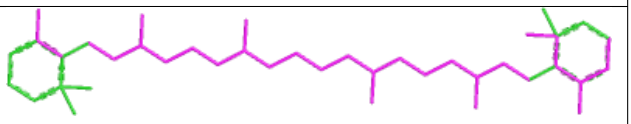
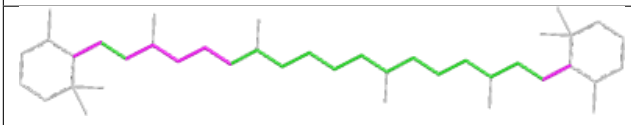
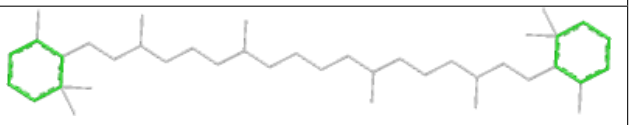


Bond angles

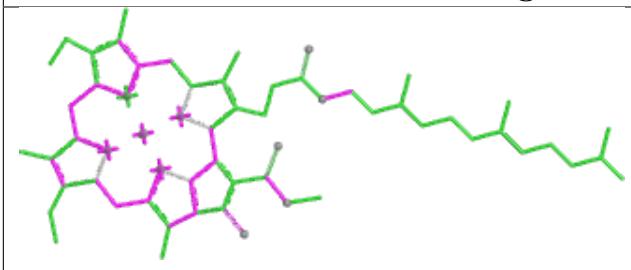


Torsions



Rings

Ligand CLA L 1501



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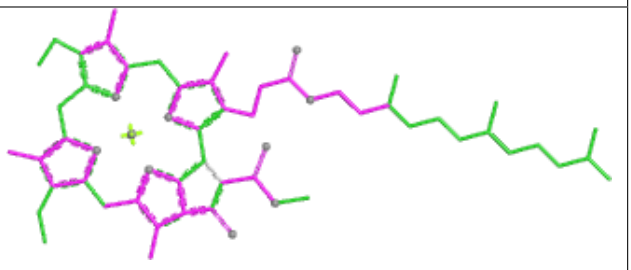
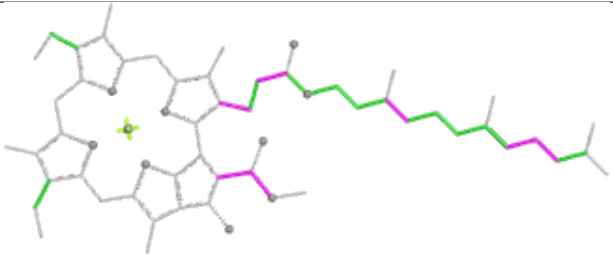


Bond angles



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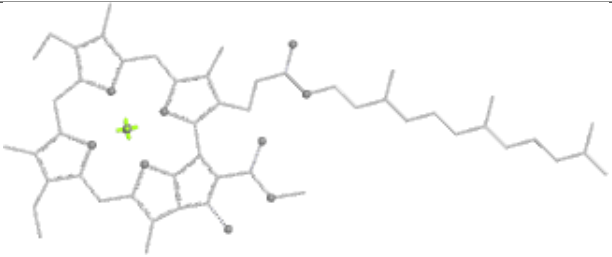
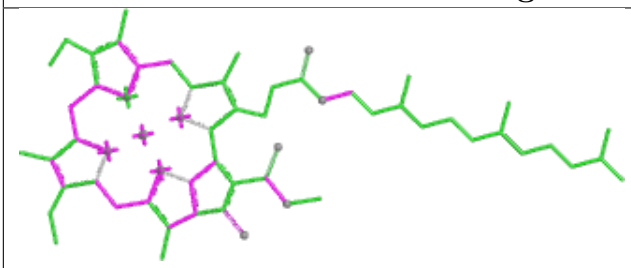


Rings

Ligand CLA L 1502



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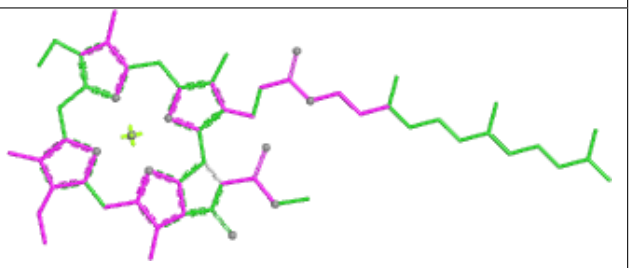
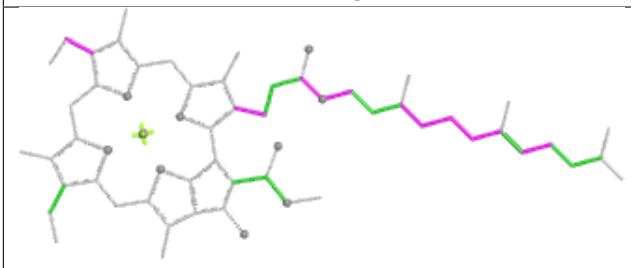
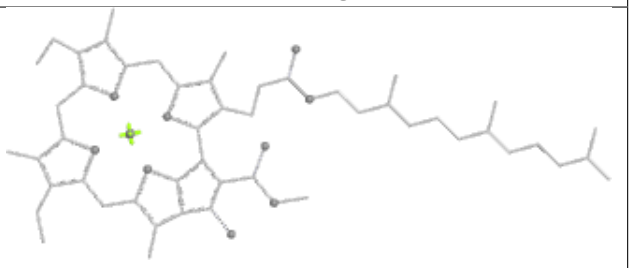


Bond angles

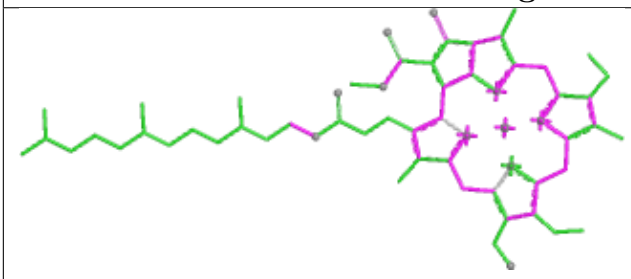


Torsions



Rings

Ligand F6C H 1237



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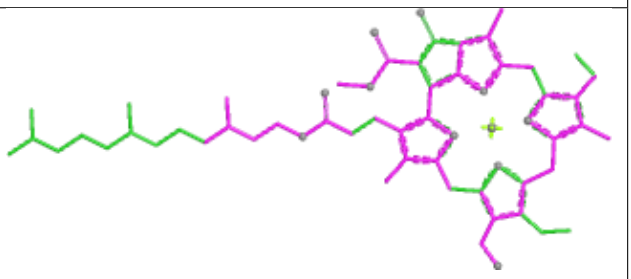
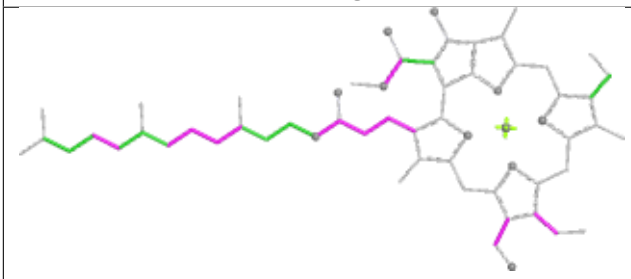
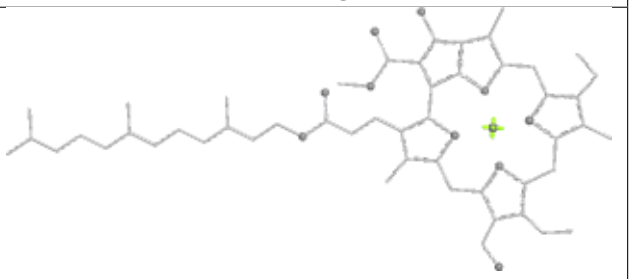


Bond angles

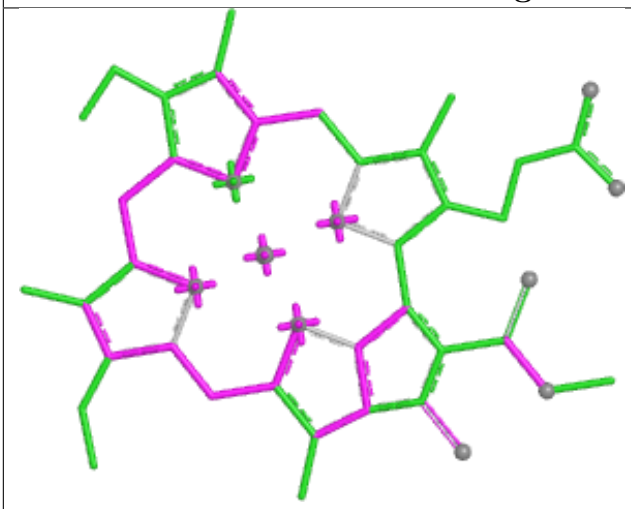


Torsions

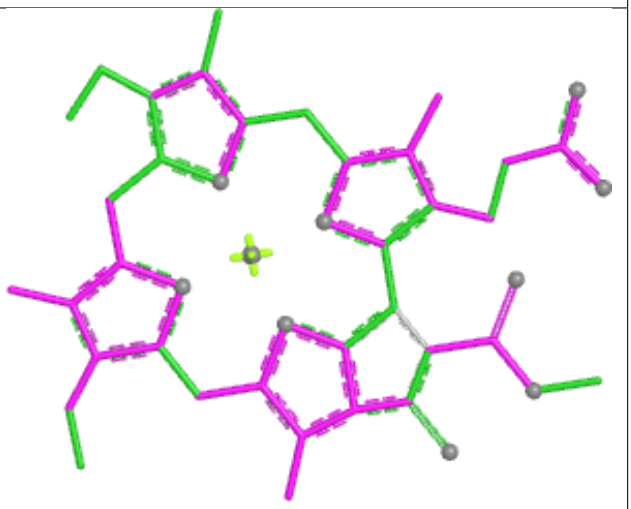


Rings

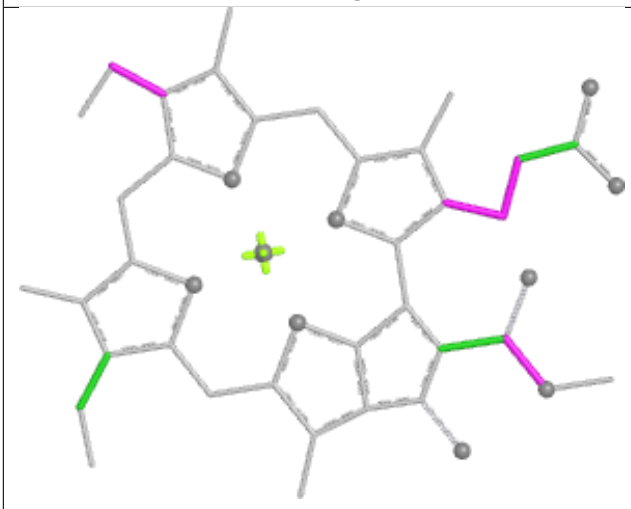
Ligand CLA H 1227



Bond lengths



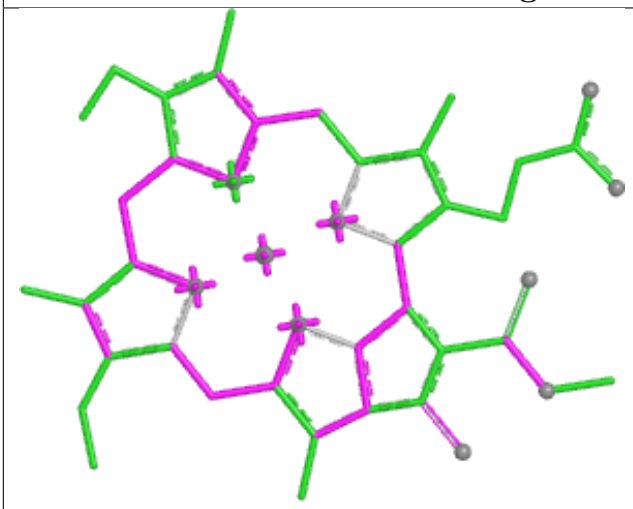
Bond angles



Torsions

Rings

Ligand CLA a 1106



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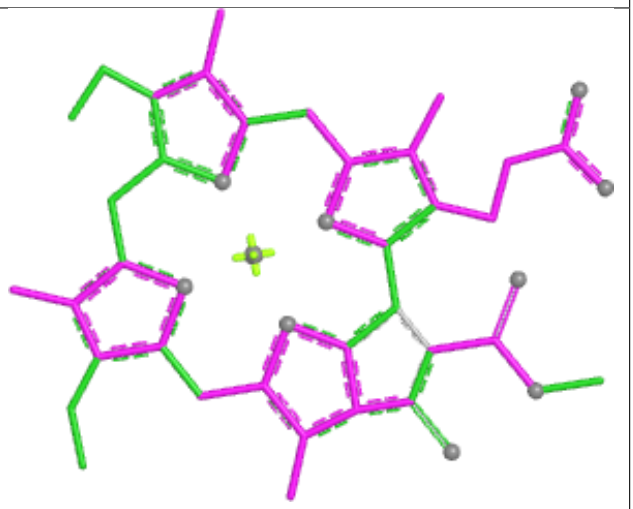
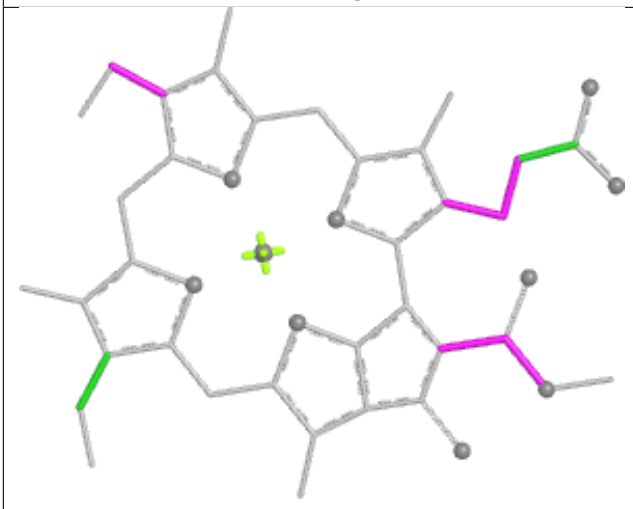


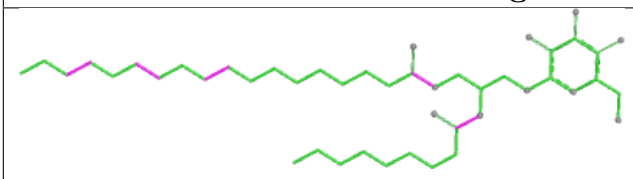
Bond angles



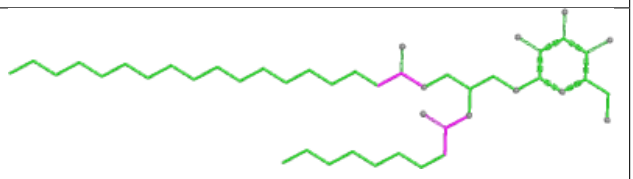
Torsions

Rings

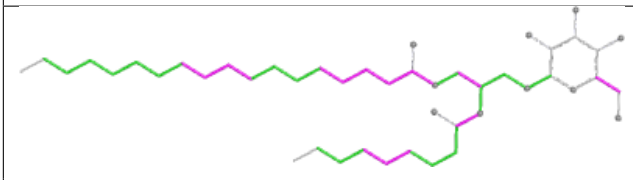
Ligand LMG G 5005



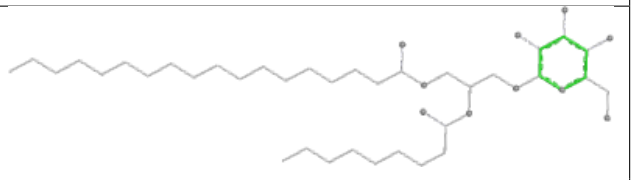
Bond lengths



Bond angles

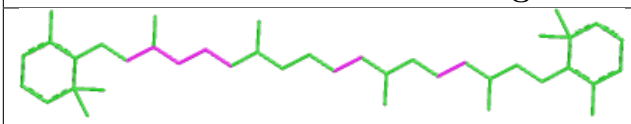


Torsions



Rings

Ligand BCR H 4016



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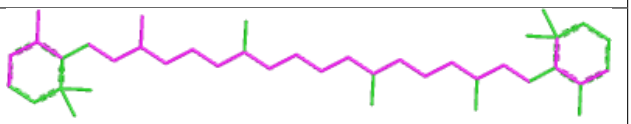
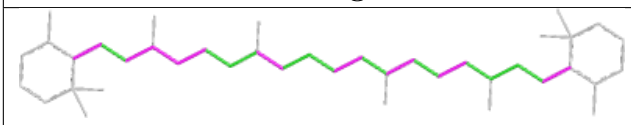
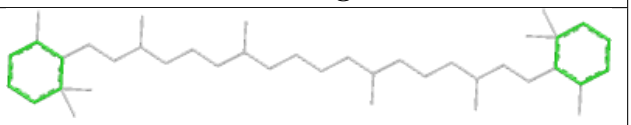


Bond angles

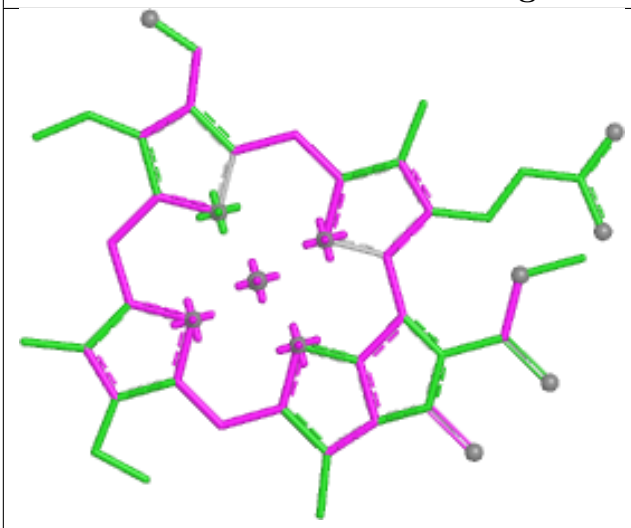


Torsions



Rings

Ligand F6C A 1120



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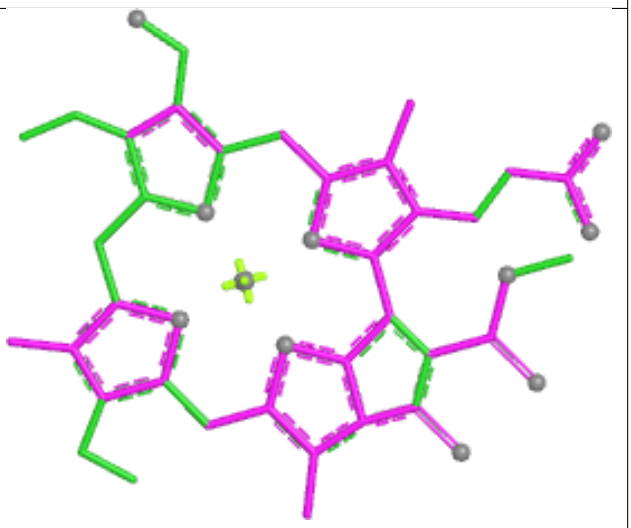
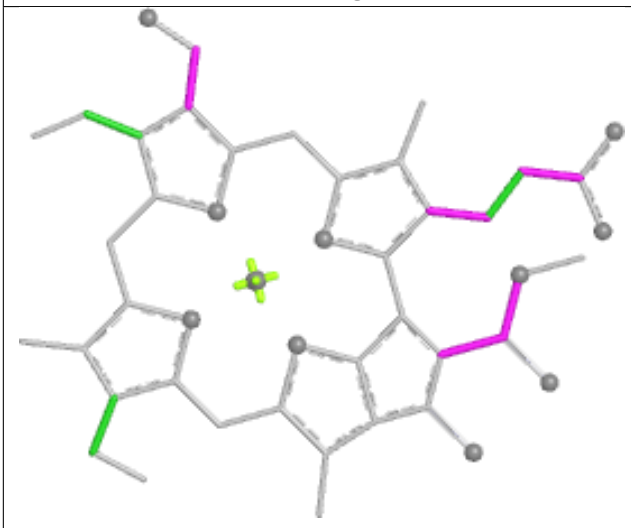


Bond angles



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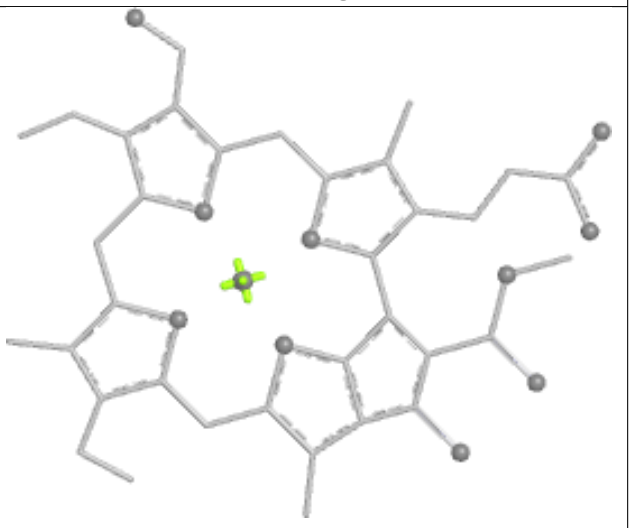
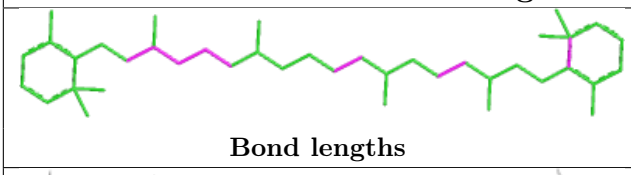


Rings

Ligand BCR b 4004



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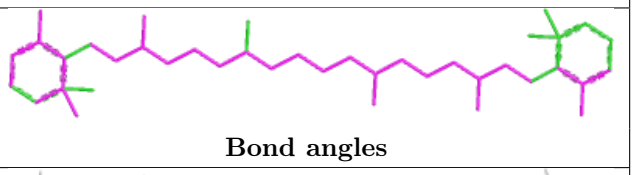
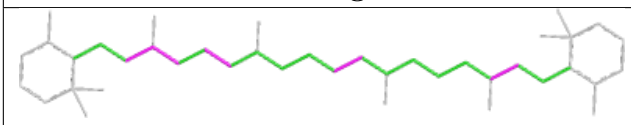
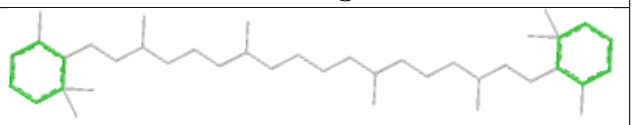


Bond angles

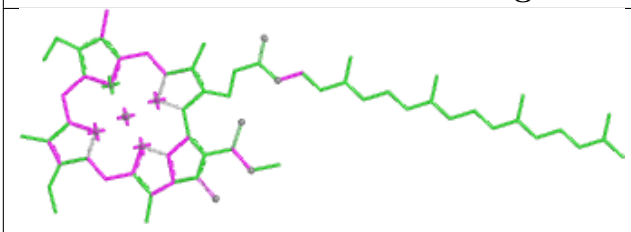


Torsions

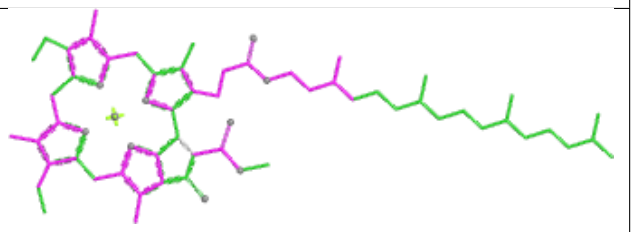


Rings

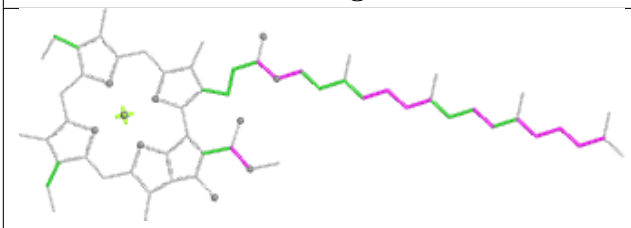
Ligand CLA H 1226



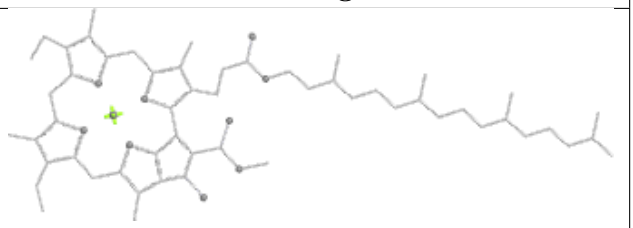
Bond lengths



Bond angles

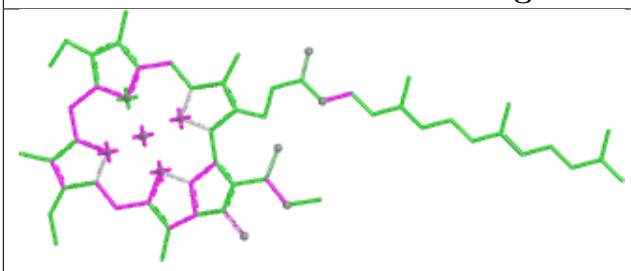


Torsions



Rings

Ligand CLA H 1215



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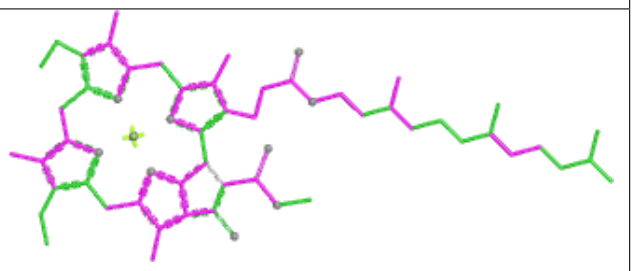
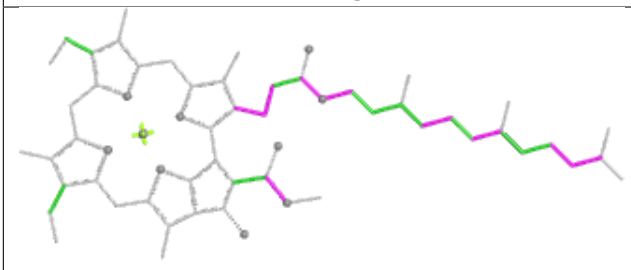
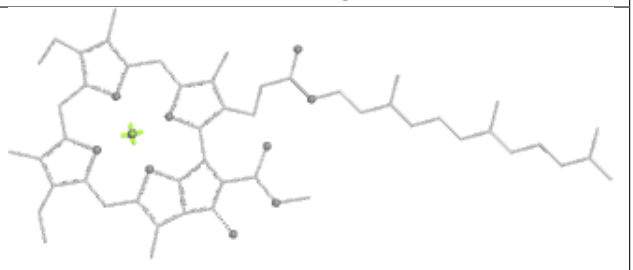


Bond angles

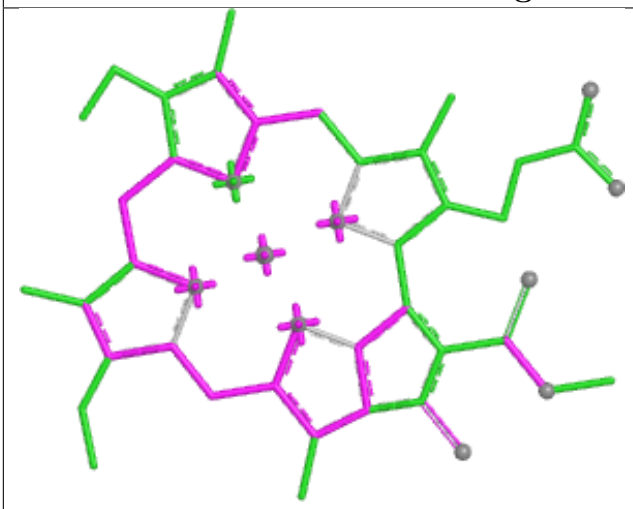


Torsions

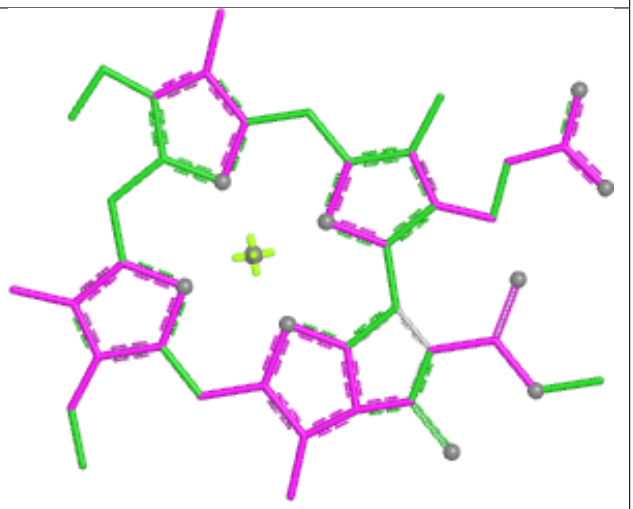


Rings

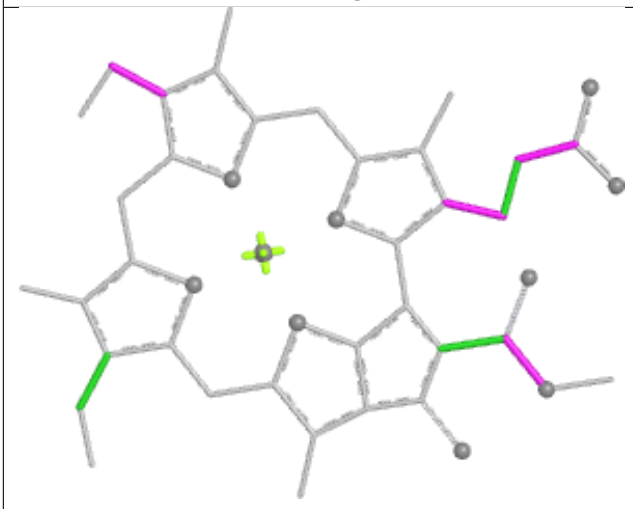
Ligand CLA A 1105



Bond lengths



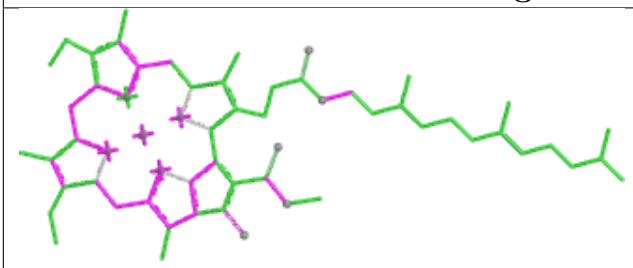
Bond angles



Torsions

Rings

Ligand CLA H 1229



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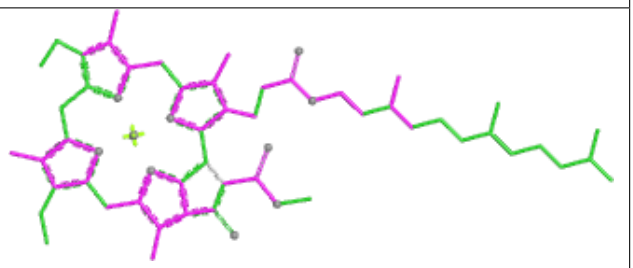
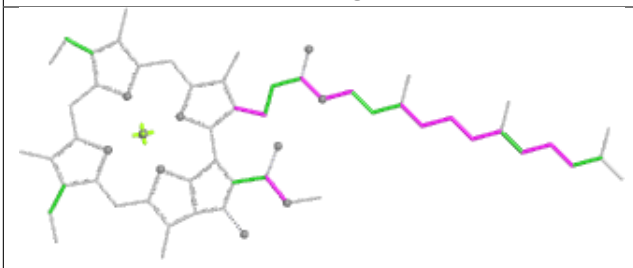
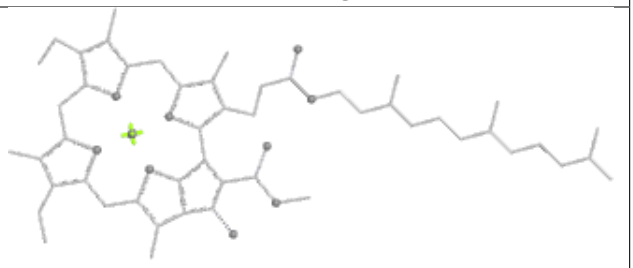


Bond angles

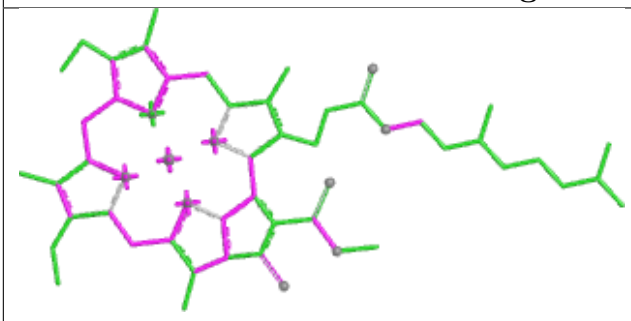


Torsions



Rings

Ligand CLA a 1136



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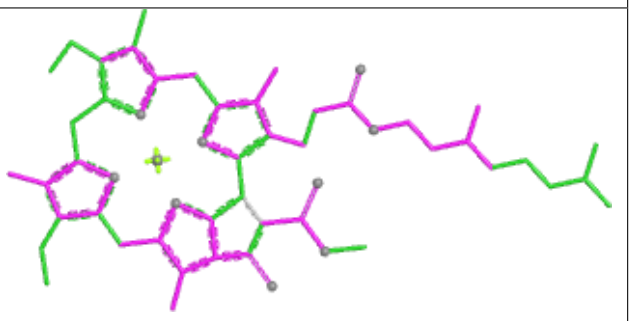
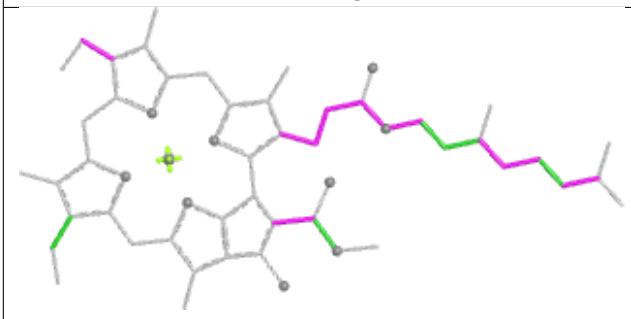
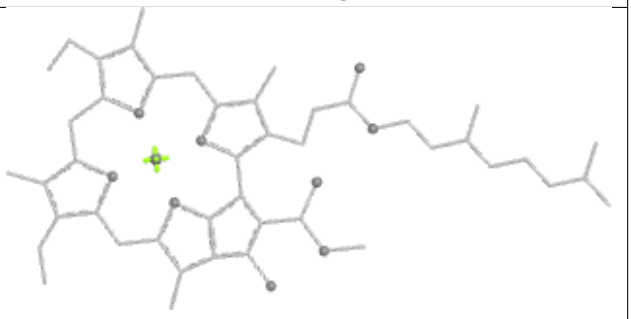


Bond angles

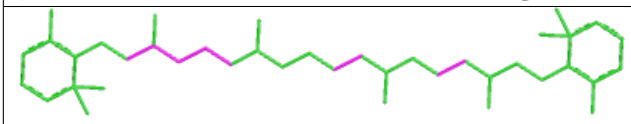


Torsions



Rings

Ligand BCR b 4017



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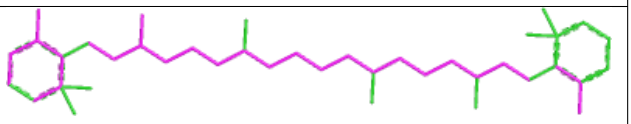
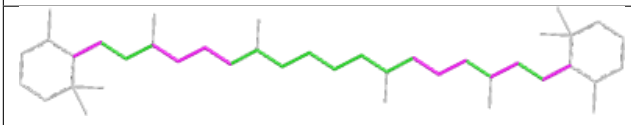
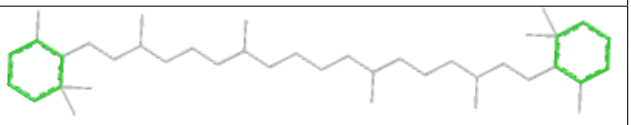


Bond angles

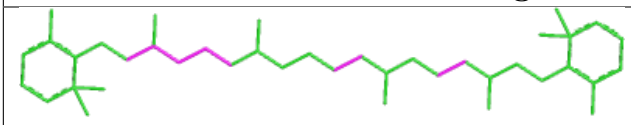


Torsions

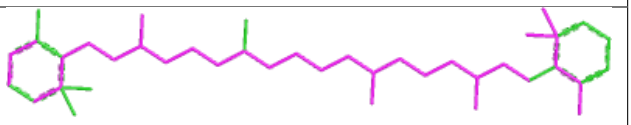


Rings

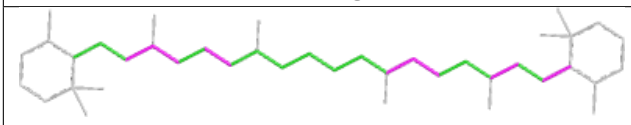
Ligand BCR V 4021



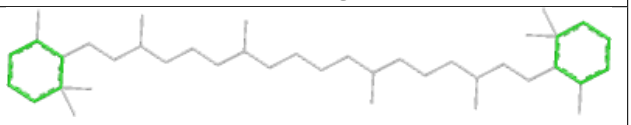
Bond lengths



Bond angles

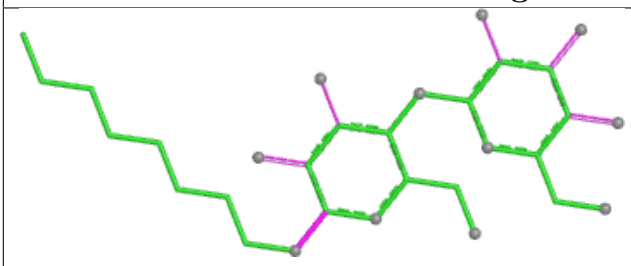


Torsions

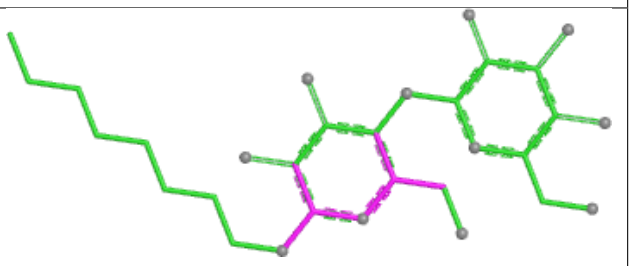


Rings

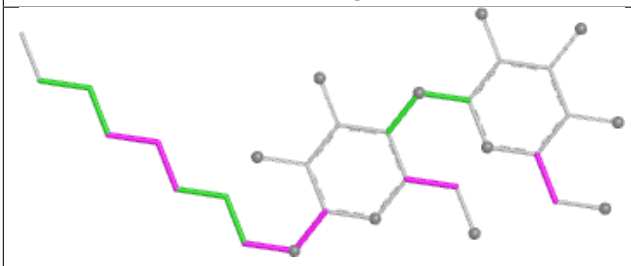
Ligand LMT G 6001



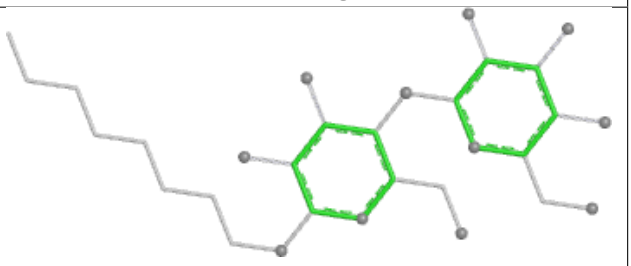
Bond lengths



Bond angles

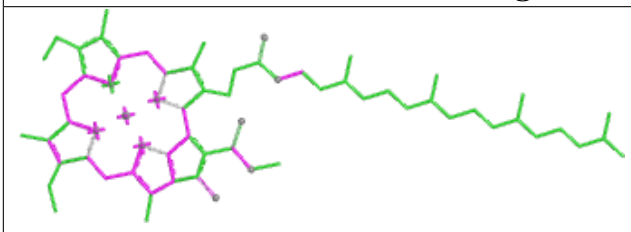


Torsions

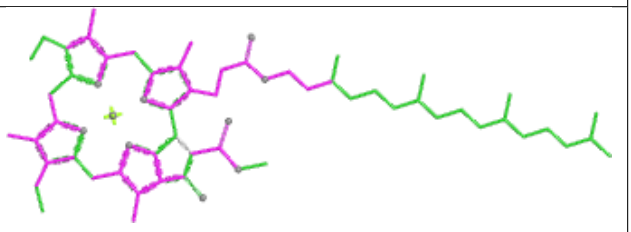


Rings

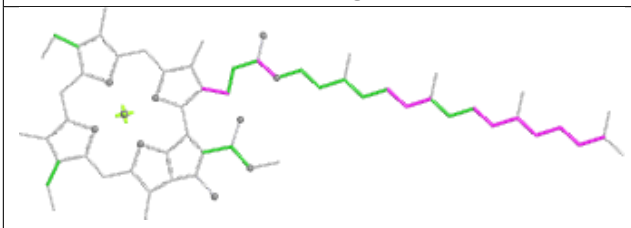
Ligand CLA G 1117



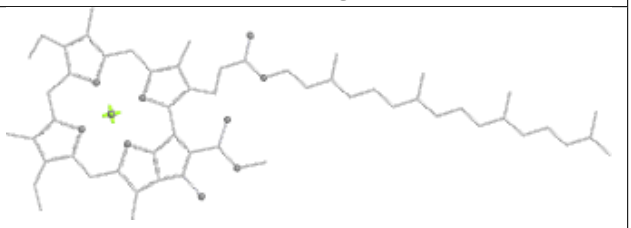
Bond lengths



Bond angles

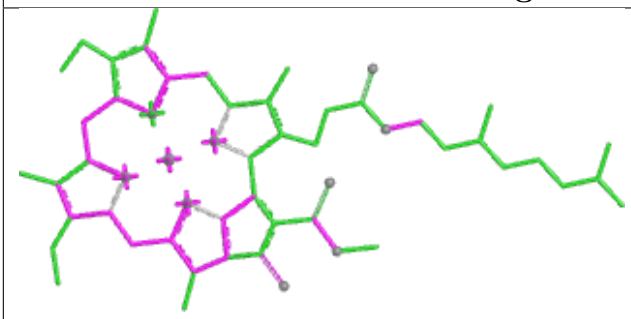


Torsions



Rings

Ligand CLA B 1216



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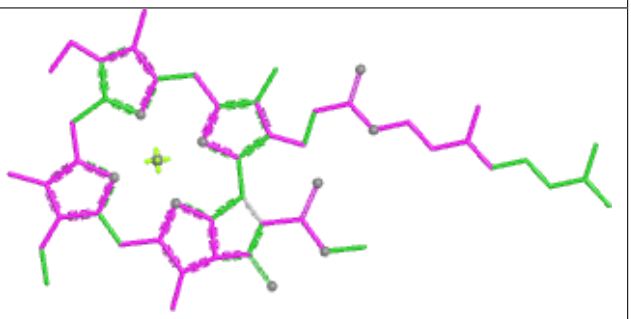

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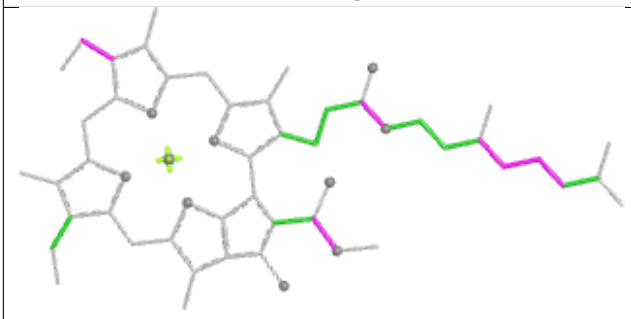
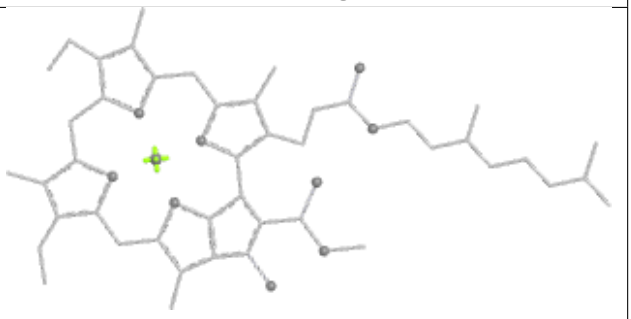
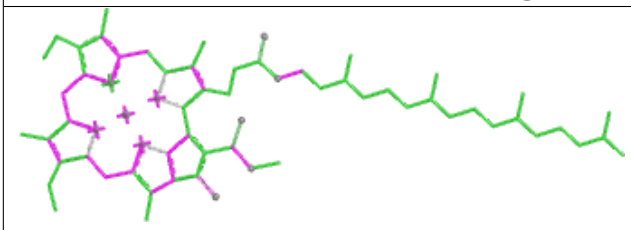


Torsions



Rings

Ligand CLA b 1021



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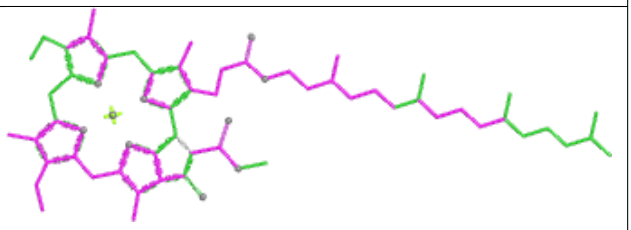

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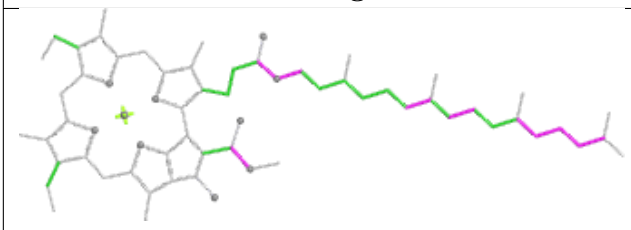
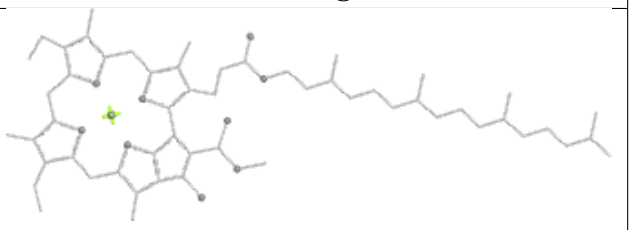
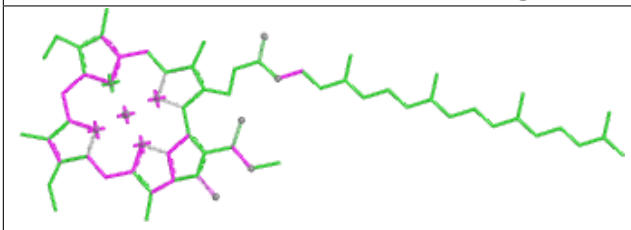


Torsions



Rings

Ligand CLA H 1222



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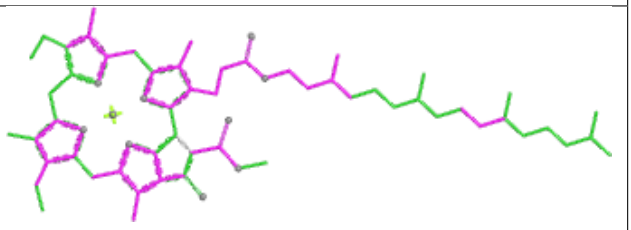
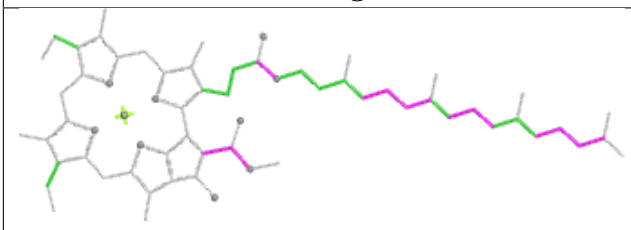


Bond angles



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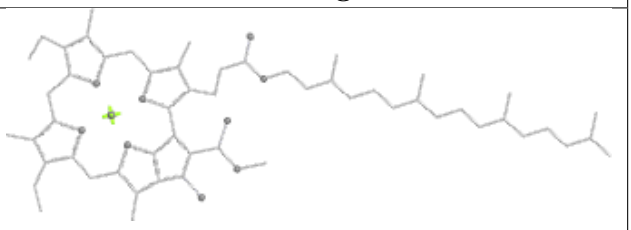
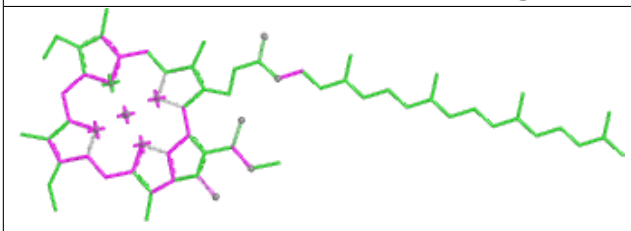


Rings

Ligand CLA H 1239



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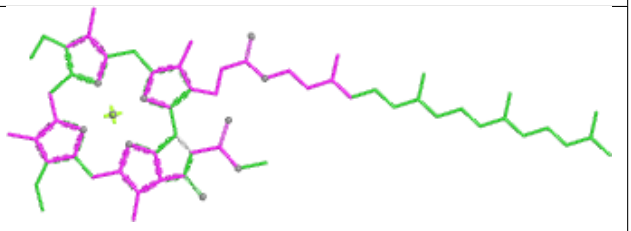
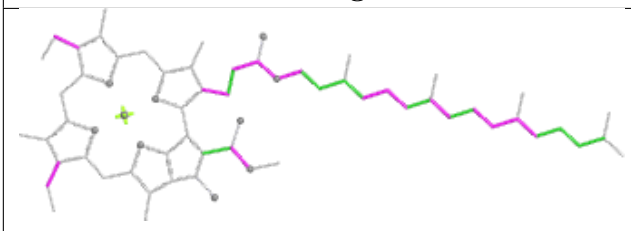


Bond angles



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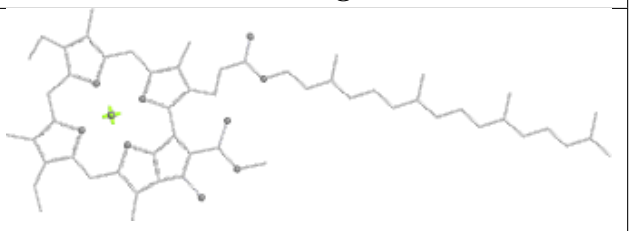
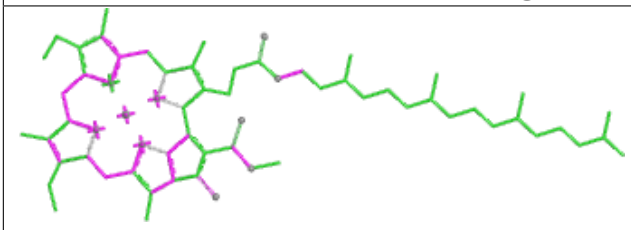


Rings

Ligand CLA b 1022



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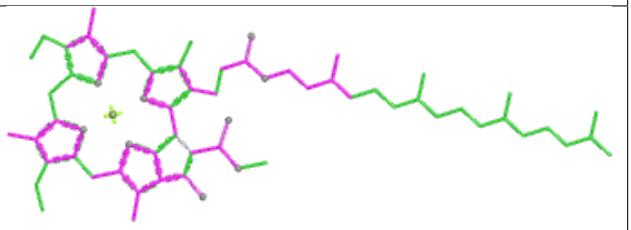
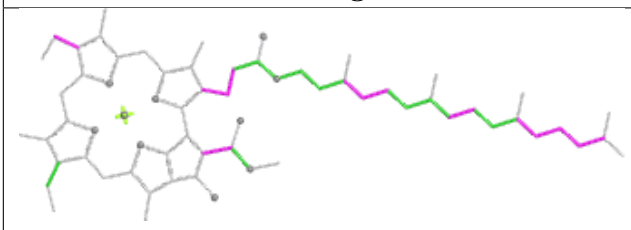


Bond angles



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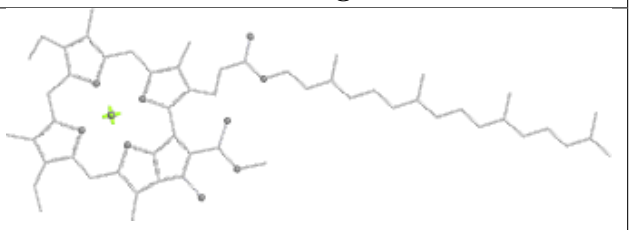
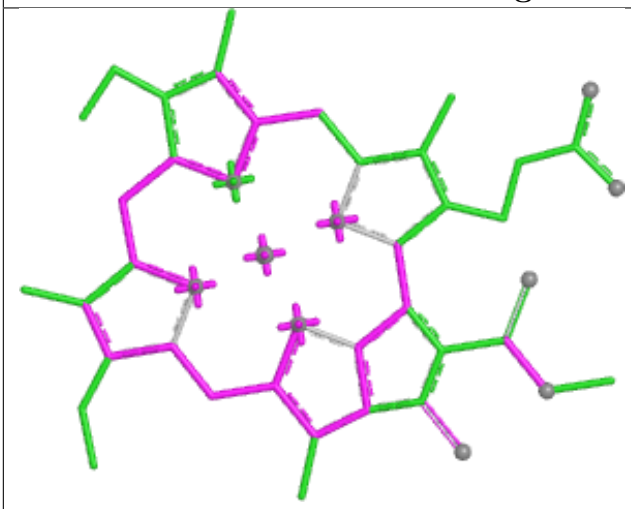


Rings

Ligand CLA A 1112



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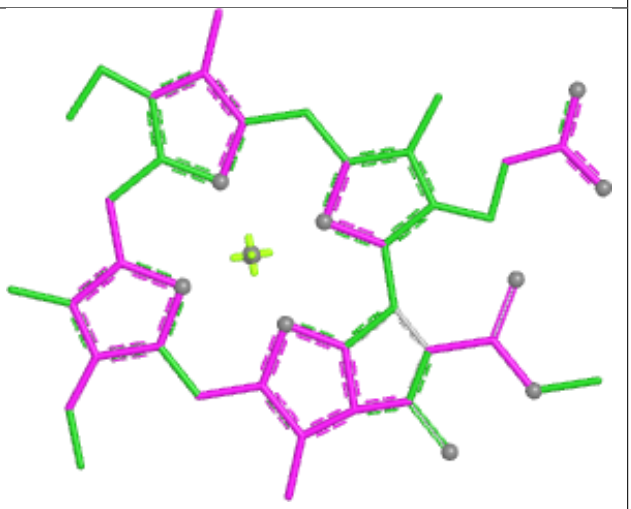

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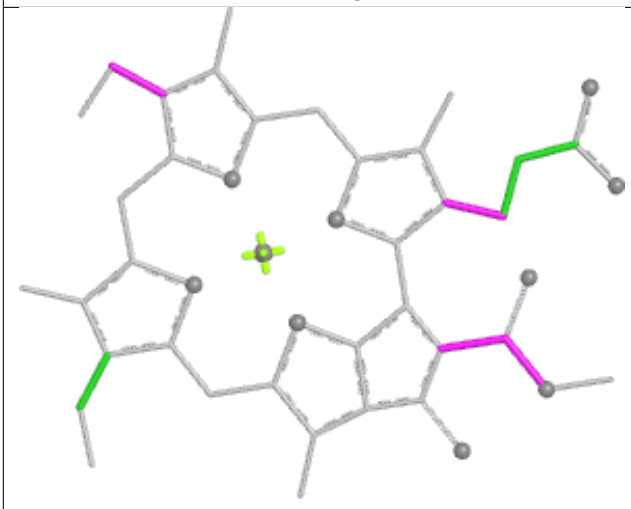
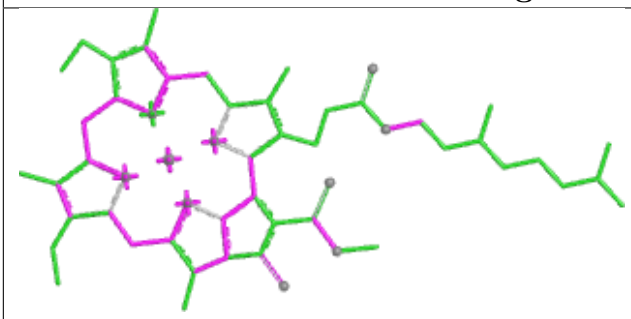


Torsions

Rings

Ligand CLA B 1217



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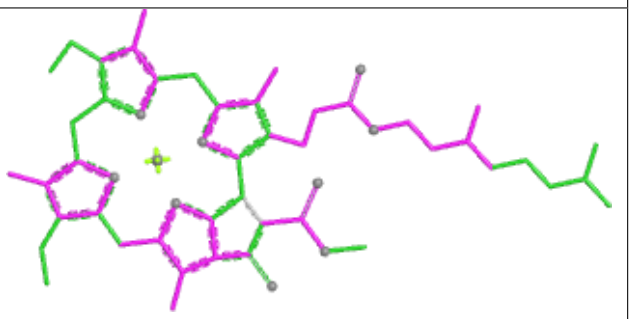
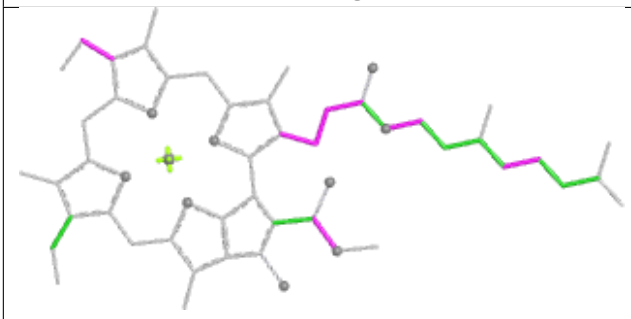


Bond angles



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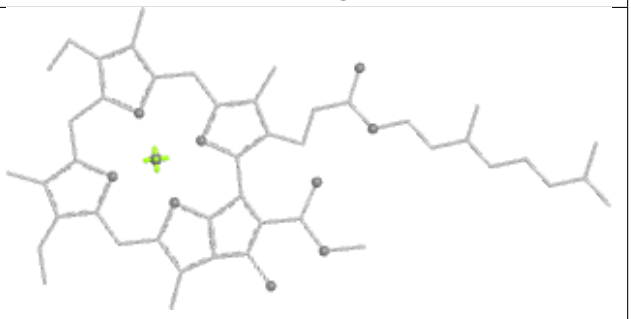
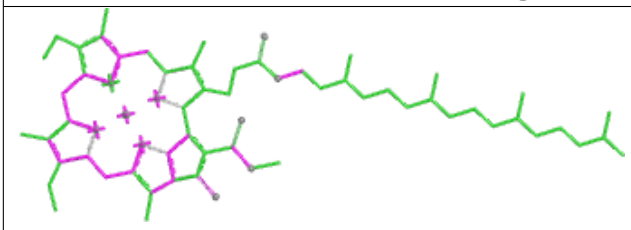


Rings

Ligand CLA H 1210



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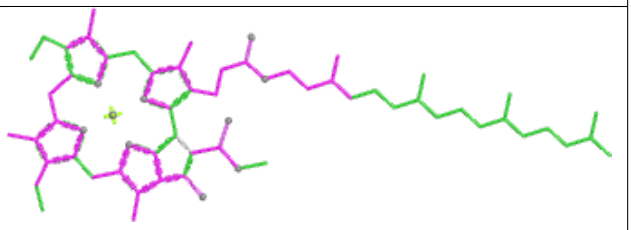
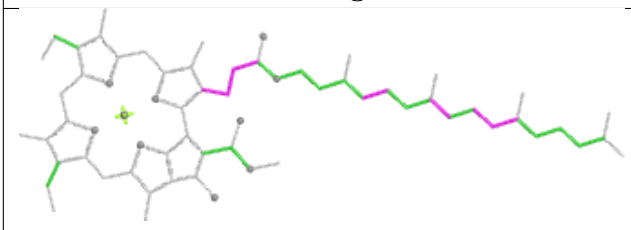


Bond angles



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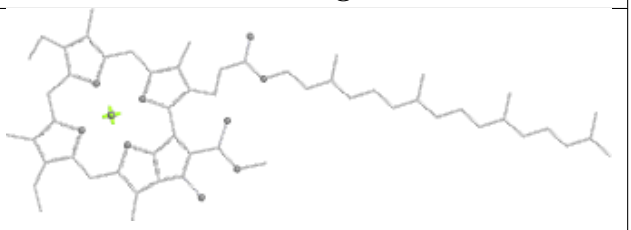
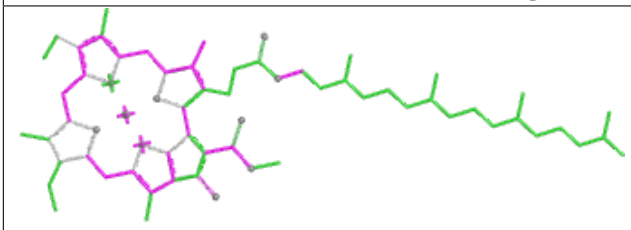


Rings

Ligand CL0 a 1011



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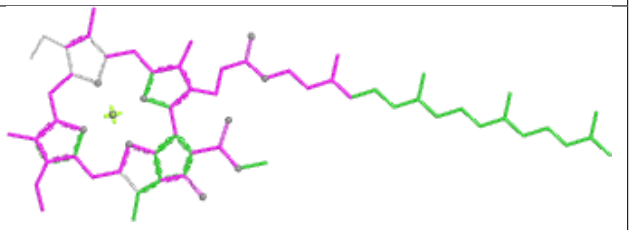
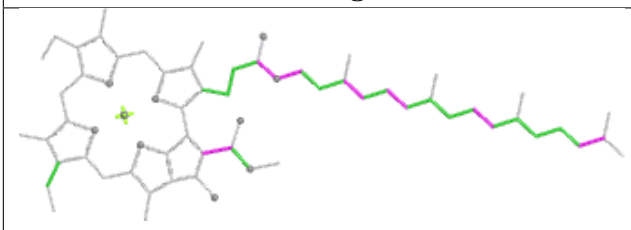


Bond angles



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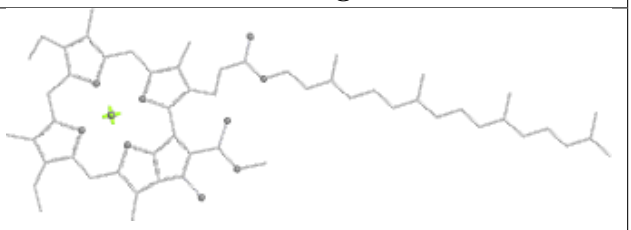
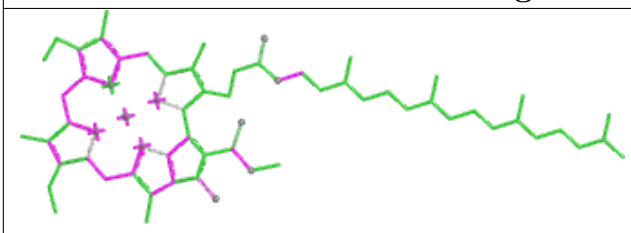


Rings

Ligand CLA A 1140



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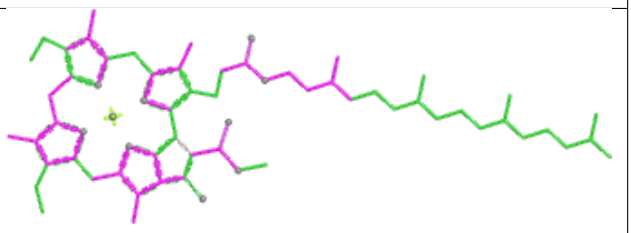
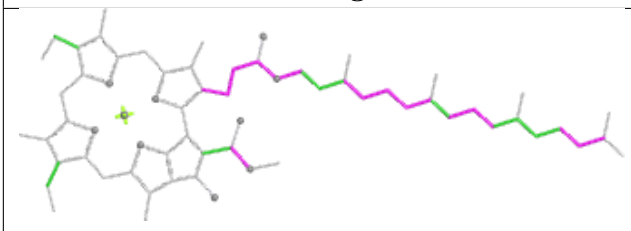


Bond angles



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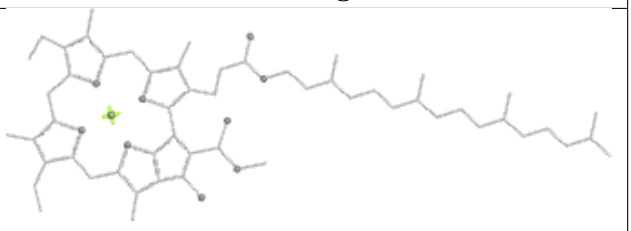
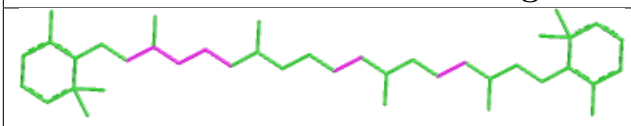


Rings

Ligand BCR l 4019



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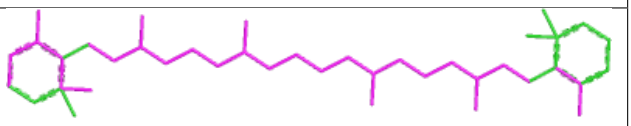
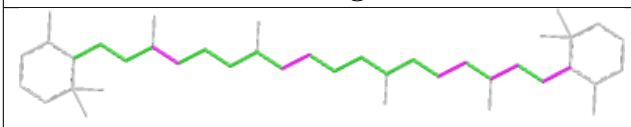
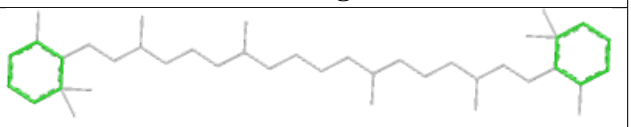


Bond angles

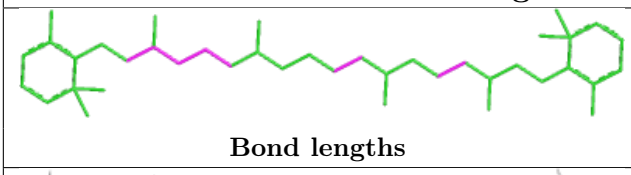


Torsions



Rings

Ligand BCR H 4012



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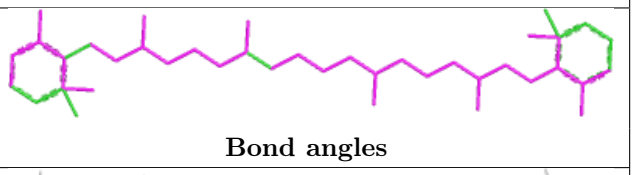
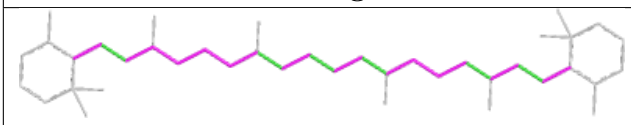
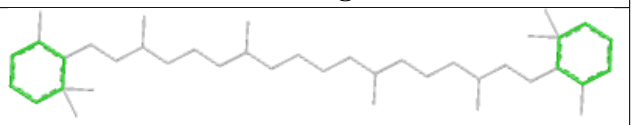


Bond angles

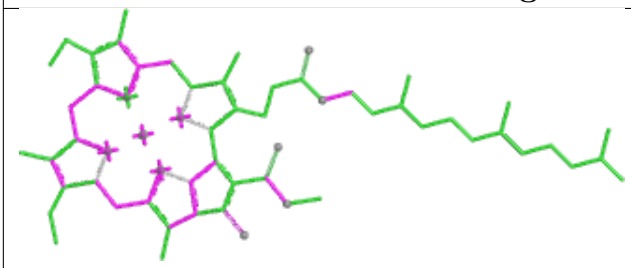


Torsions



Rings

Ligand CLA a 1102



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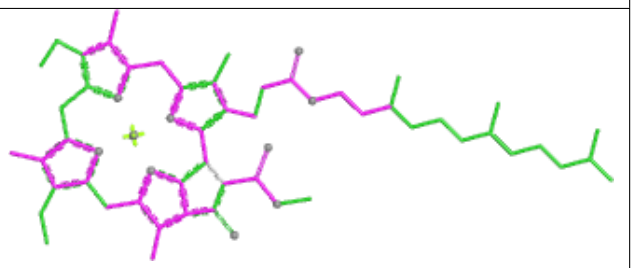
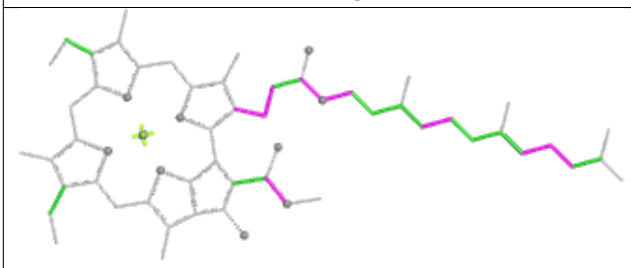


Bond angles



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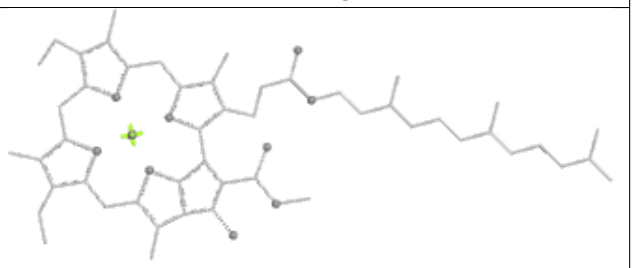
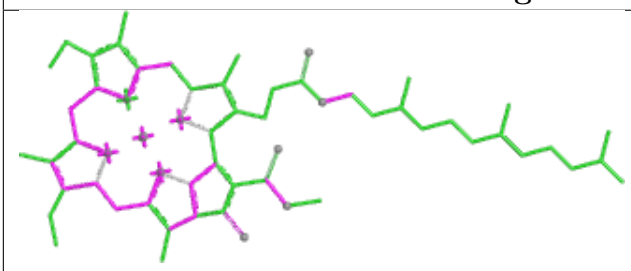
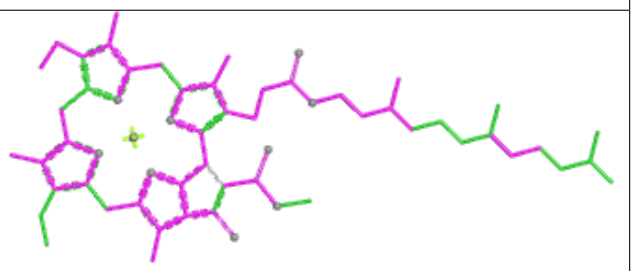


Rings

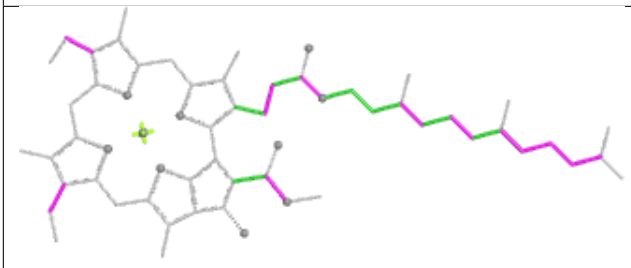
Ligand CLA H 1214



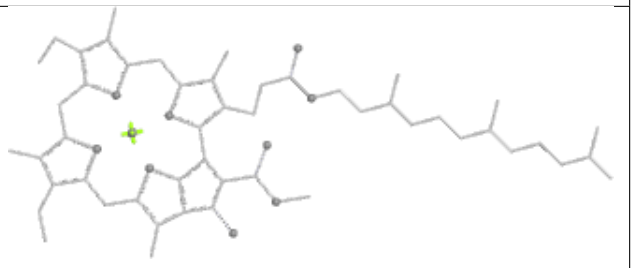
Bond lengths



Bond angles

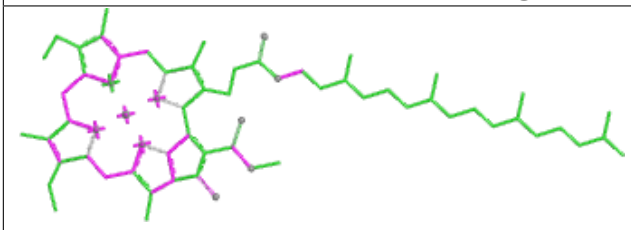


Torsions



Rings

Ligand CLA B 1224



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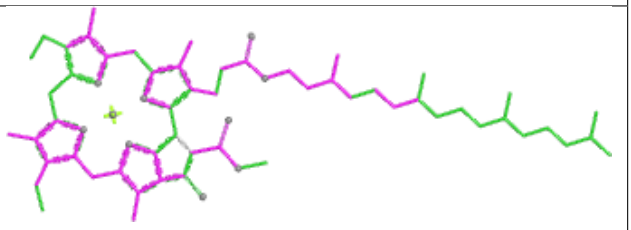
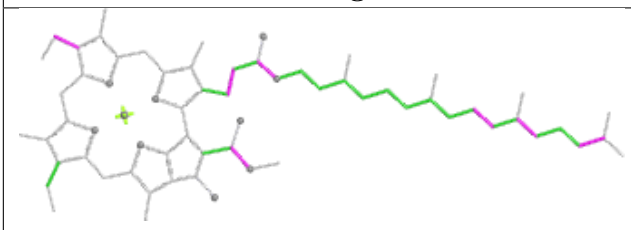
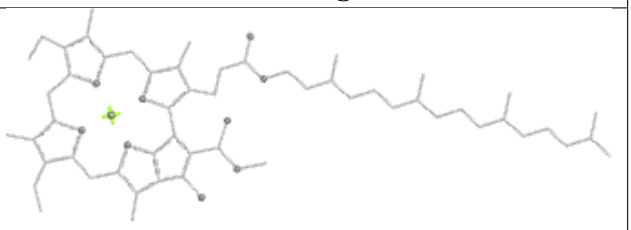


Bond angles

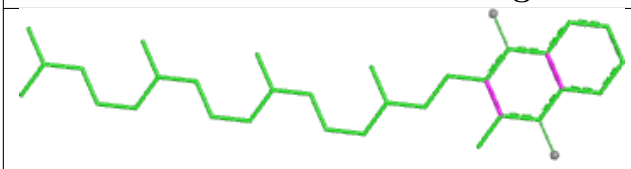


Torsions



Rings

Ligand PQN B 2002



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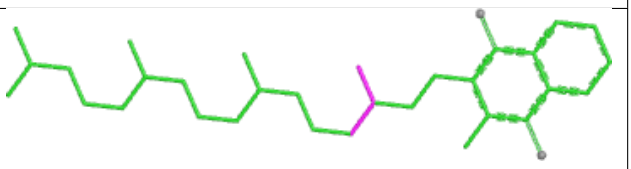
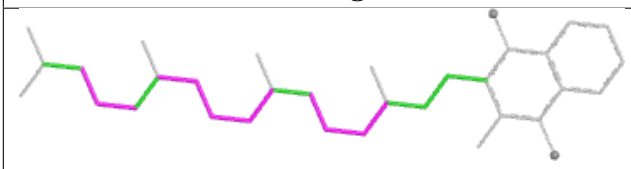
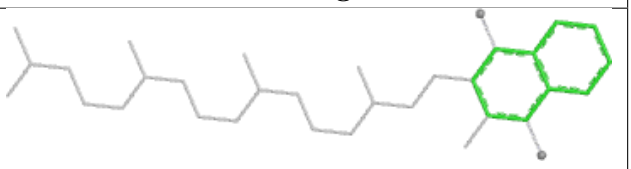


Bond angles

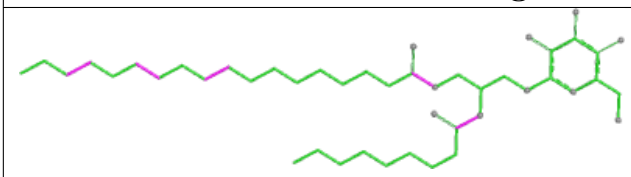


Torsions



Rings

Ligand LMG A 5005



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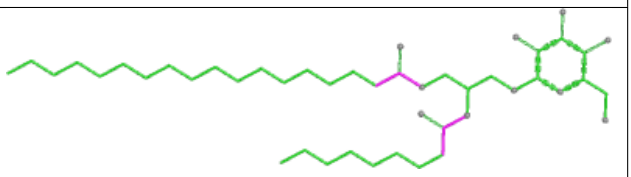
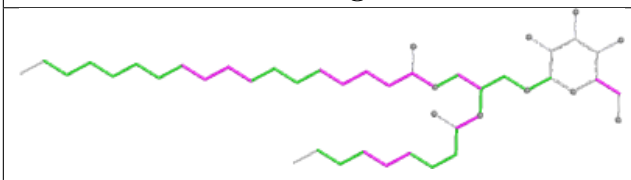
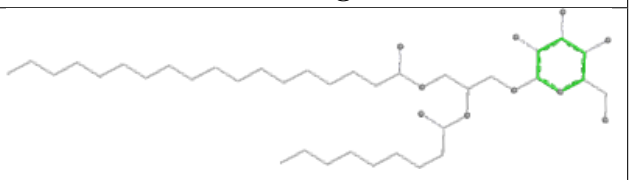


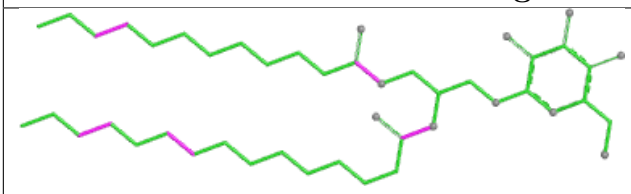
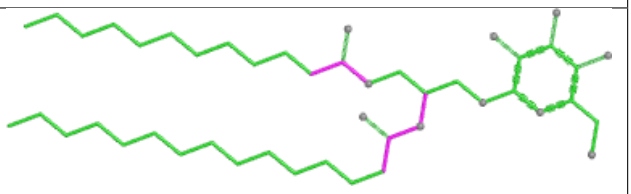
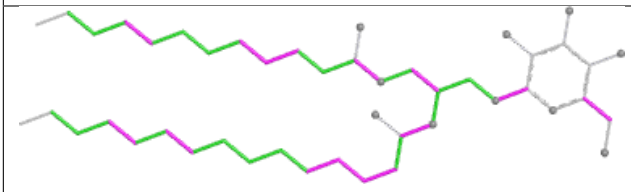
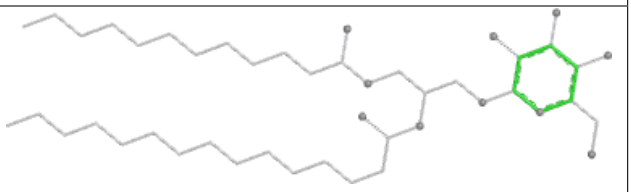
Bond angles

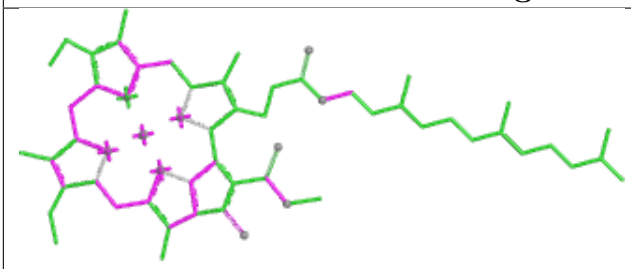
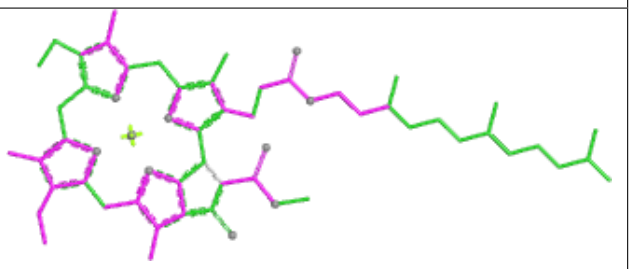
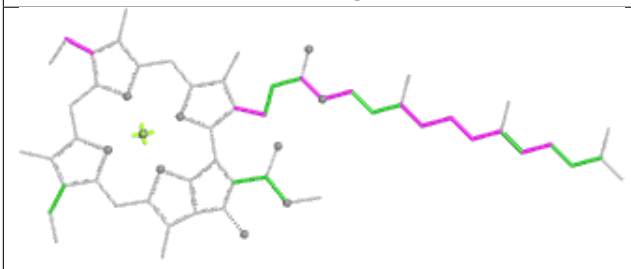
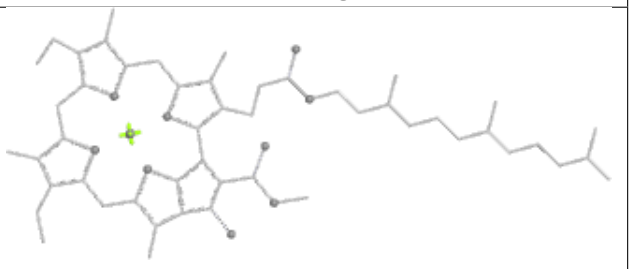


Torsions

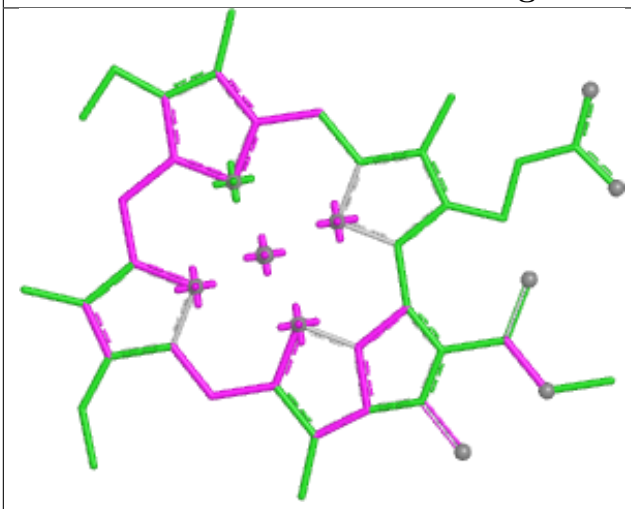


Rings

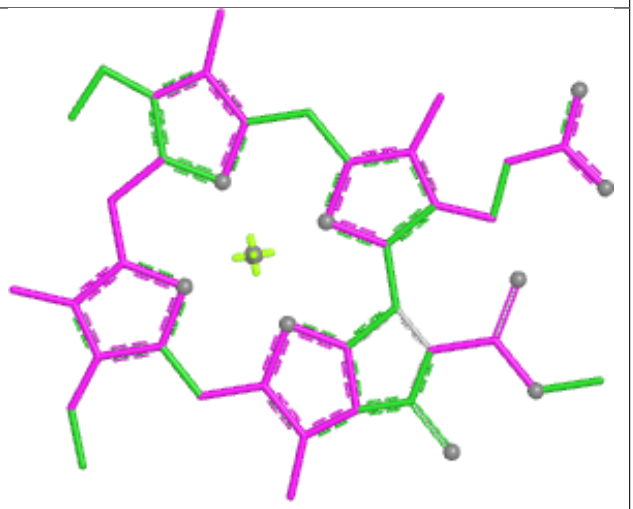
Ligand LMG b 5002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 1502	
 Bond lengths	 Bond angles
 Torsions	 Rings

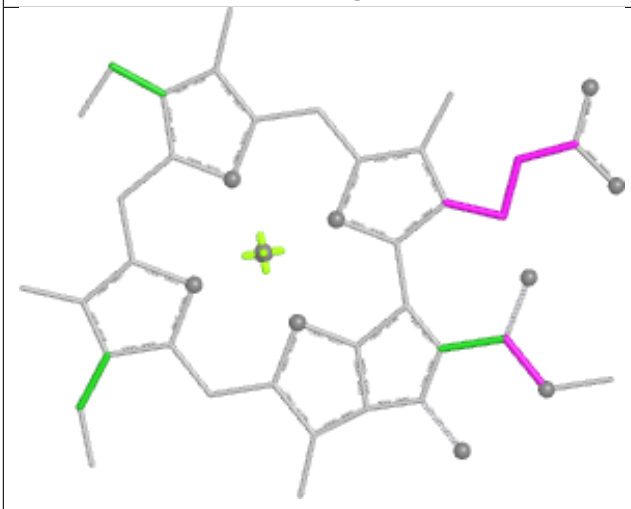
Ligand CLA b 1207



Bond lengths



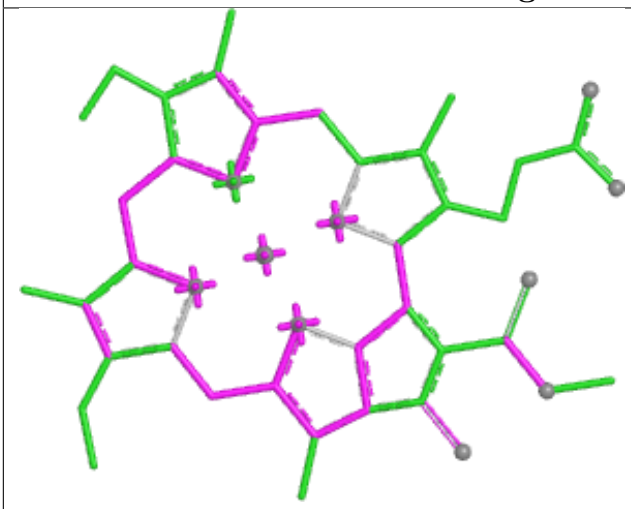
Bond angles



Torsions

Rings

Ligand CLA b 1209



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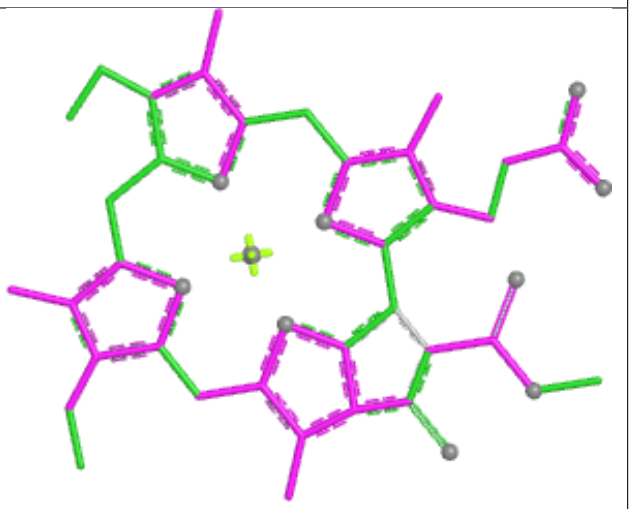
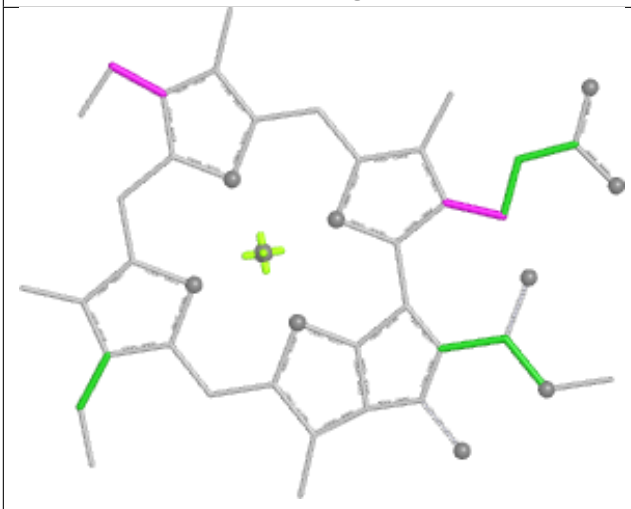


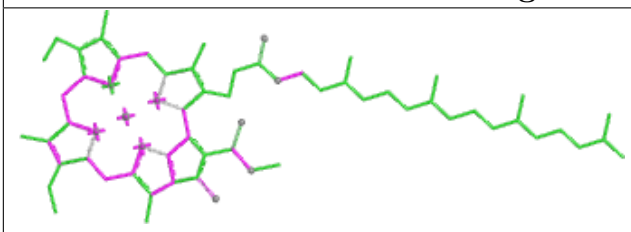
Bond angles



Torsions

Rings

Ligand CLA b 1205



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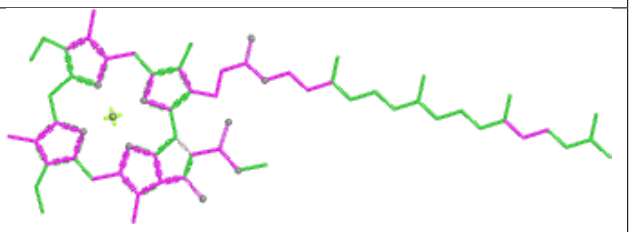
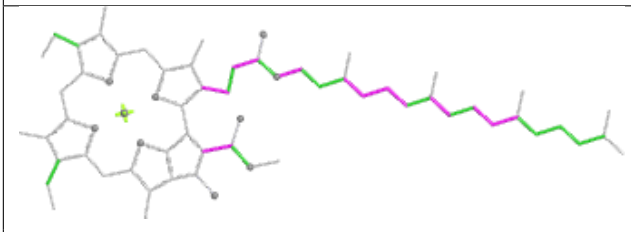
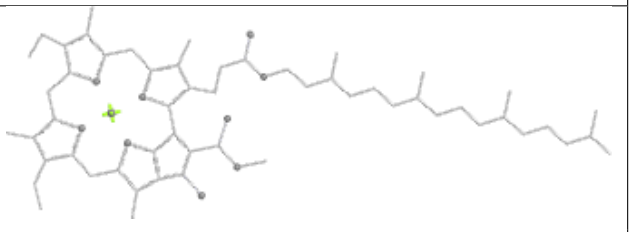


Bond angles

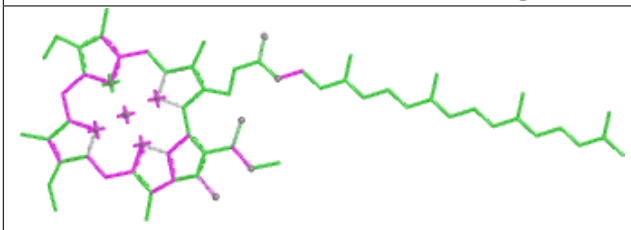


Torsions

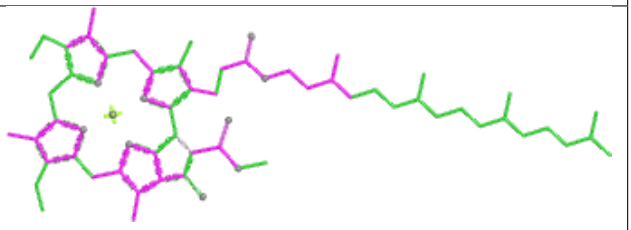


Rings

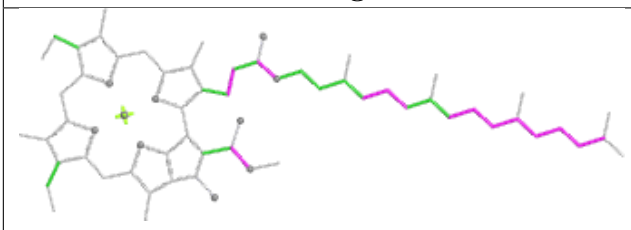
Ligand CLA H 1211



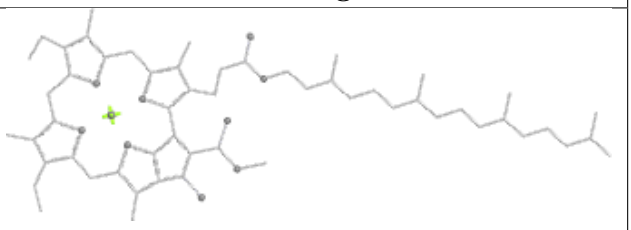
Bond lengths



Bond angles

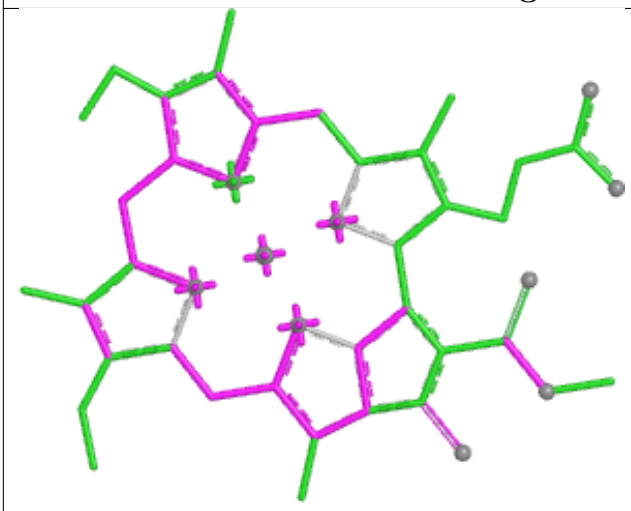


Torsions



Rings

Ligand CLA a 1108



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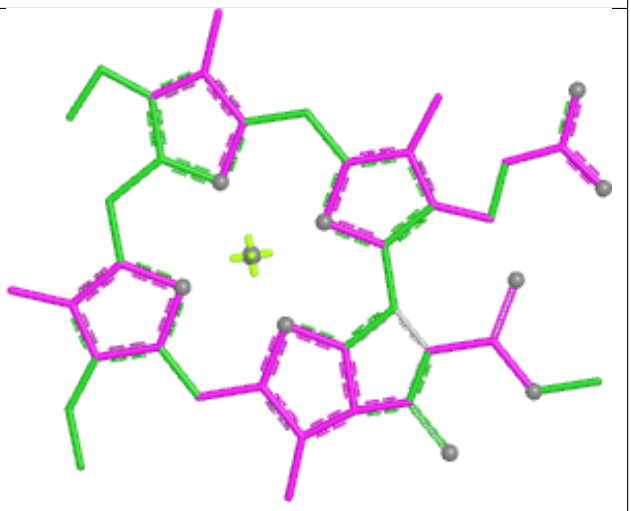
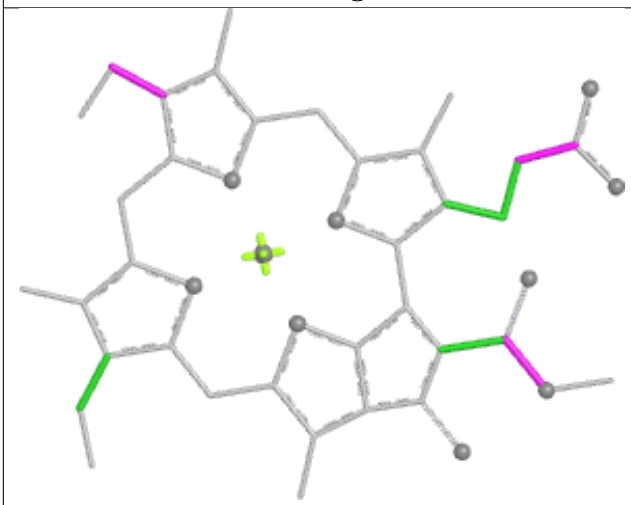


Bond angles



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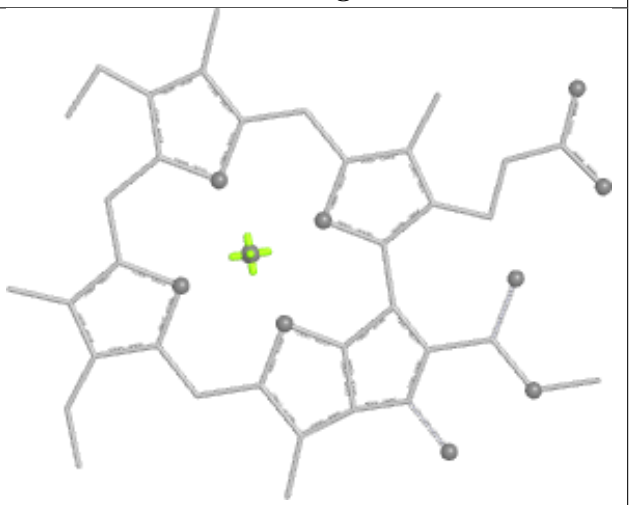
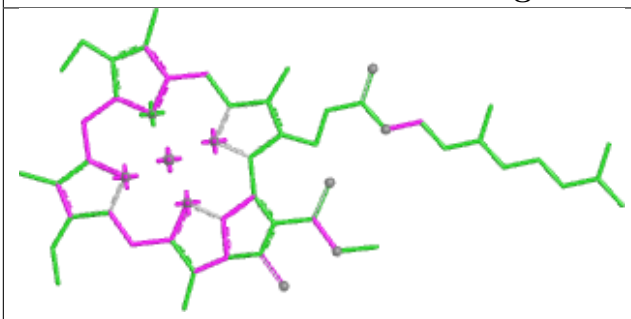


Rings

Ligand CLA G 1116



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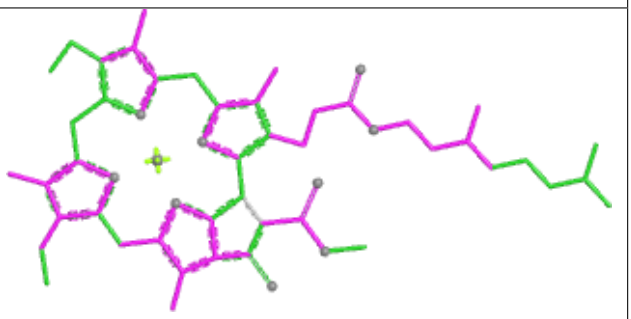
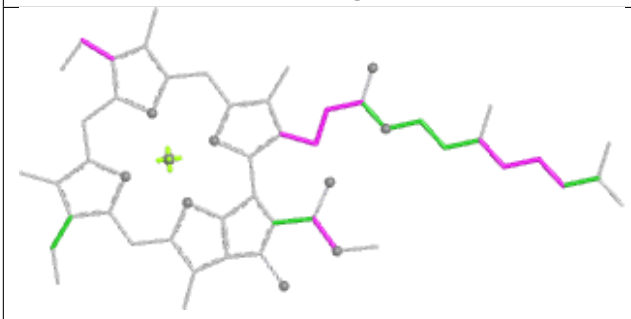
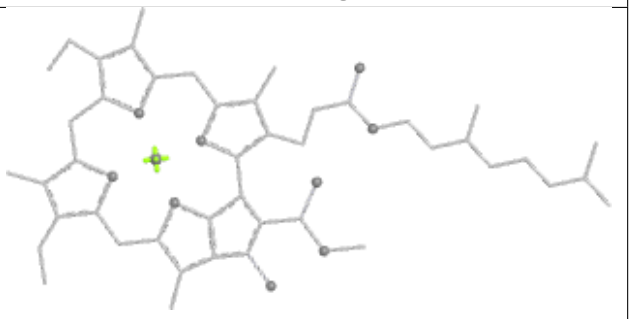


Bond angles

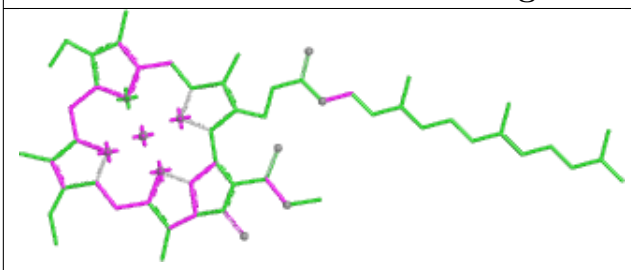


Torsions

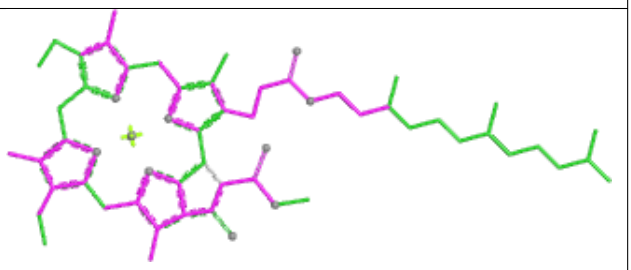


Rings

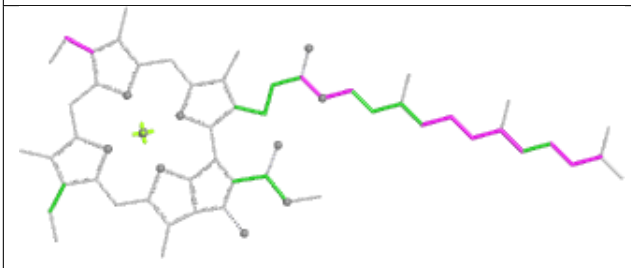
Ligand CLA b 1221



Bond lengths



Bond angles



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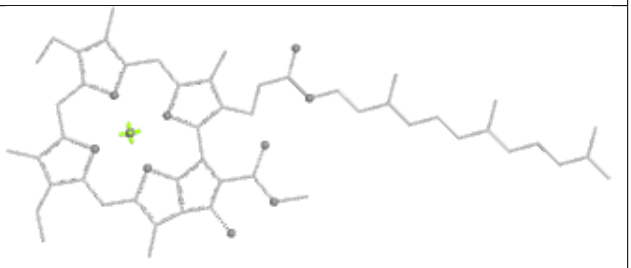
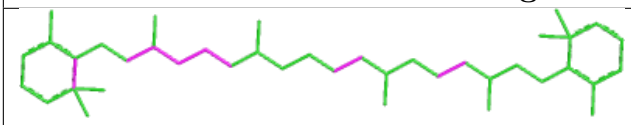
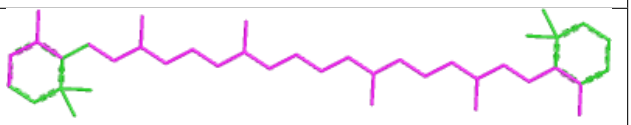


Rings

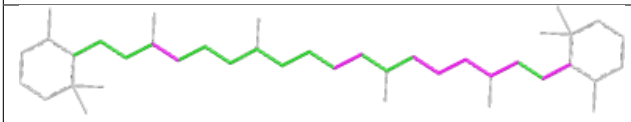
Ligand BCR I 4020



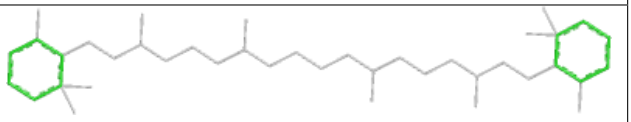
Bond lengths



Bond angles

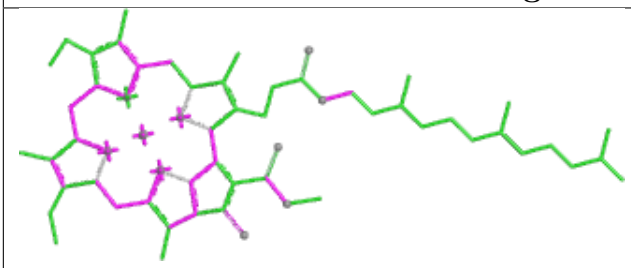


Torsions

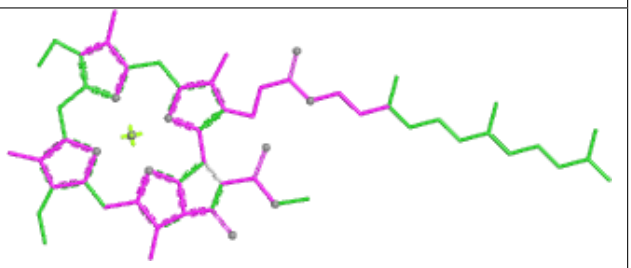


Rings

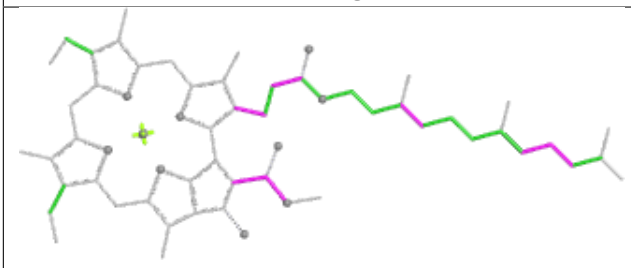
Ligand CLA l 1501



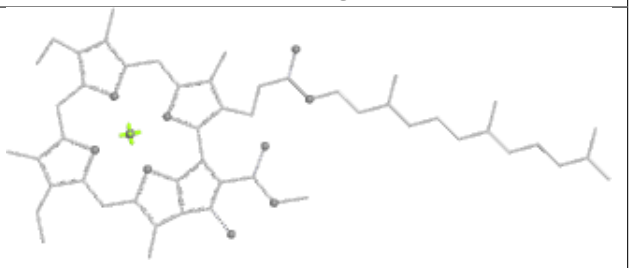
Bond lengths



Bond angles

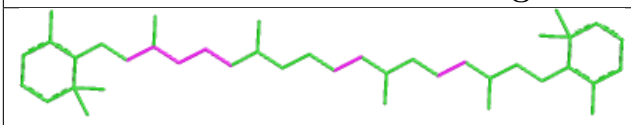


Torsions

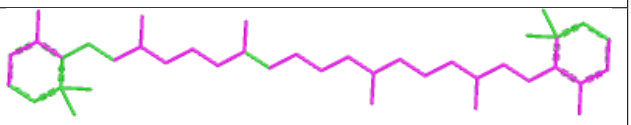


Rings

Ligand BCR G 4002

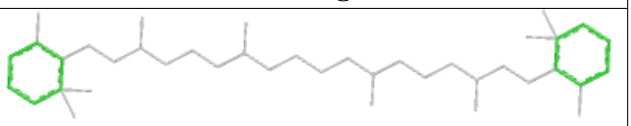


Bond lengths



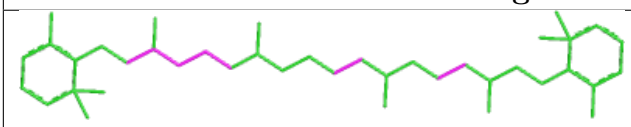
Bond angles

Torsions

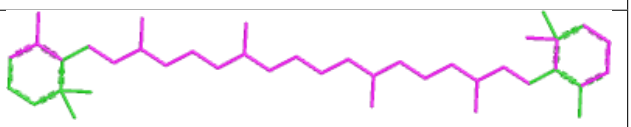


Rings

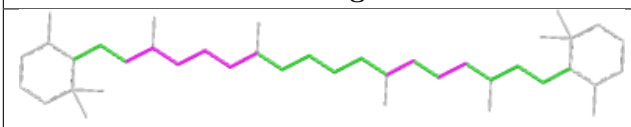
Ligand BCR H 4014



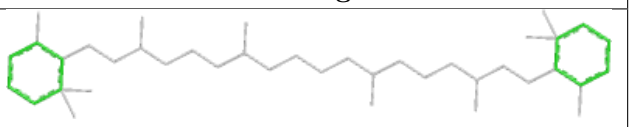
Bond lengths



Bond angles

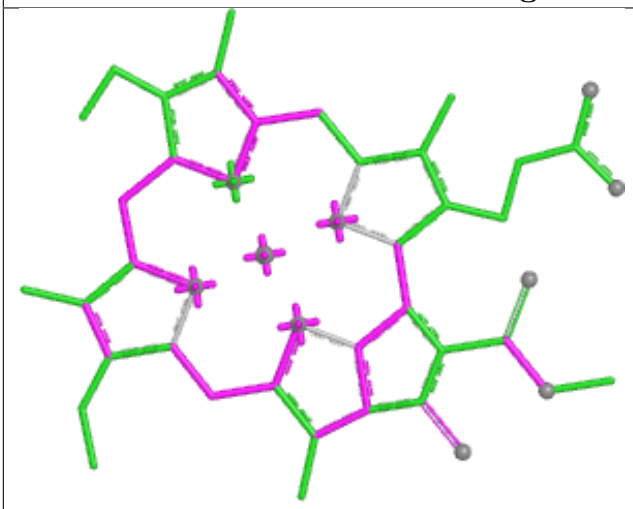


Torsions



Rings

Ligand CLA a 1110



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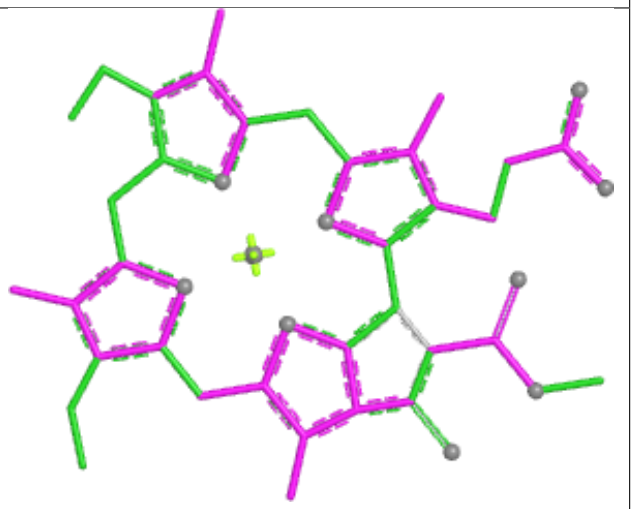
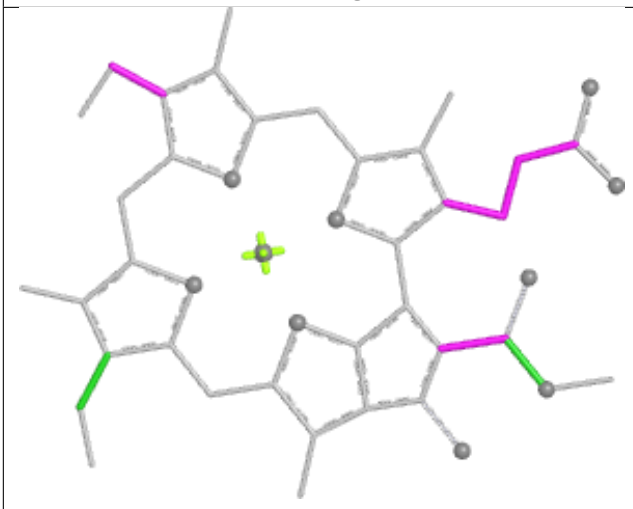


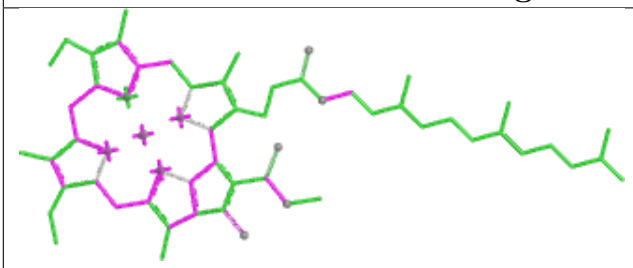
Bond angles



Torsions

Rings

Ligand CLA A 1131



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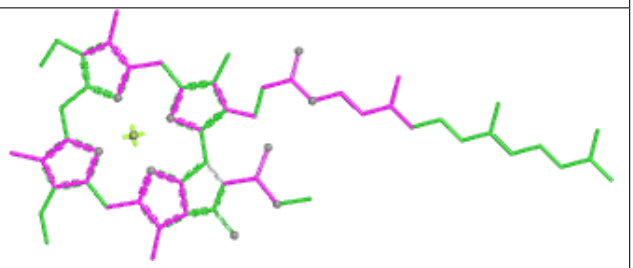
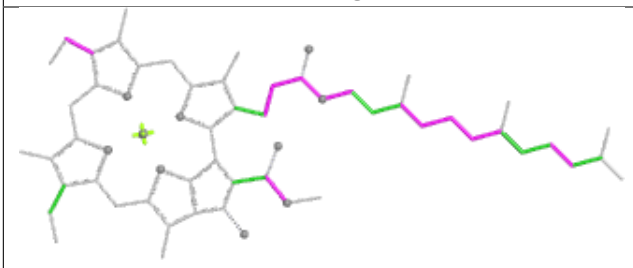
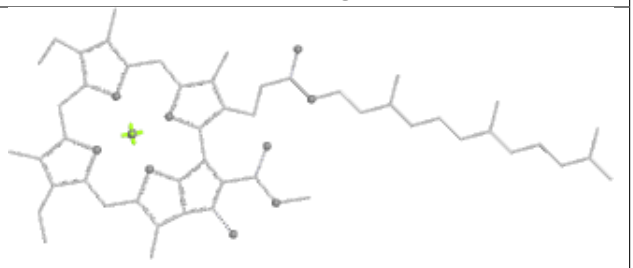


Bond angles

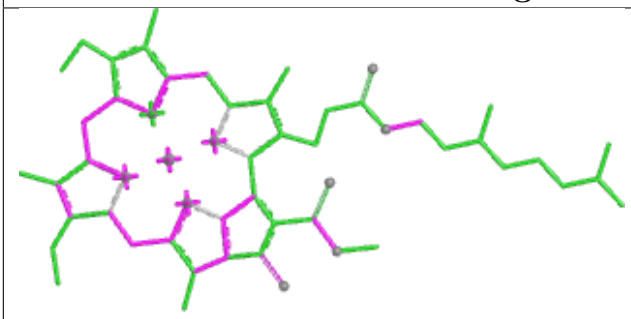


Torsions

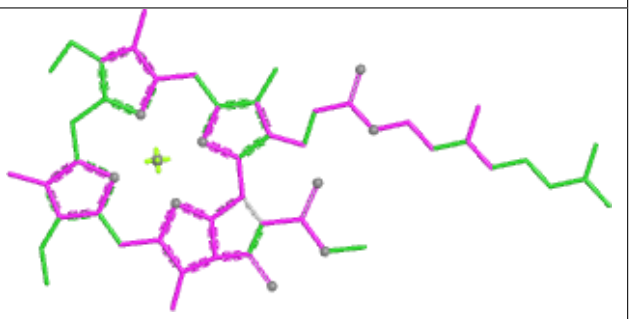


Rings

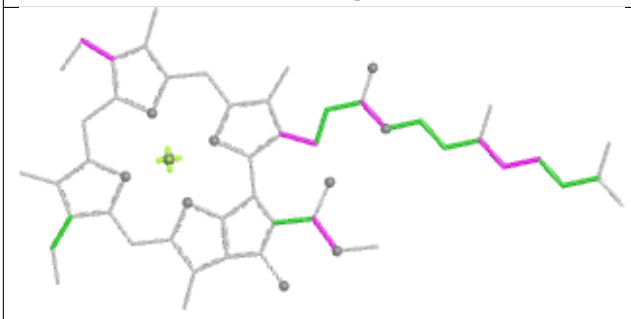
Ligand CLA G 1130



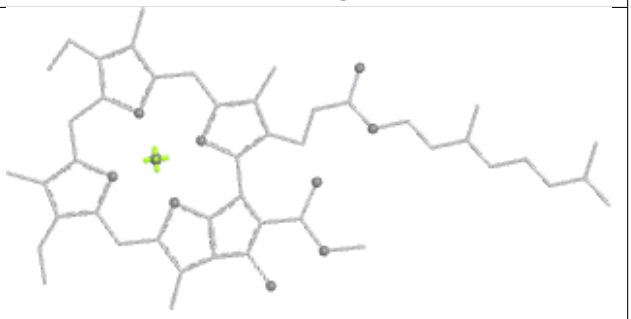
Bond lengths



Bond angles

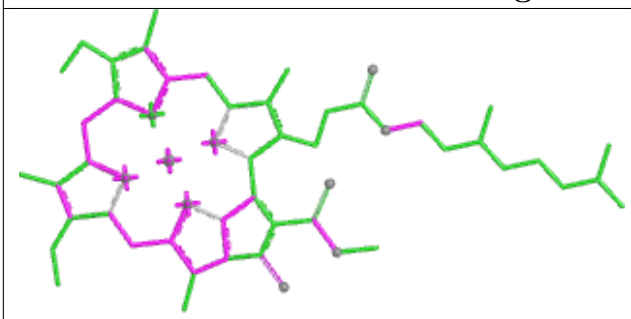


Torsions



Rings

Ligand CLA H 1213



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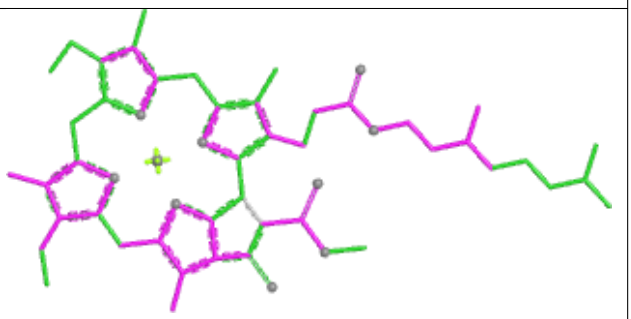
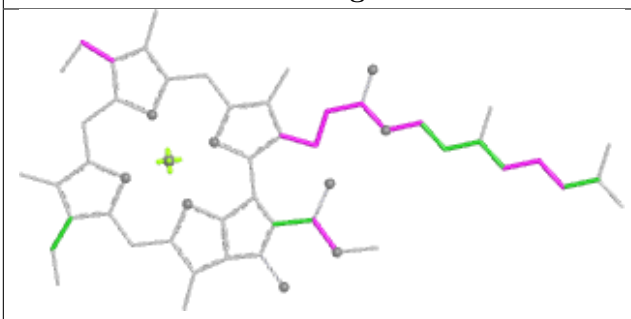
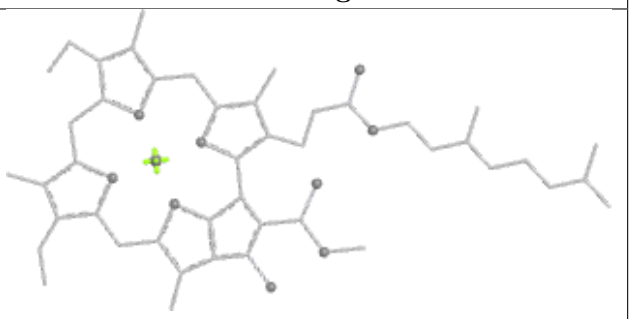


Bond angles

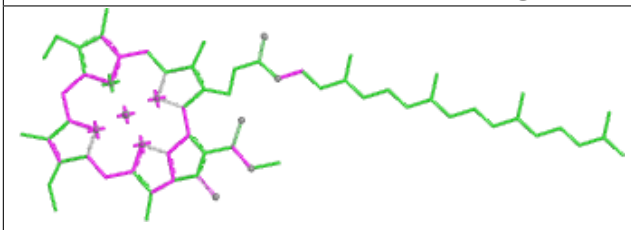


Torsions



Rings

Ligand CLA H 1223



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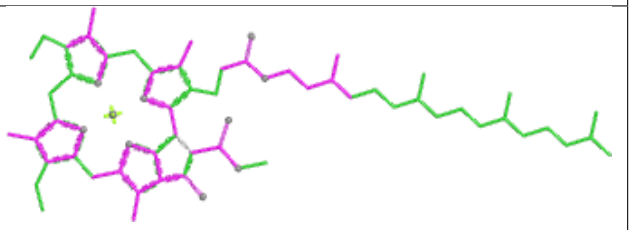
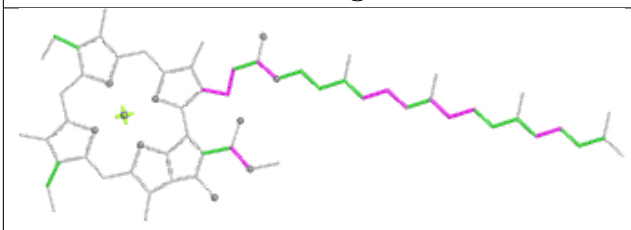
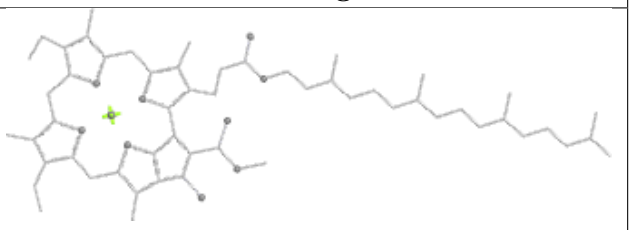


Bond angles

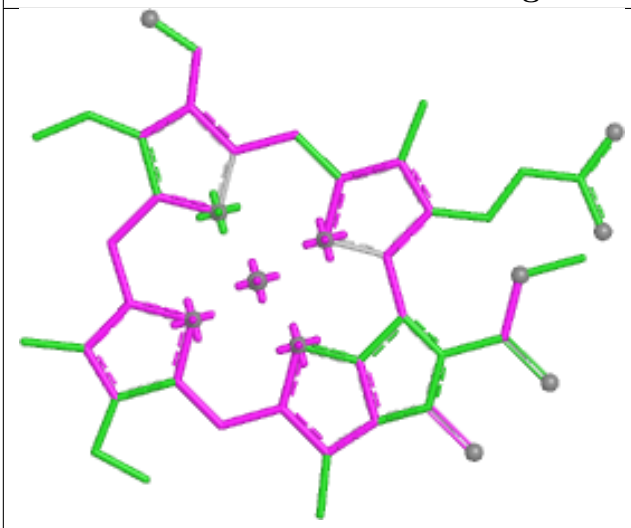


Torsions



Rings

Ligand F6C b 1230



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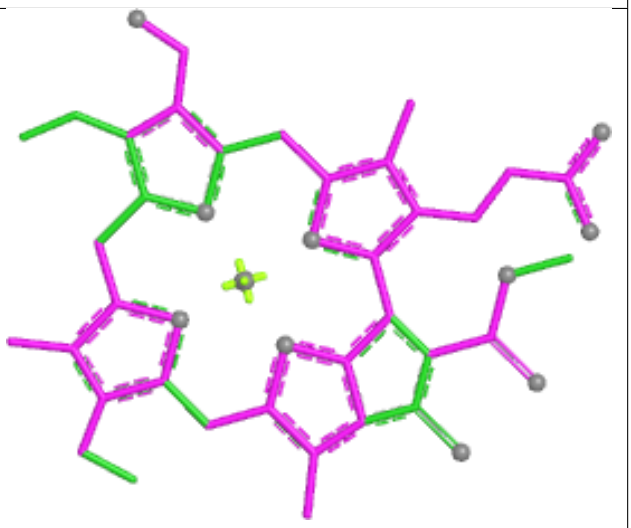
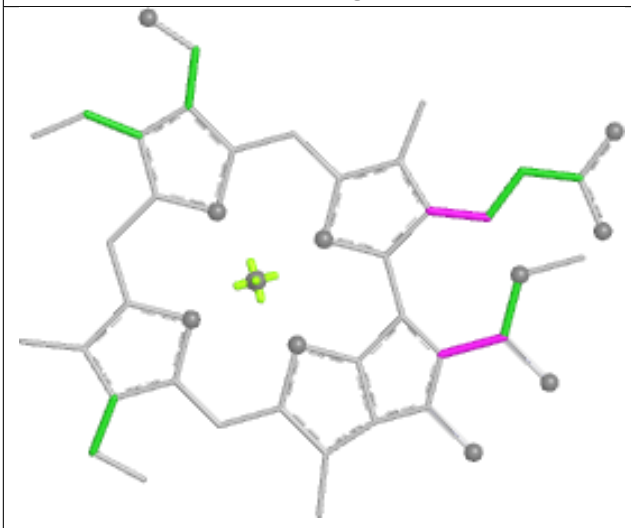
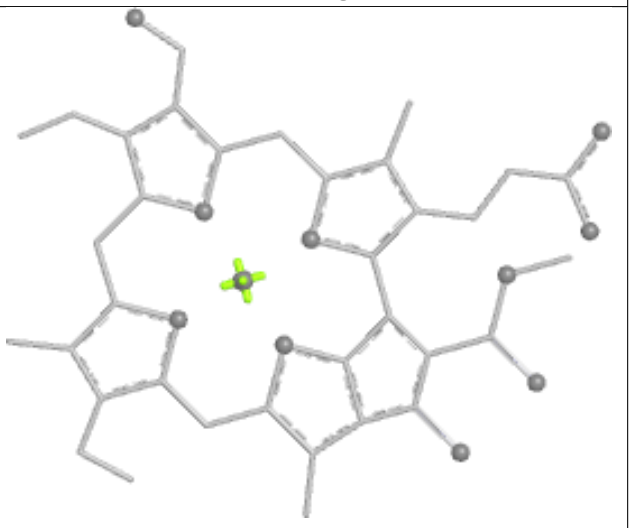


Bond angles

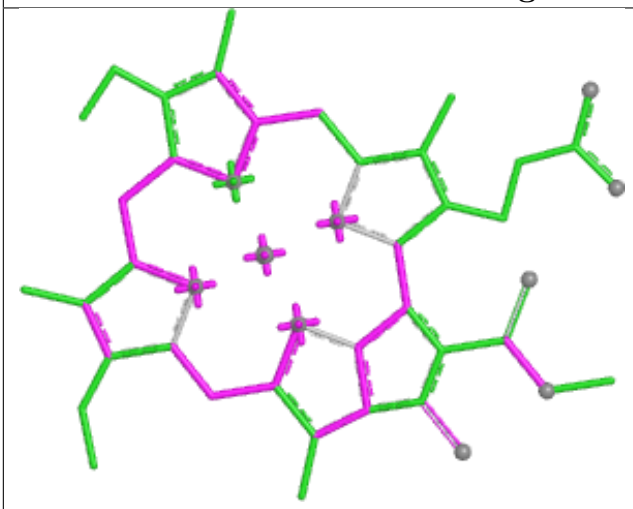


Torsions



Rings

Ligand CLA b 1219



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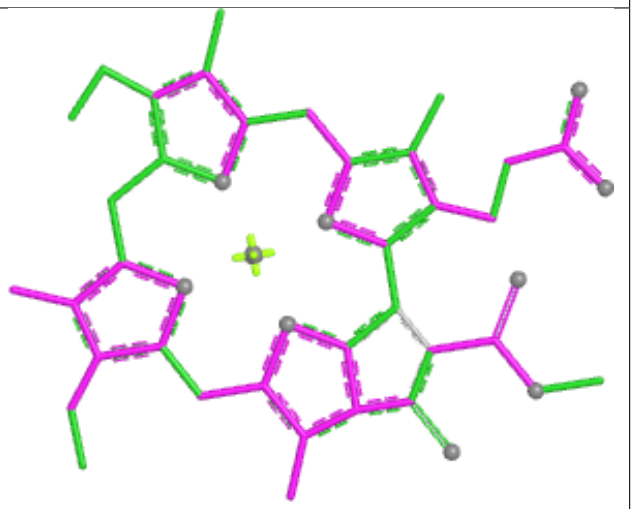
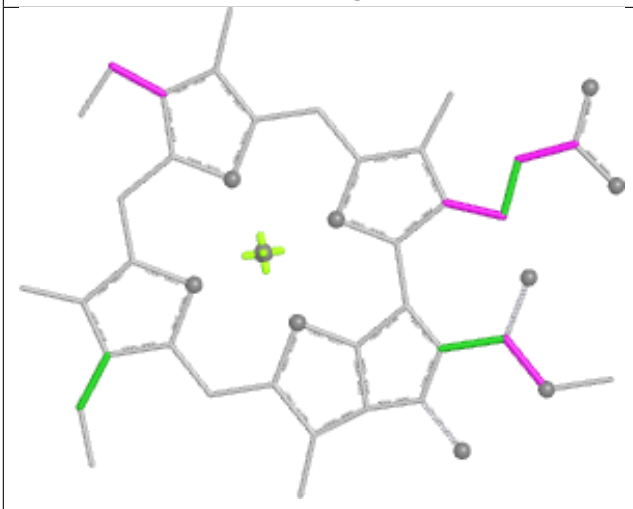


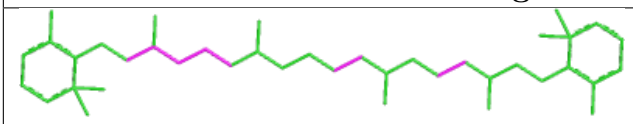
Bond angles



Torsions

Rings

Ligand BCR H 4006



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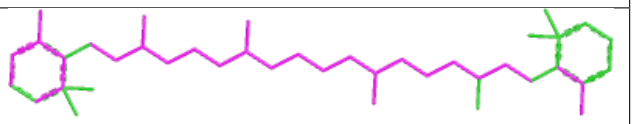
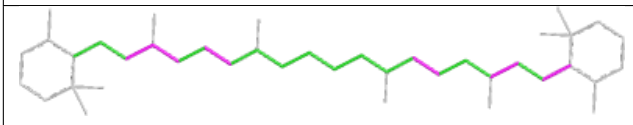
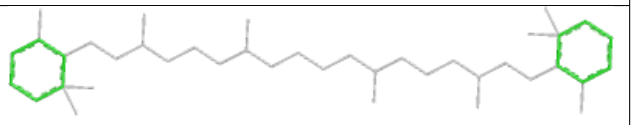


Bond angles

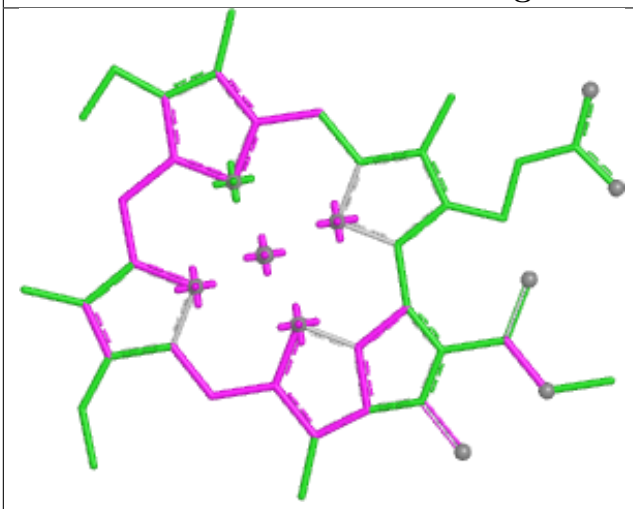


Torsions



Rings

Ligand CLA G 1108



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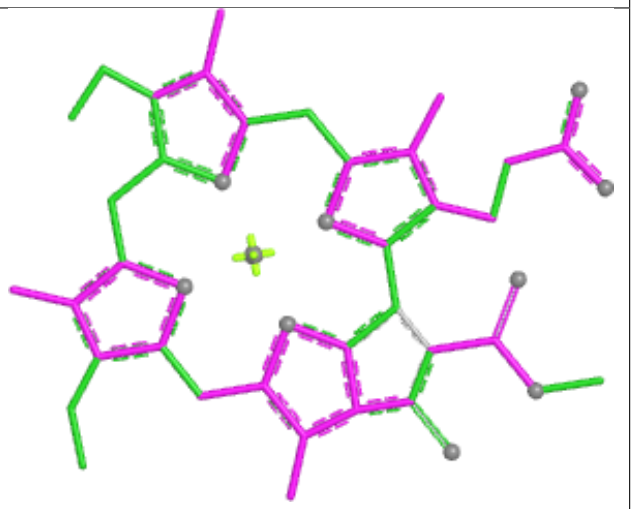
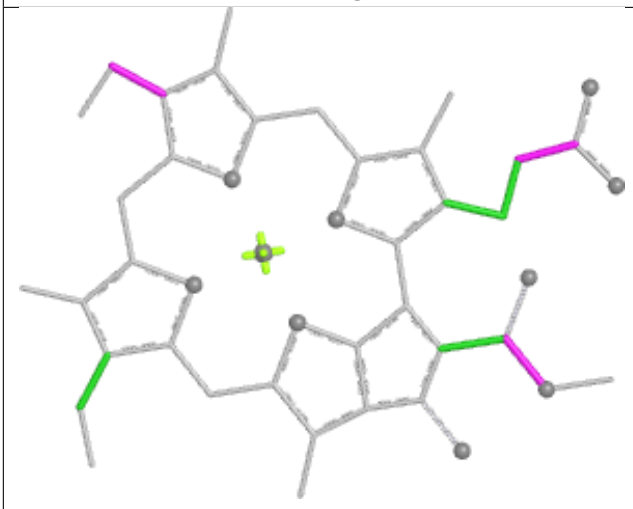


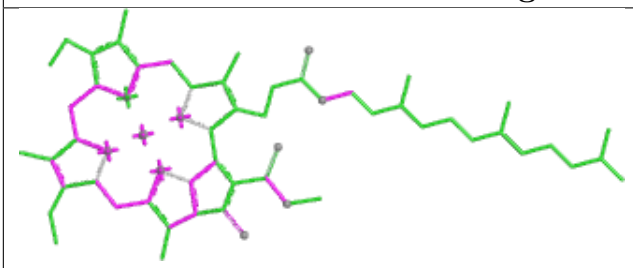
Bond angles



Torsions

Rings

Ligand CLA b 1215



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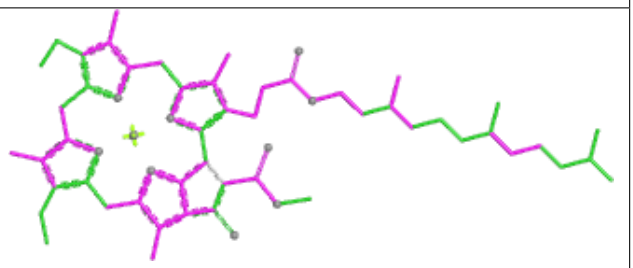
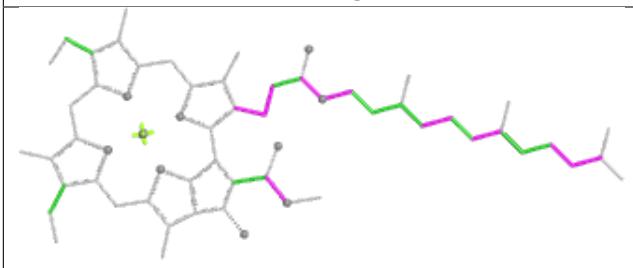
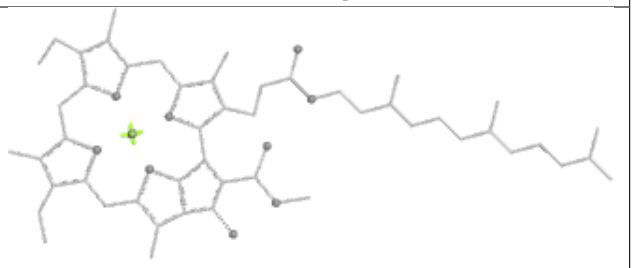


Bond angles

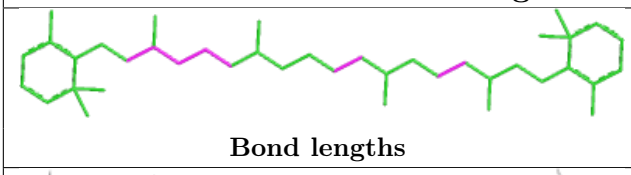


Torsions



Rings

Ligand BCR H 4013



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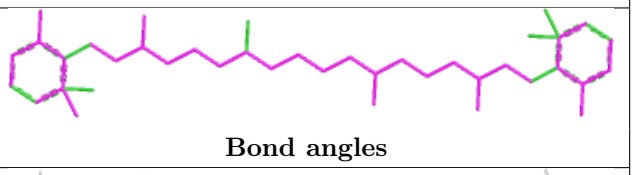
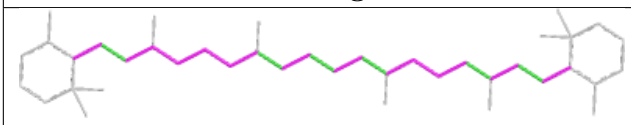
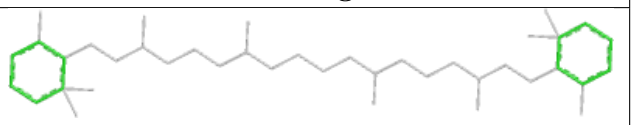


Bond angles

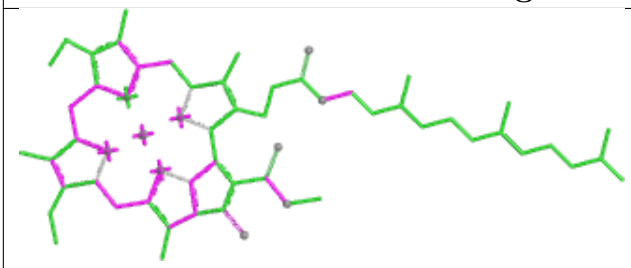


Torsions

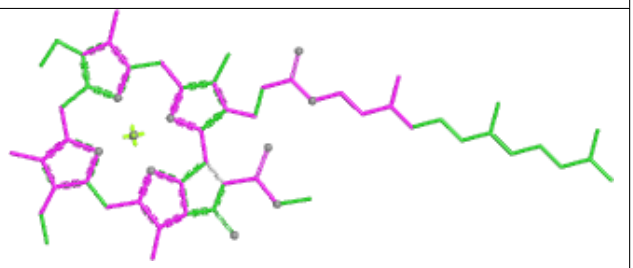


Rings

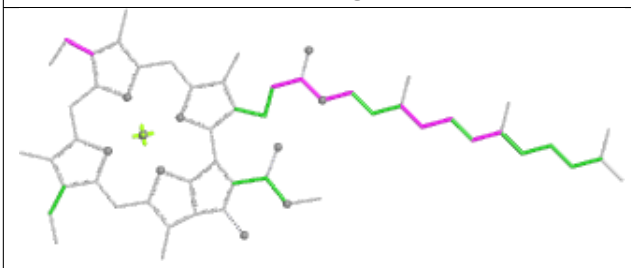
Ligand CLA B 1202



Bond lengths



Bond angles



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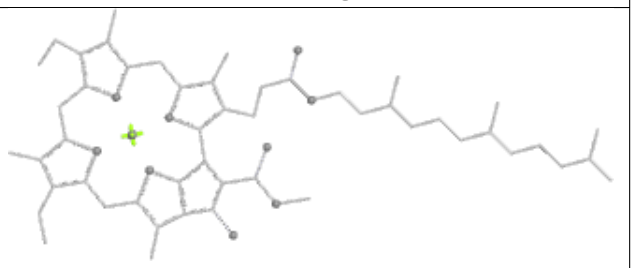
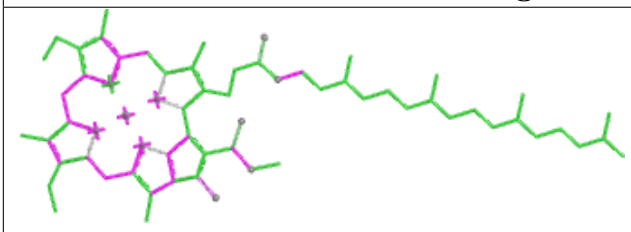
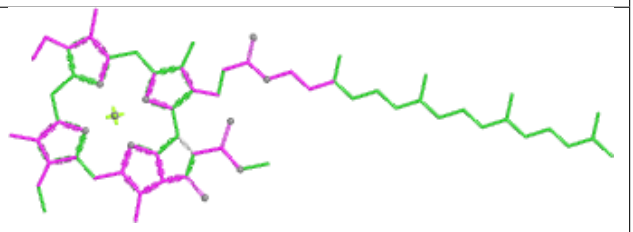


Rings

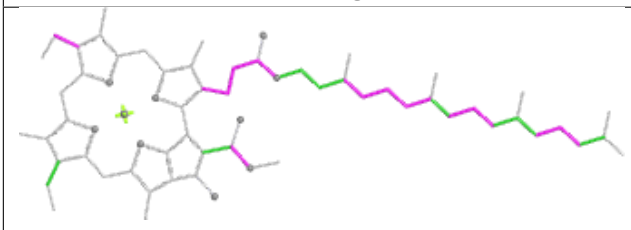
Ligand CLA B 1204



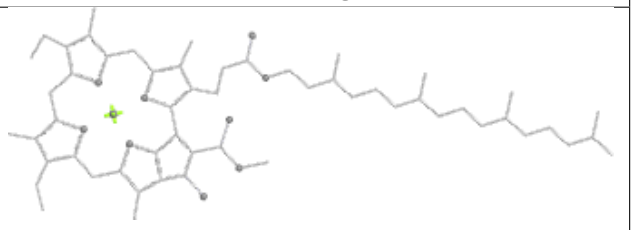
Bond lengths



Bond angles

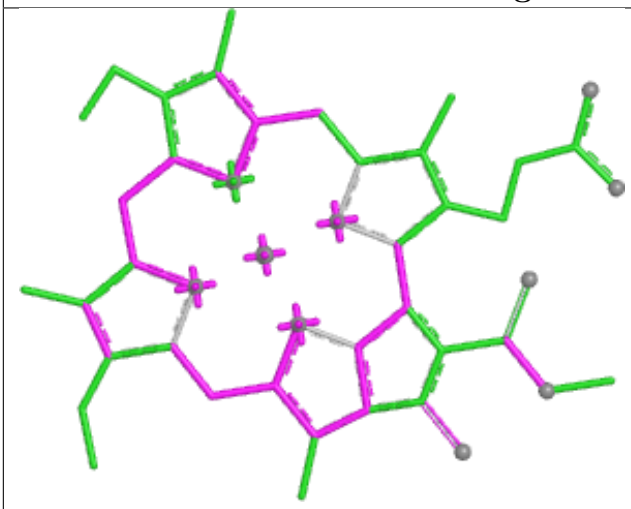


Torsions

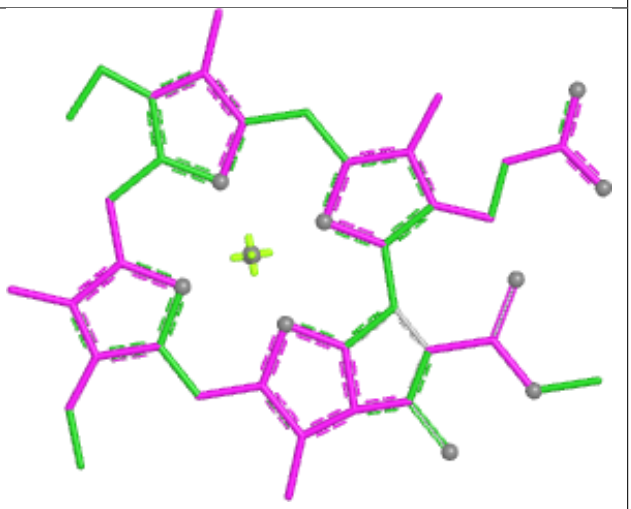


Rings

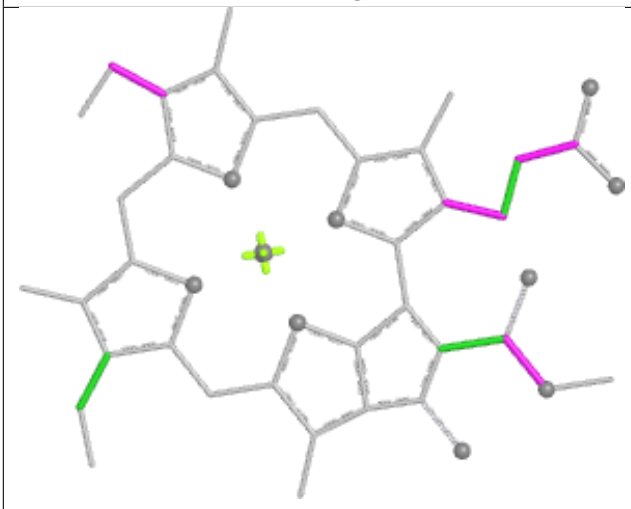
Ligand CLA G 1109



Bond lengths



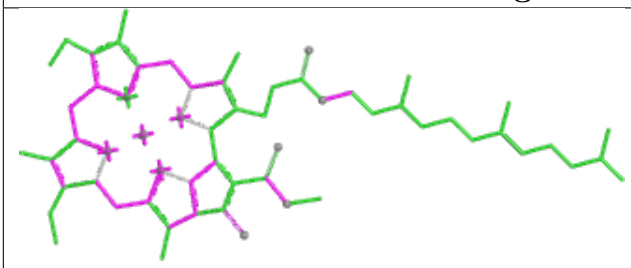
Bond angles



Torsions

Rings

Ligand CLA G 1013



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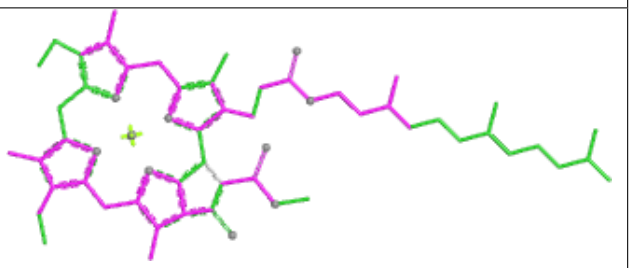
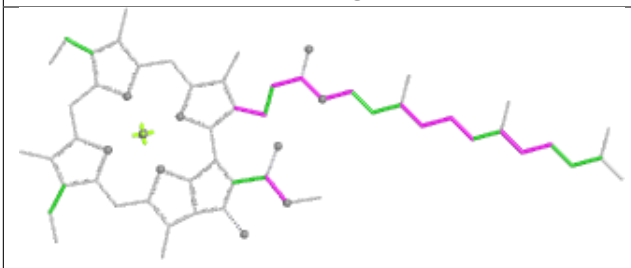
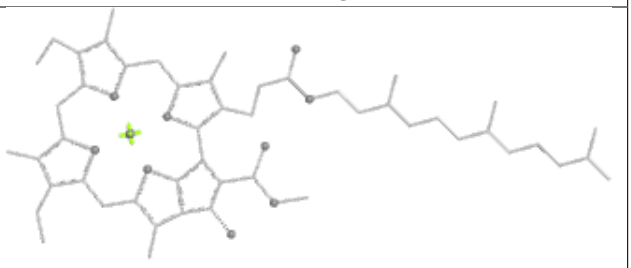


Bond angles

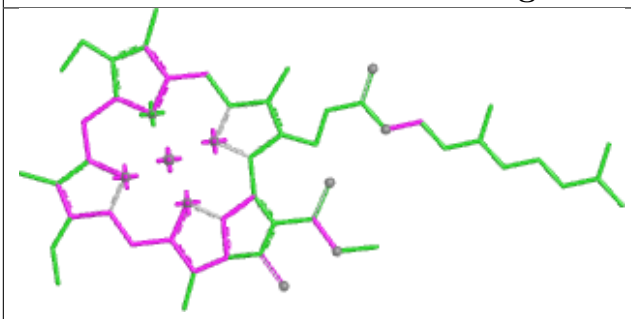


Torsions



Rings

Ligand CLA b 1216



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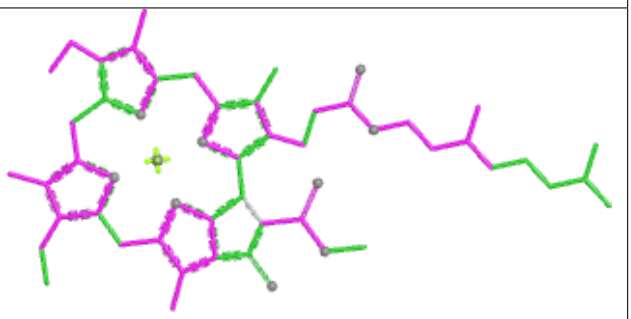
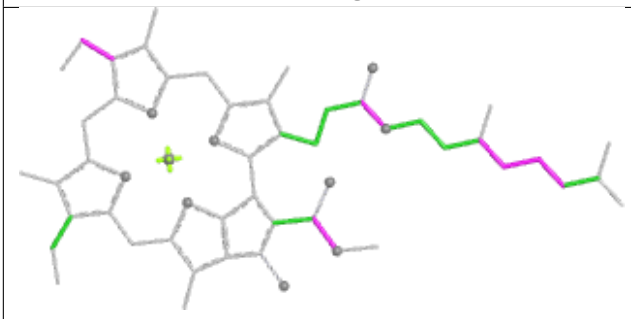
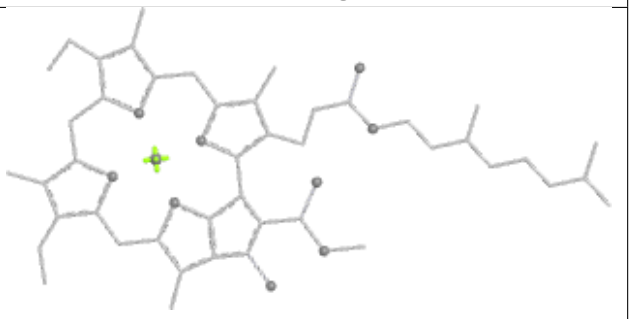


Bond angles

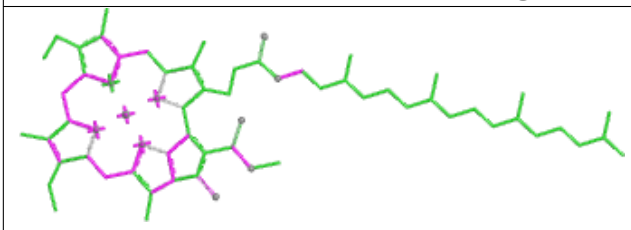


Torsions



Rings

Ligand CLA H 1204



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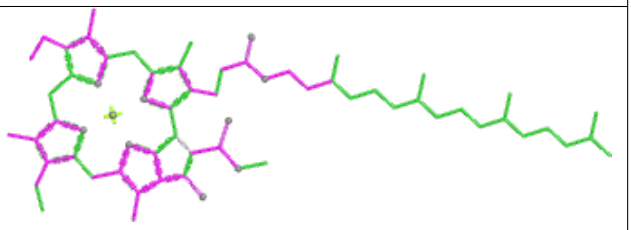
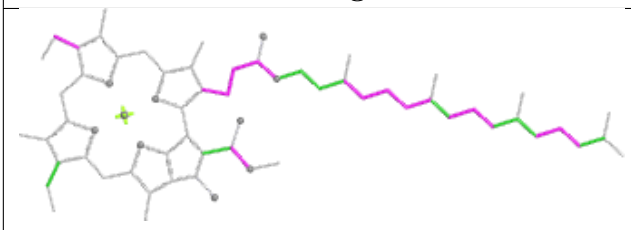
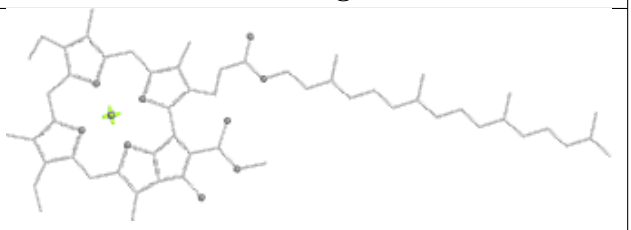


Bond angles

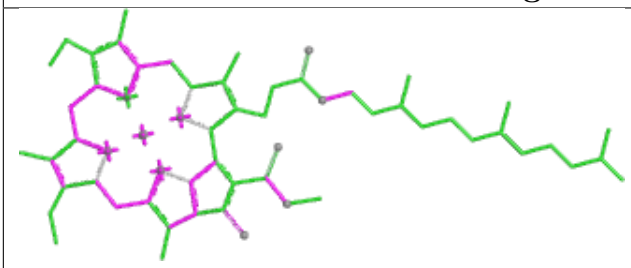


Torsions



Rings

Ligand CLA l 1502



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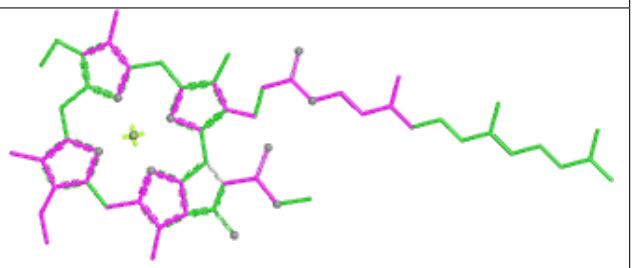
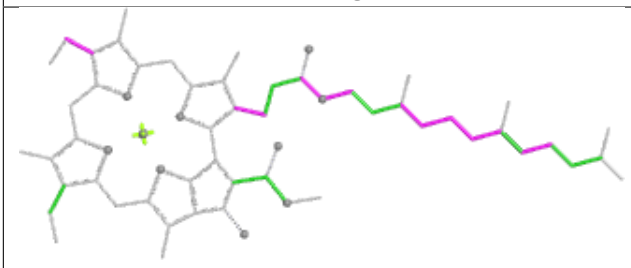
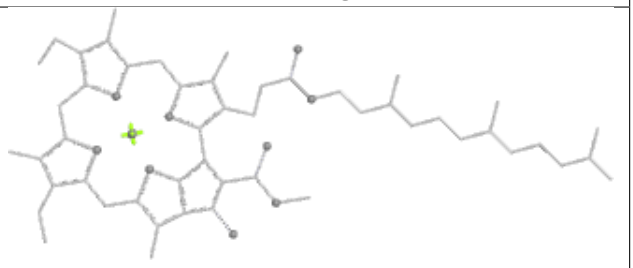


Bond angles

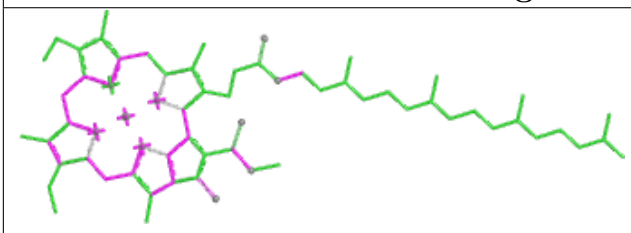


Torsions

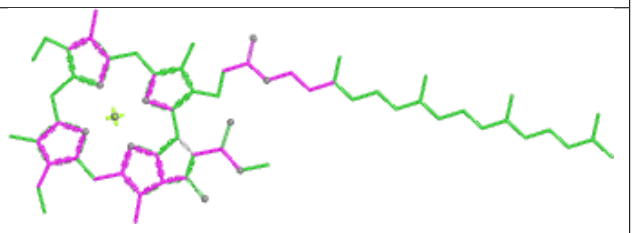


Rings

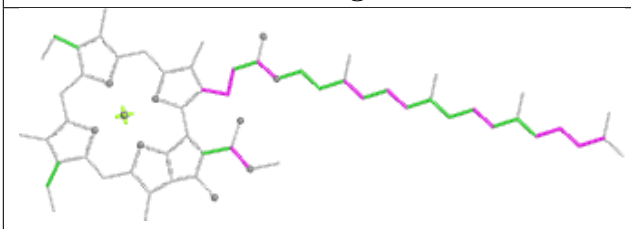
Ligand CLA B 1225



Bond lengths



Bond angles



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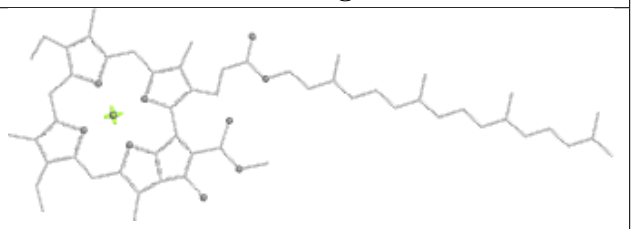
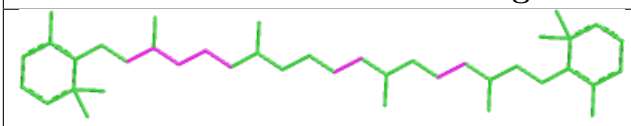


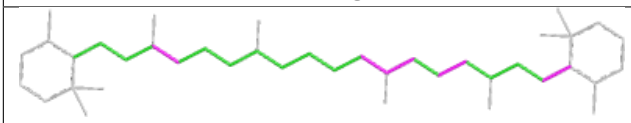
Rings

Ligand BCR H 4010

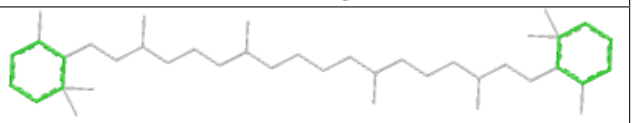


Bond lengths

Bond angles

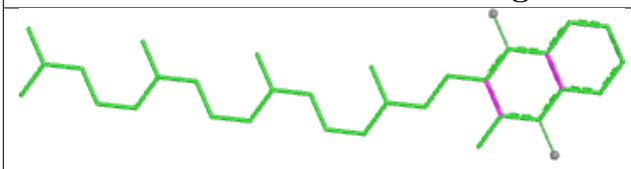


Torsions



Rings

Ligand PQN G 2001



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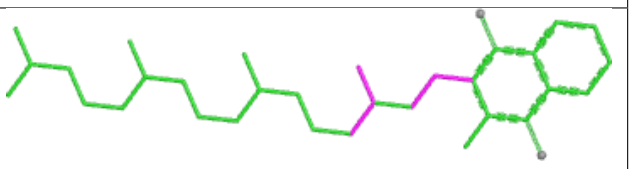
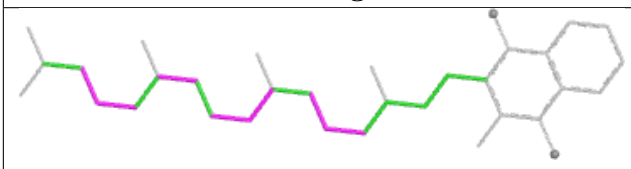
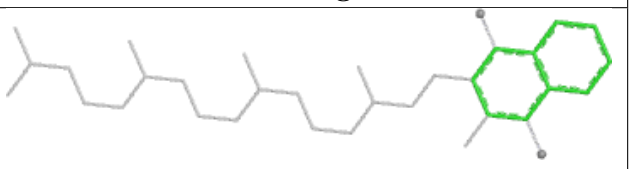


Bond angles

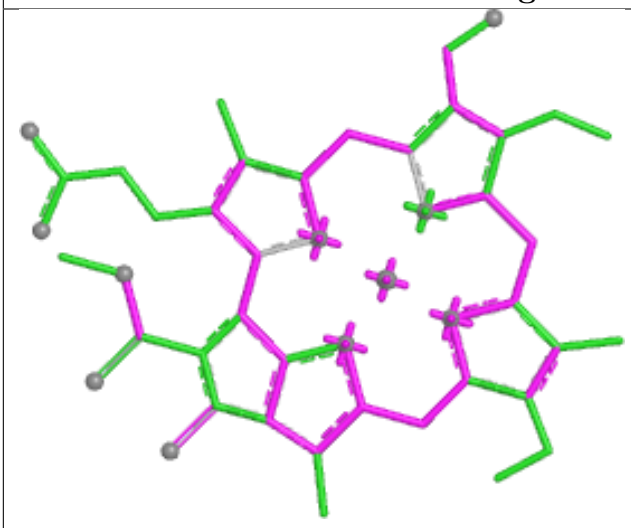


Torsions

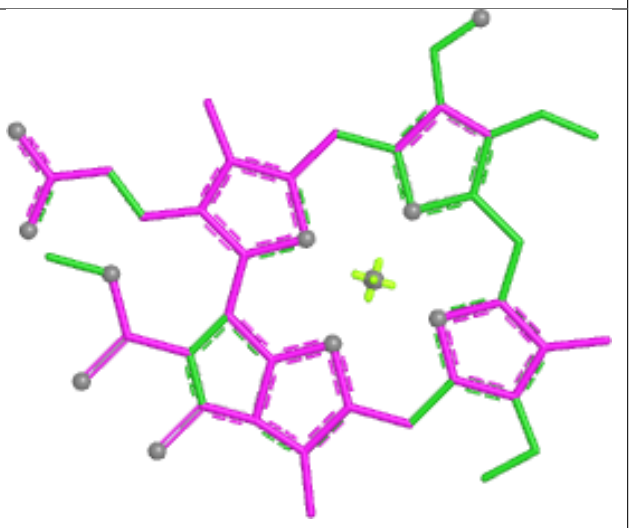


Rings

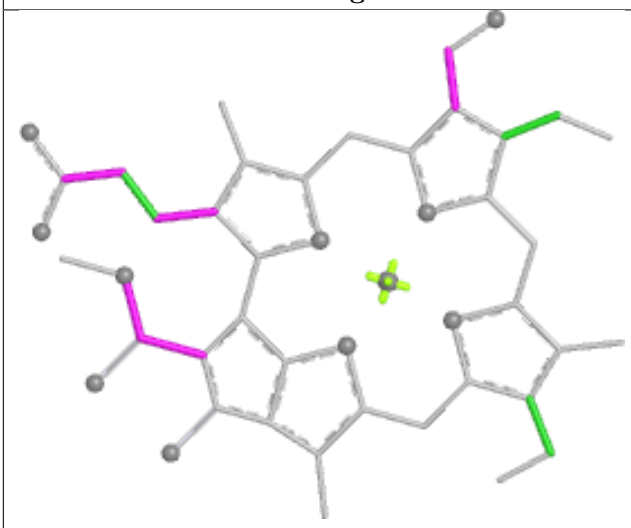
Ligand F6C G 1120



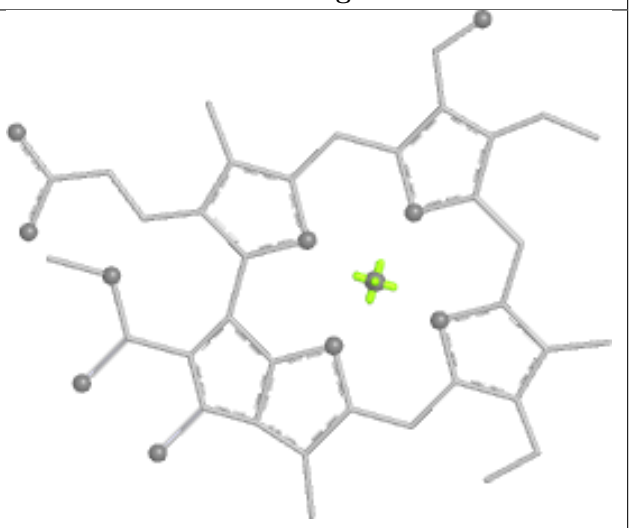
Bond lengths



Bond angles

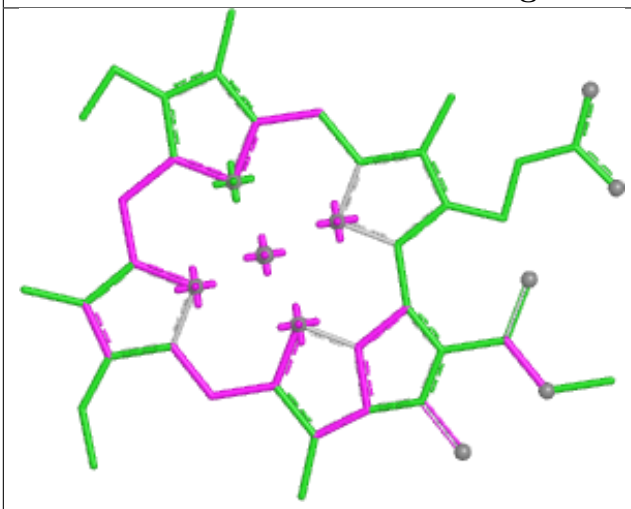


Torsions



Rings

Ligand CLA a 1129



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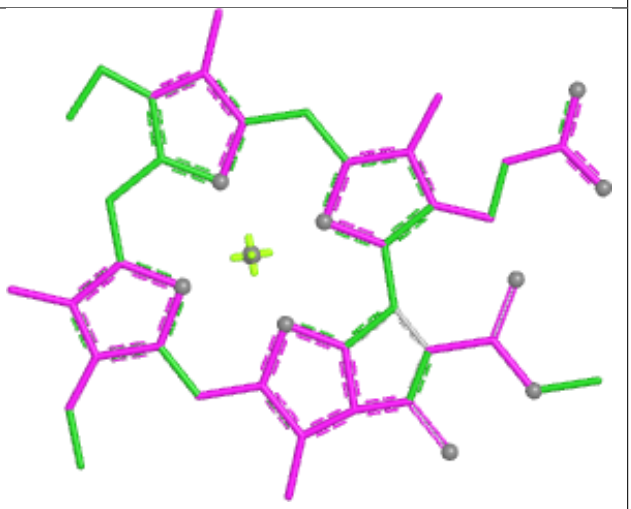
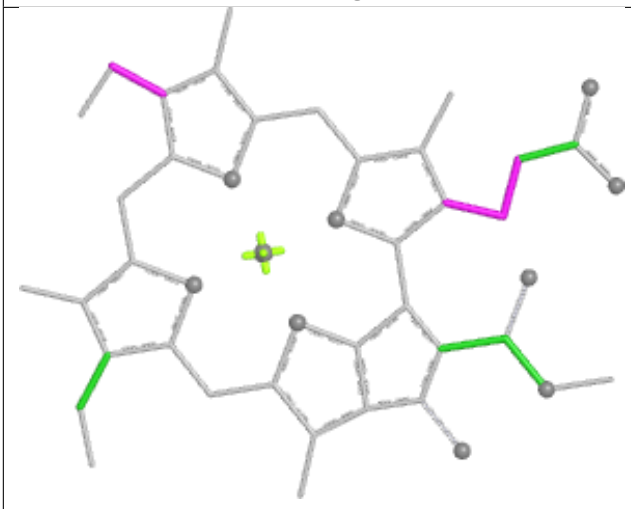


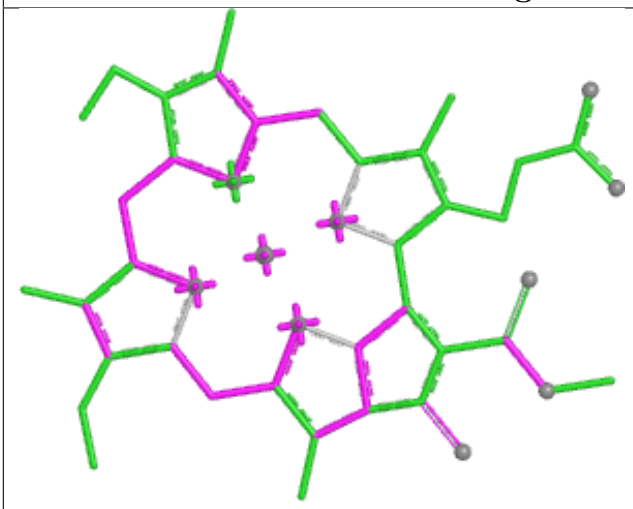
Bond angles



Torsions

Rings

Ligand CLA X 1701



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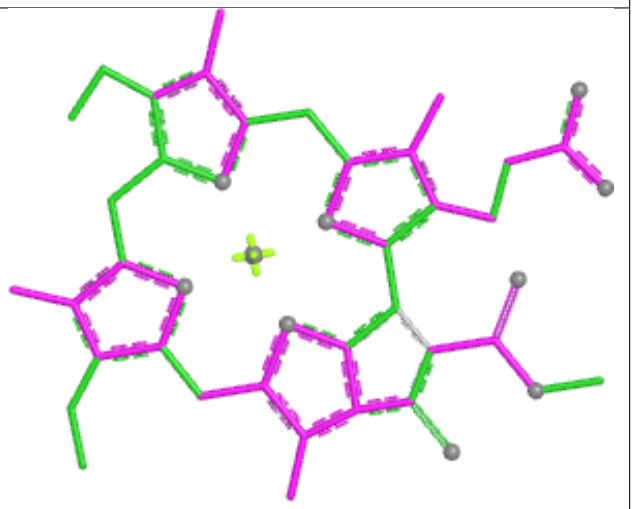
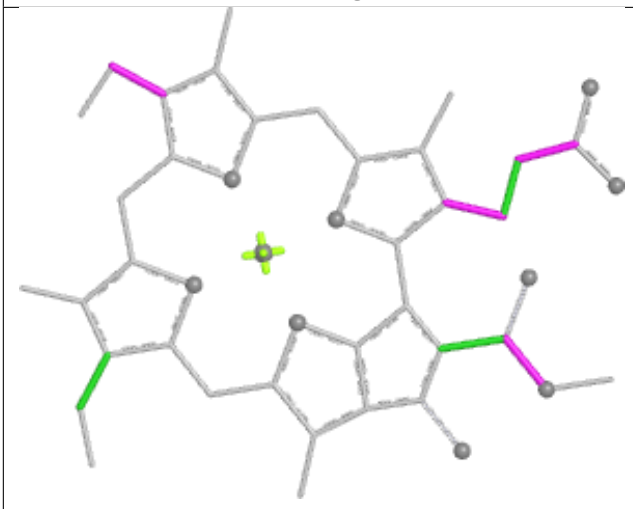


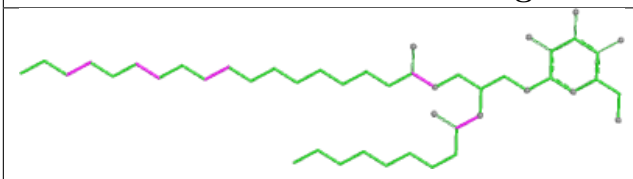
Bond angles



Torsions

Rings

Ligand LMG a 5005



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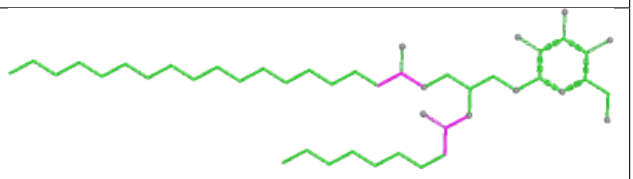
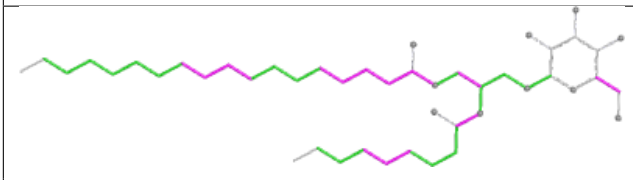


Bond angles



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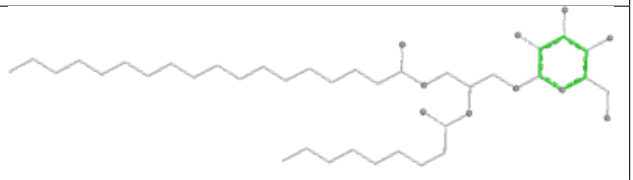
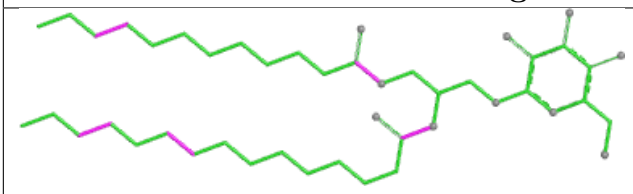
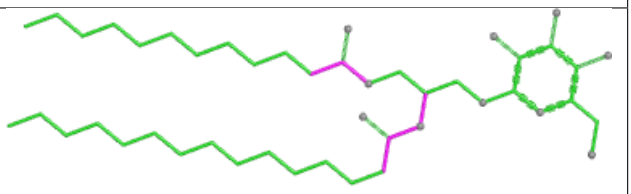


Rings

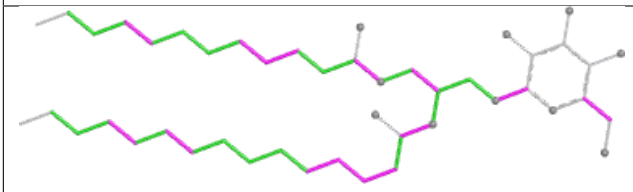
Ligand LMG H 5002



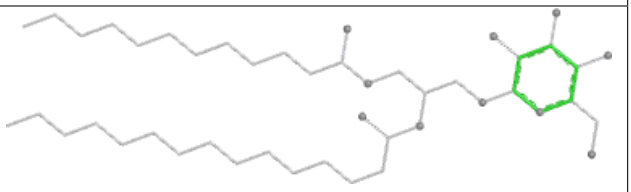
Bond lengths



Bond angles

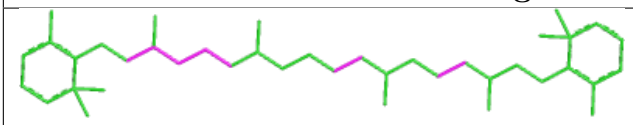


Torsions

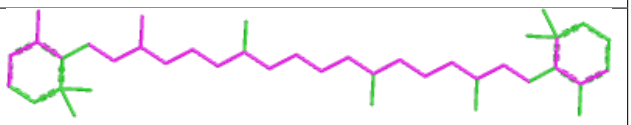


Rings

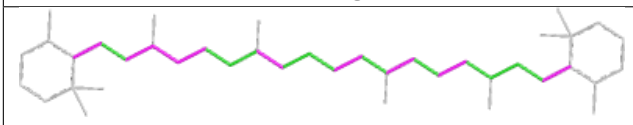
Ligand BCR B 4016



Bond lengths



Bond angles



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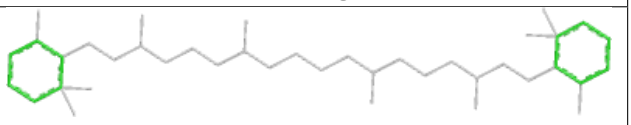
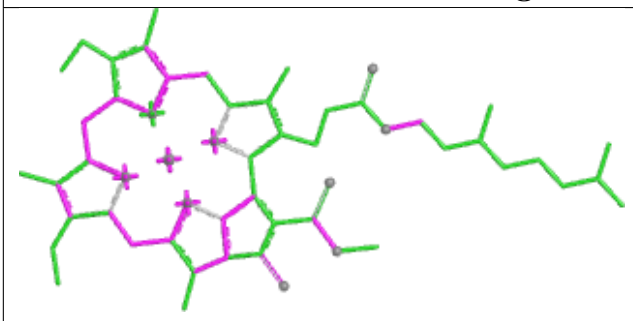
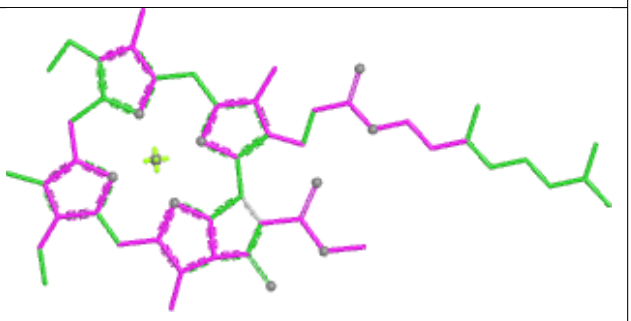


Rings

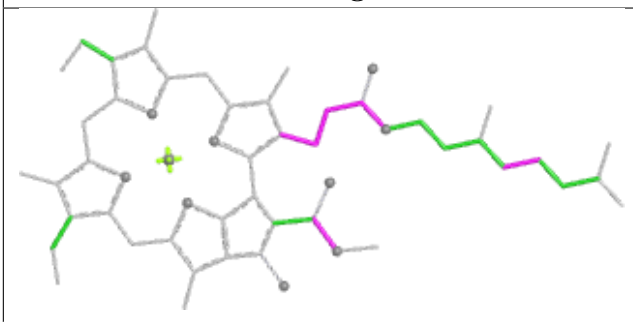
Ligand CLA B 1220



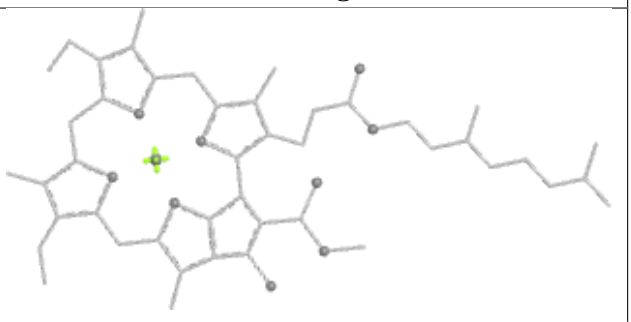
Bond lengths



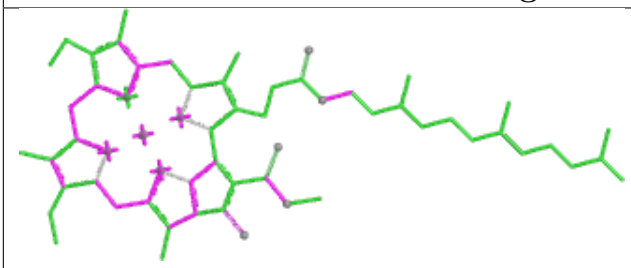
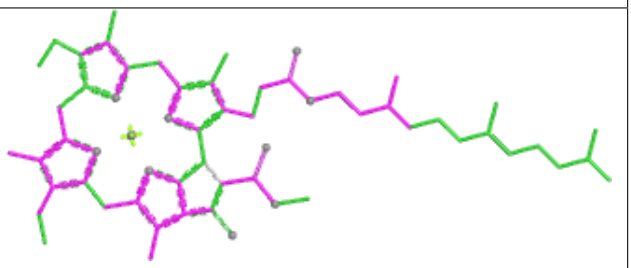
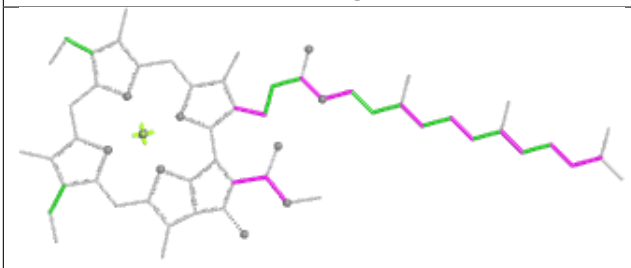
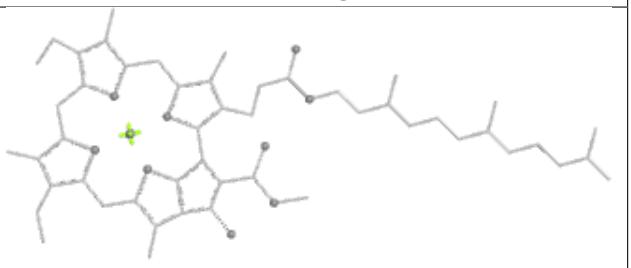
Bond angles

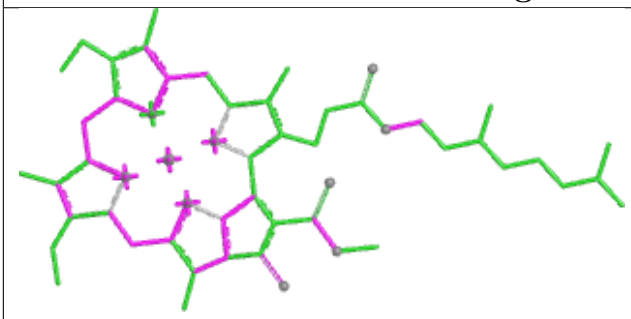
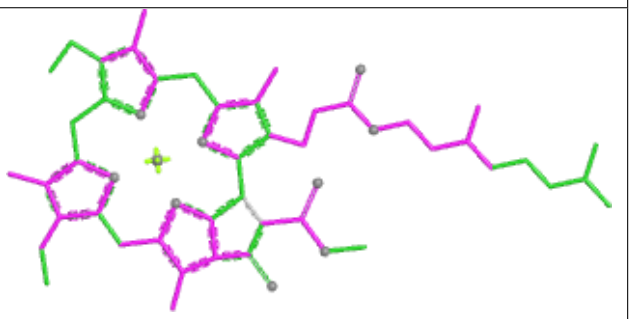
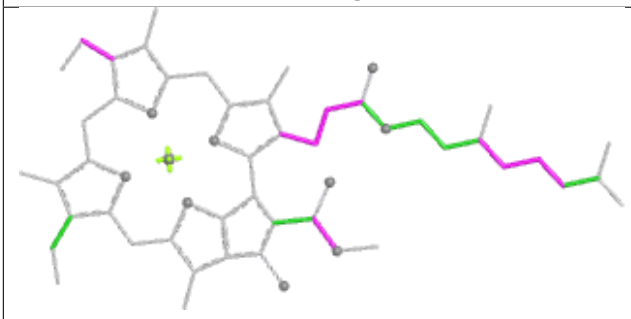
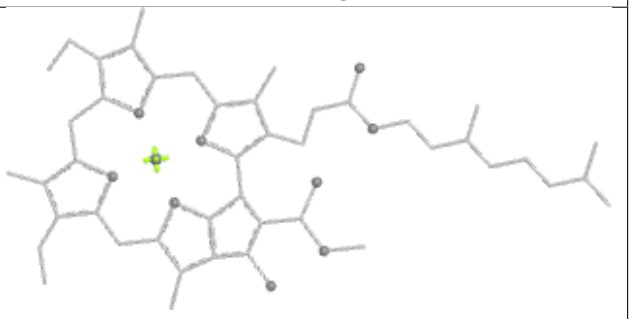


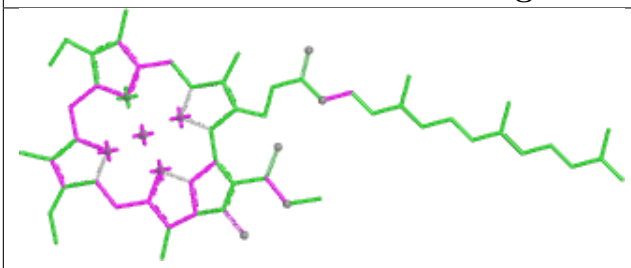
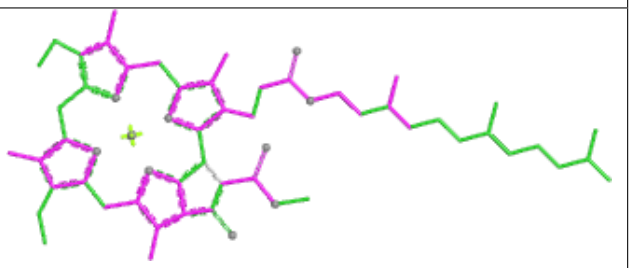
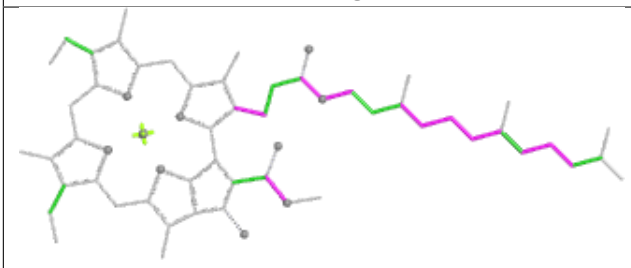
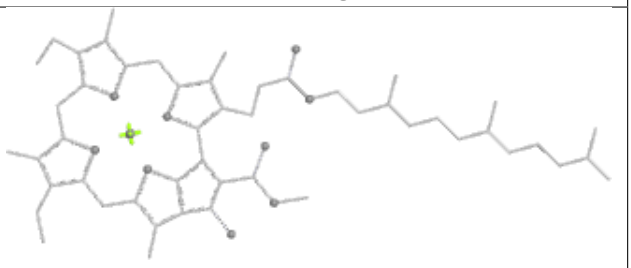
Torsions

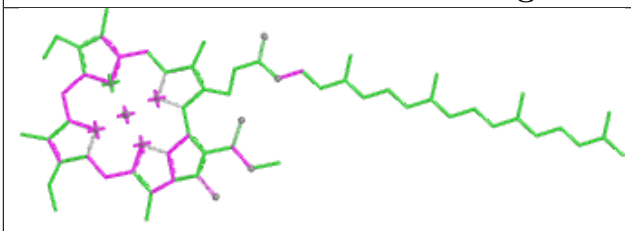
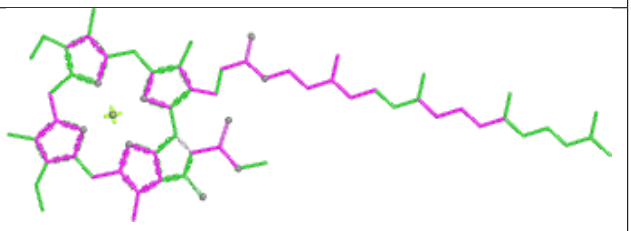
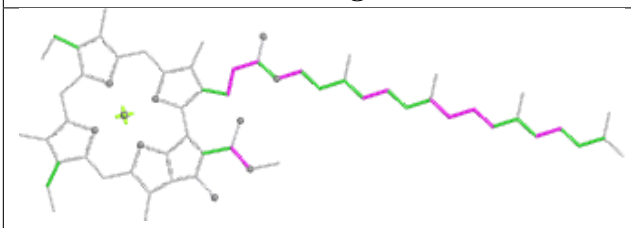
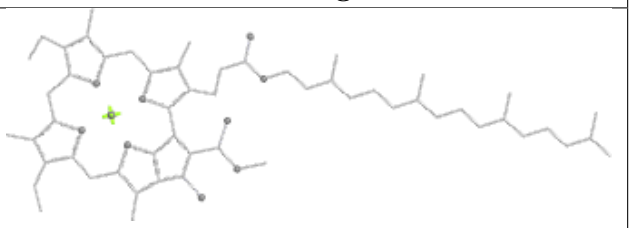


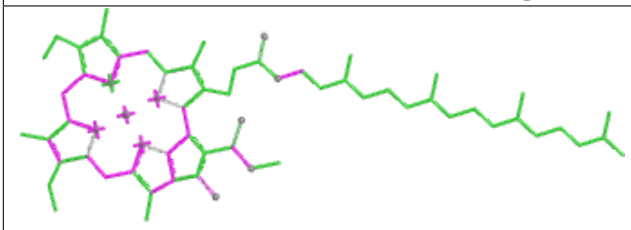
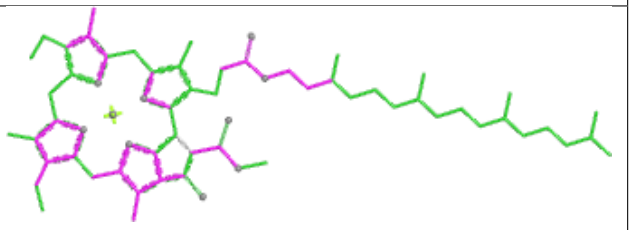
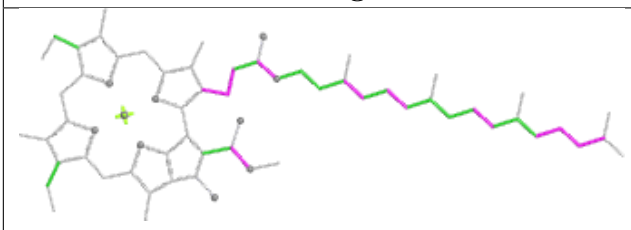
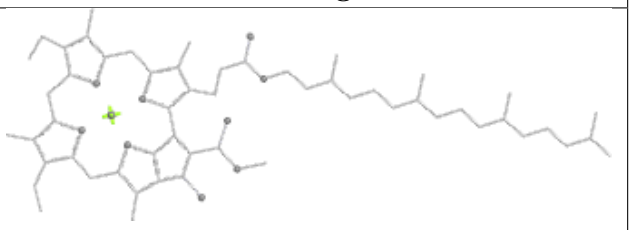
Rings

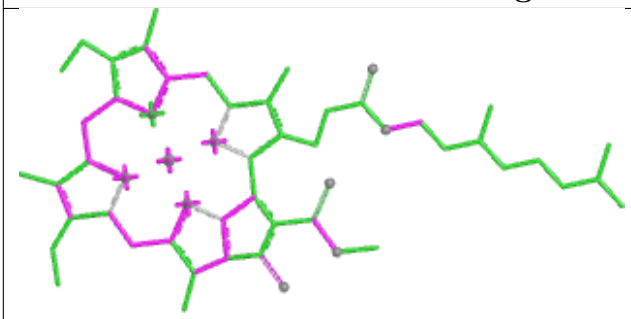
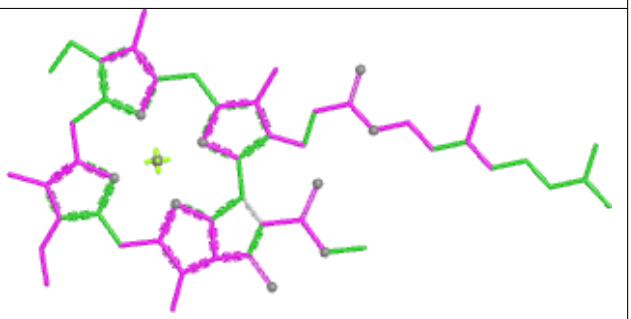
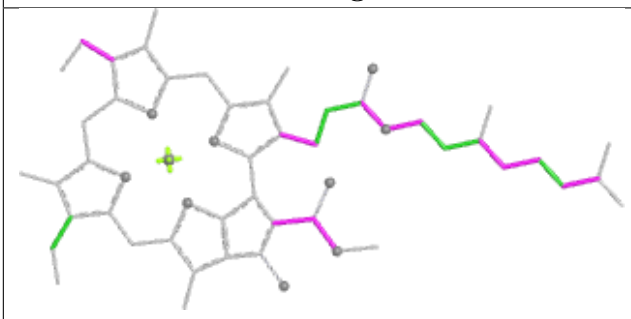
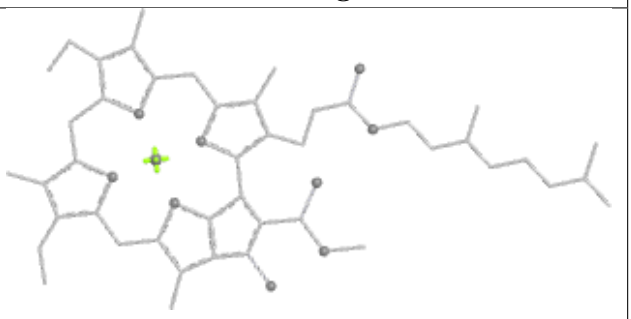
Ligand CLA a 1103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1116	
	
Bond lengths	Bond angles
	
Torsions	Rings

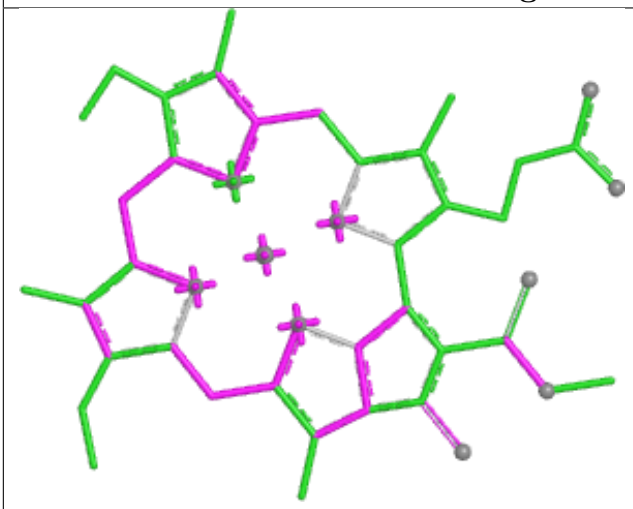
Ligand CLA B 1229	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 1503	
	
Bond lengths	Bond angles
	
Torsions	Rings

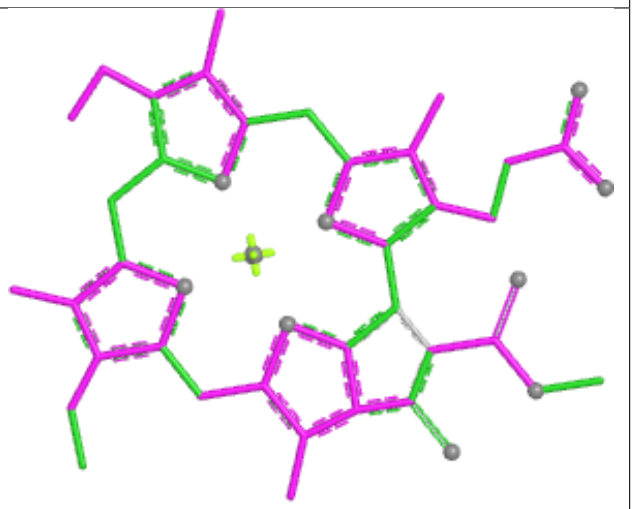
Ligand CLA b 1225	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1118	
	
Bond lengths	Bond angles
	
Torsions	Rings

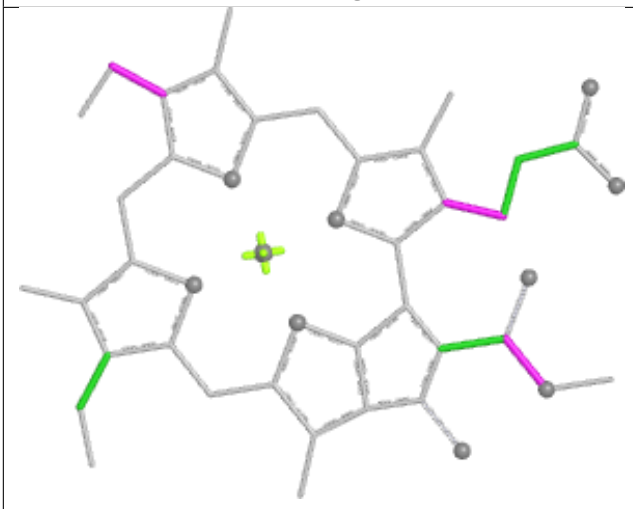
Ligand CLA a 1107



Bond lengths



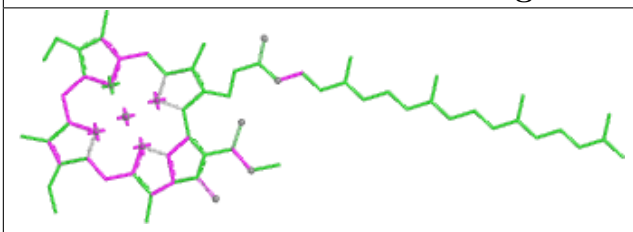
Bond angles



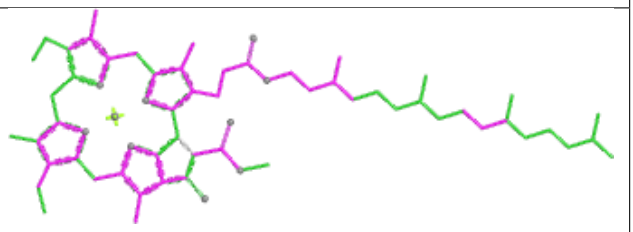
Torsions

Rings

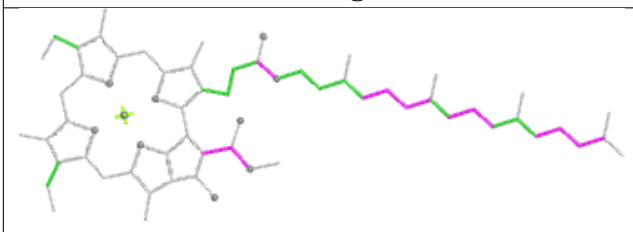
Ligand CLA B 1222



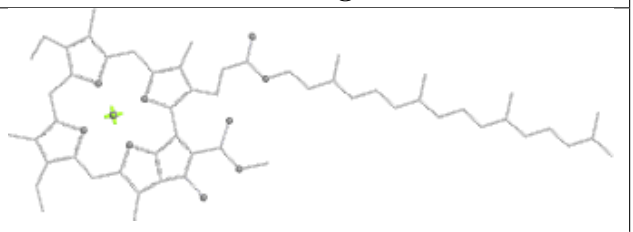
Bond lengths



Bond angles

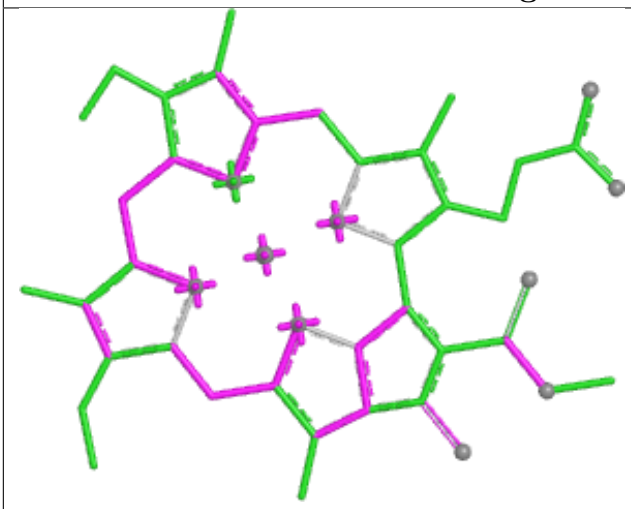


Torsions



Rings

Ligand CLA a 1137



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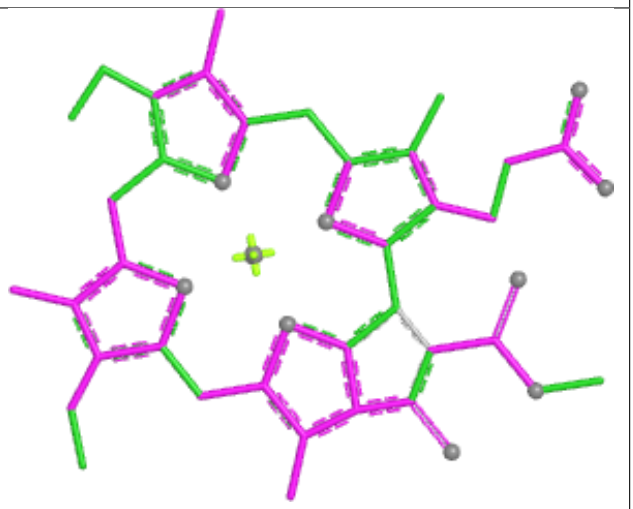
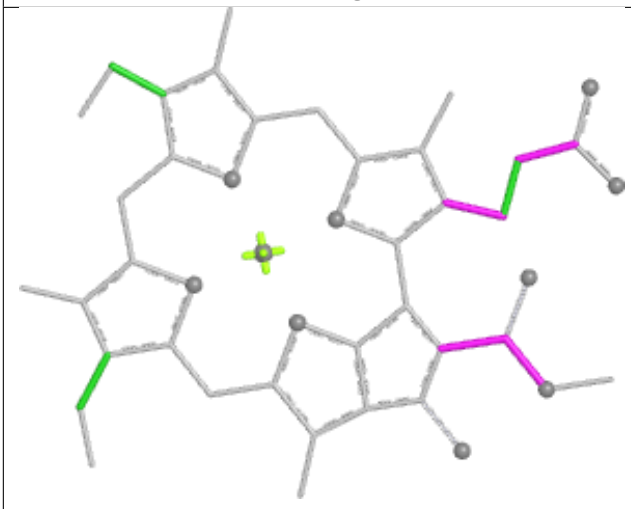


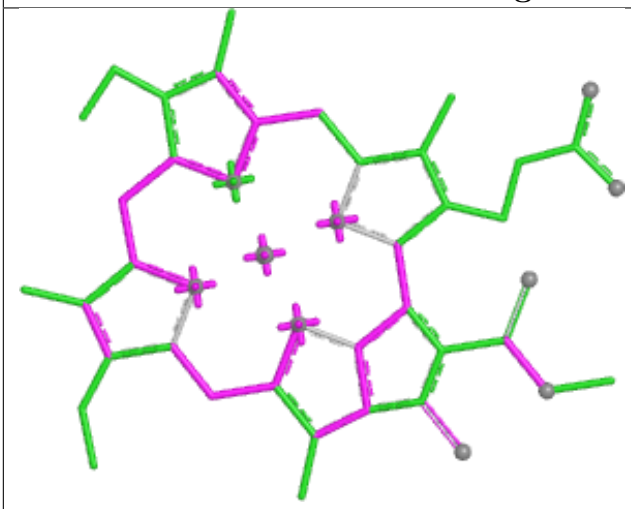
Bond angles



Torsions

Rings

Ligand CLA H 1219



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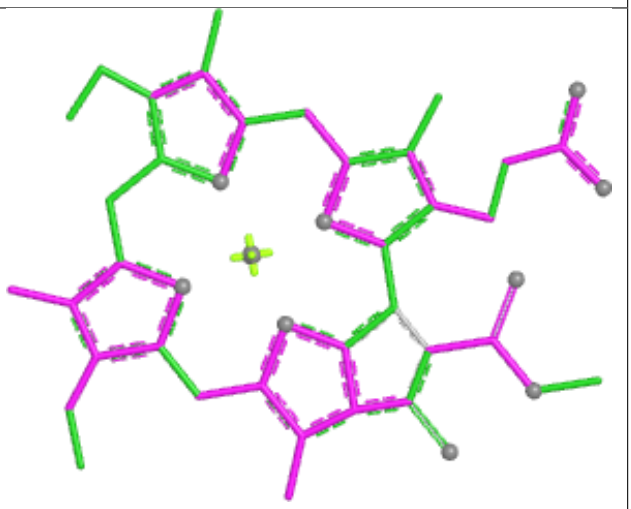

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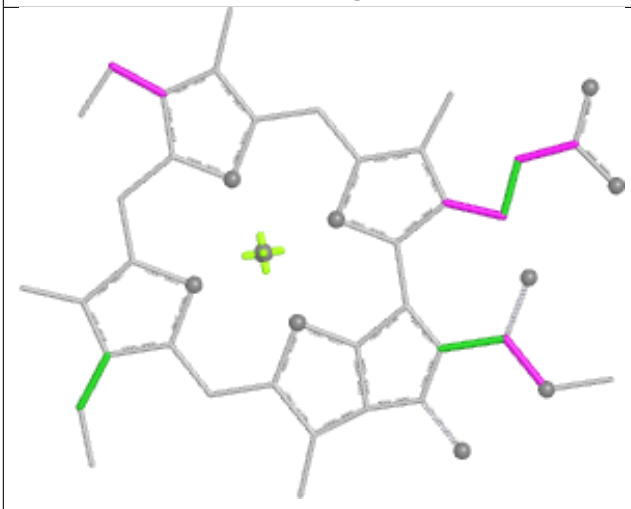
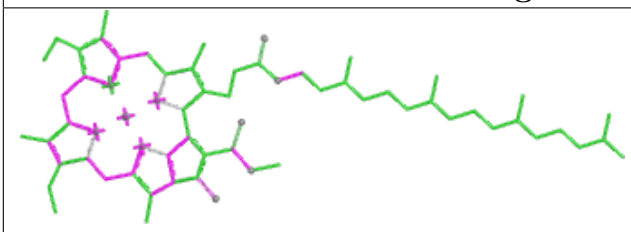


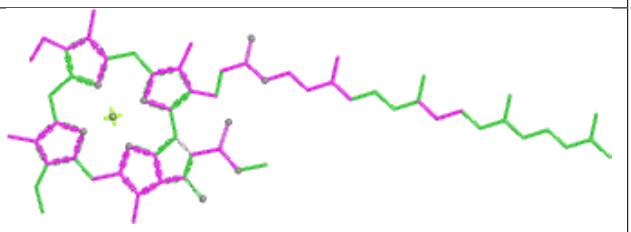
Torsions

Rings

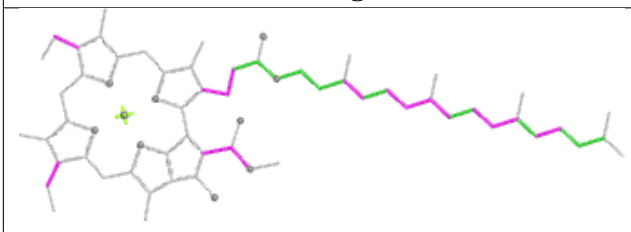
Ligand CLA A 1132



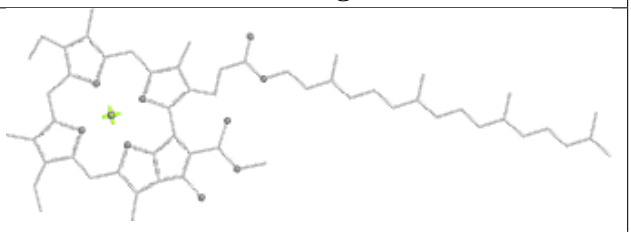
Bond lengths



Bond angles

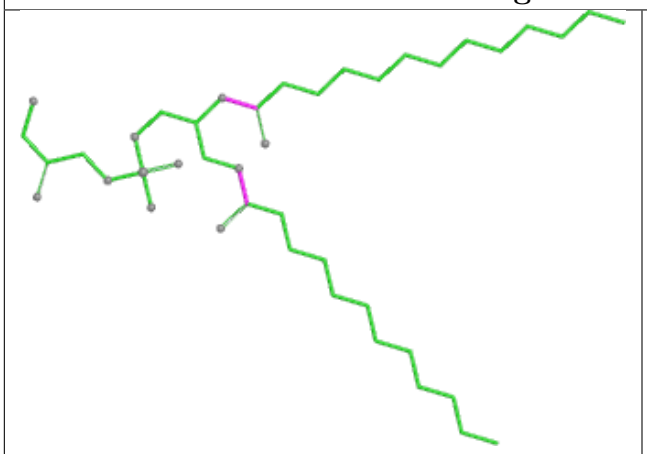


Torsions

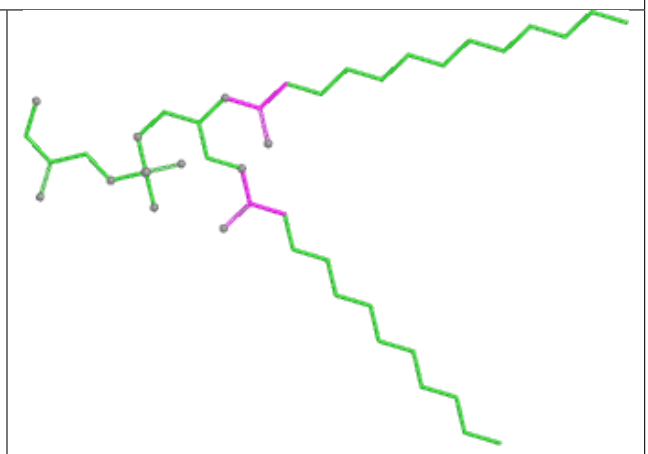


Rings

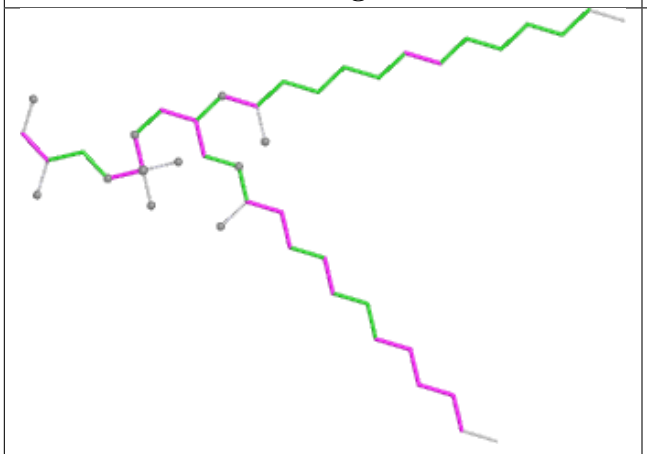
Ligand LHG G 5001



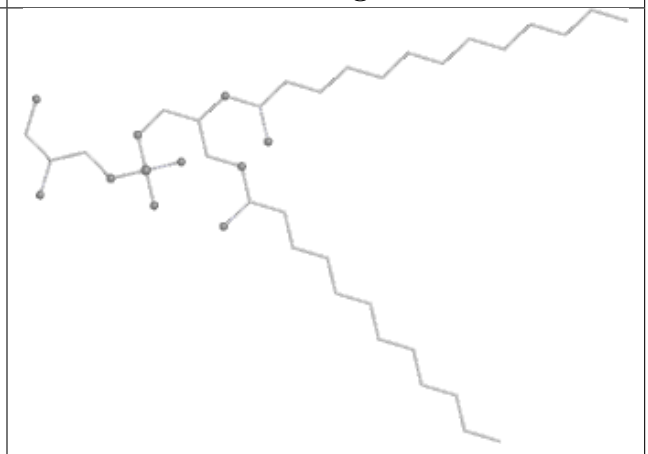
Bond lengths



Bond angles

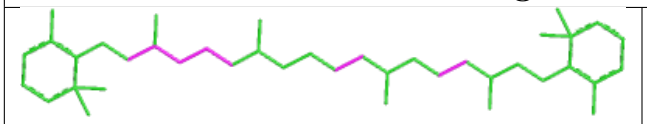


Torsions



Rings

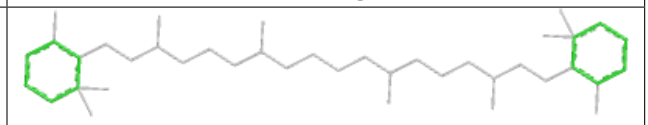
Ligand BCR A 4001



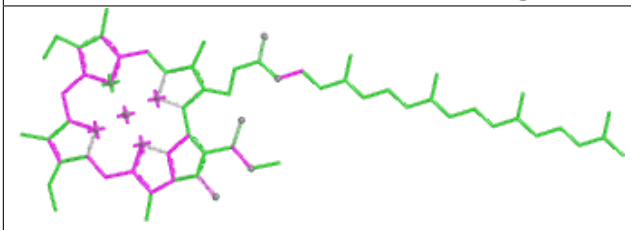
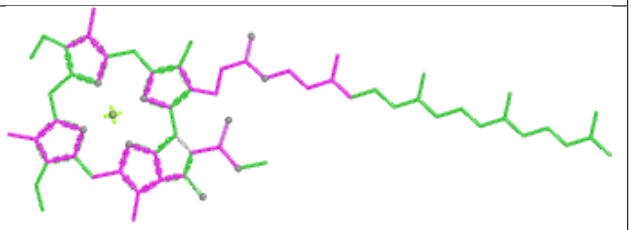
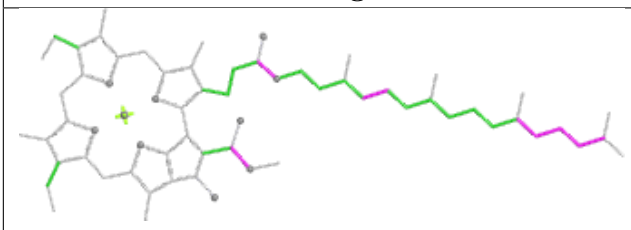
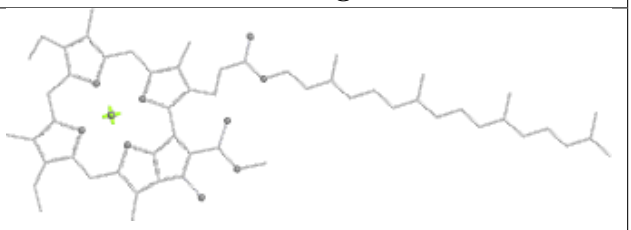
Bond lengths

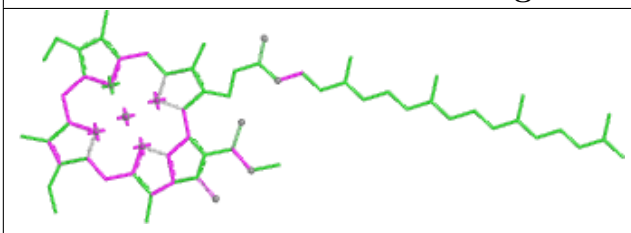
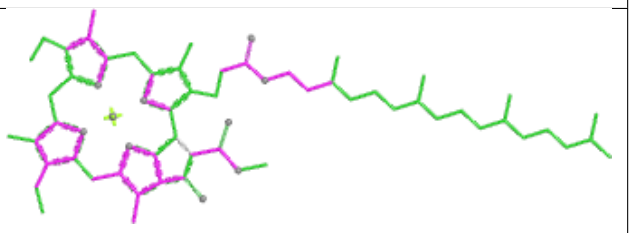
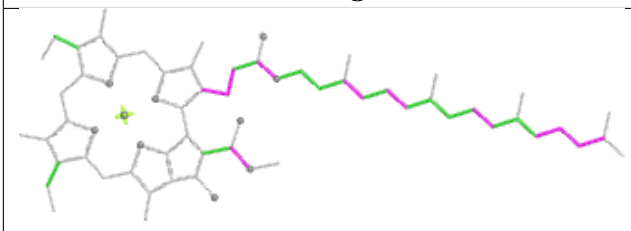
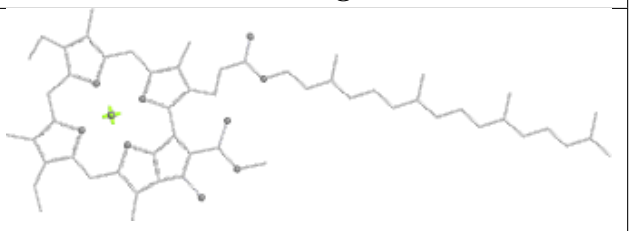
Bond angles

Torsions

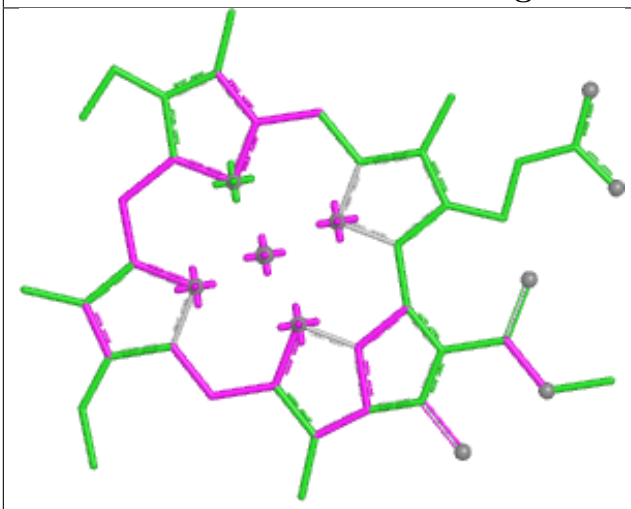


Rings

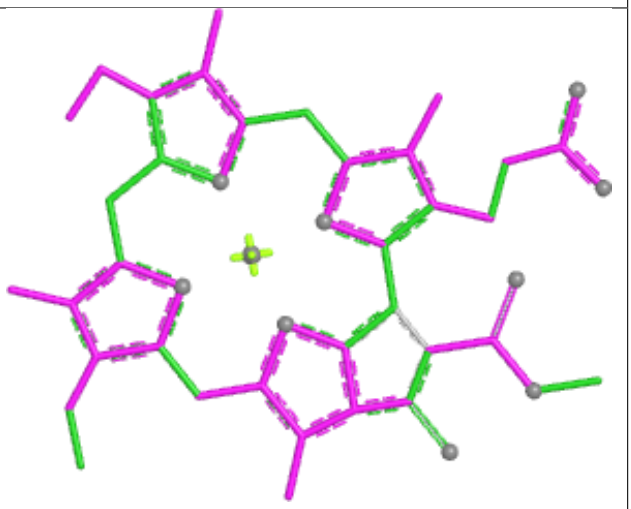
Ligand CLA H 1208	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1225	
	
Bond lengths	Bond angles
	
Torsions	Rings

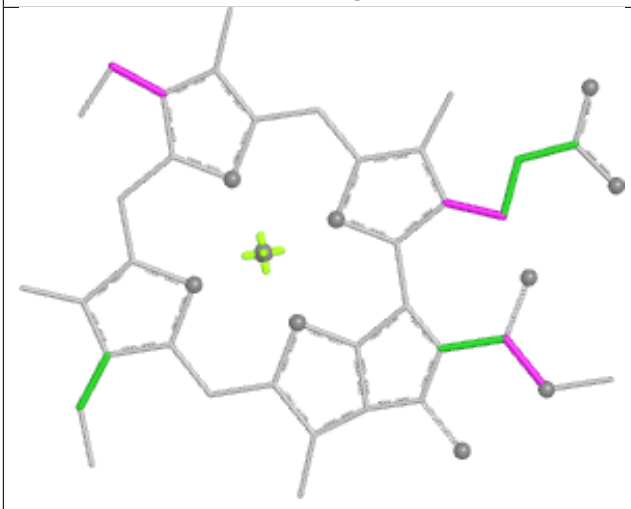
Ligand CLA A 1107



Bond lengths



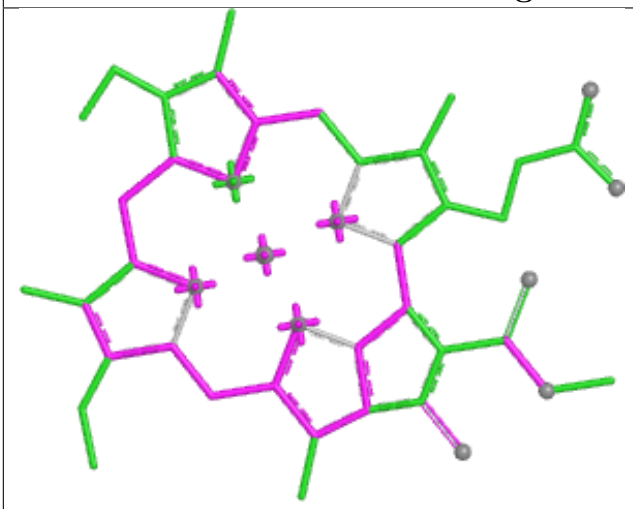
Bond angles



Torsions

Rings

Ligand CLA B 1232



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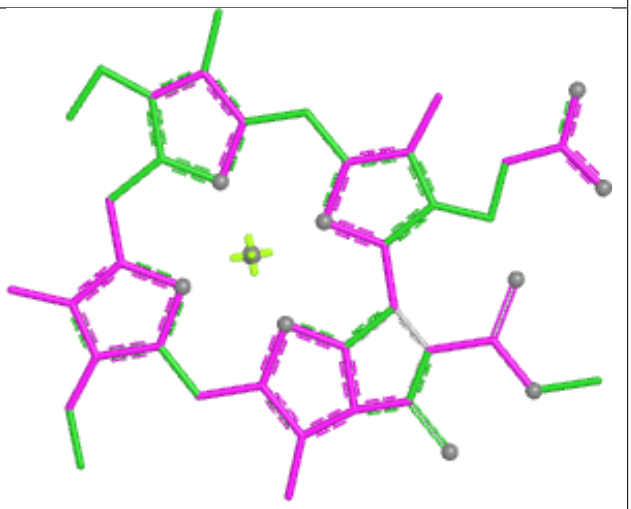
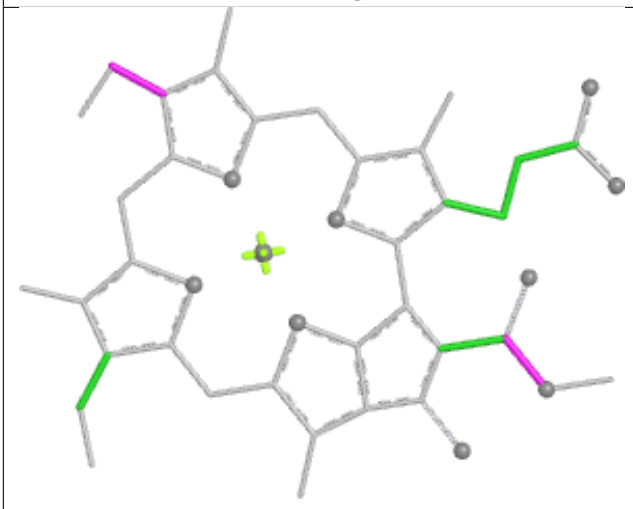


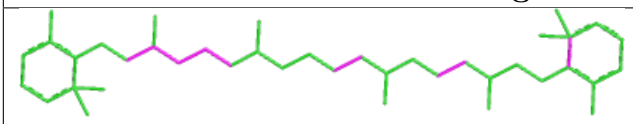
Bond angles



Torsions

Rings

Ligand BCR G 4008



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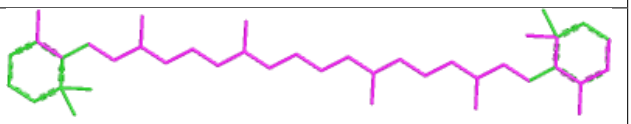
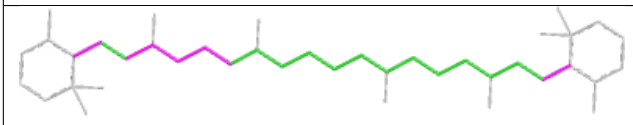
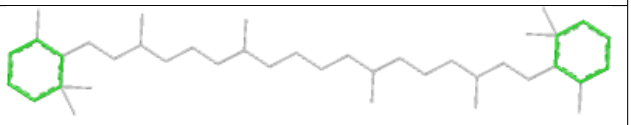


Bond angles

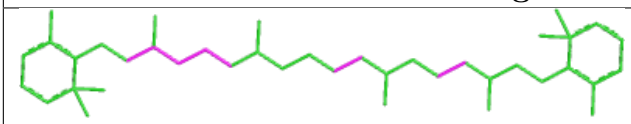


Torsions

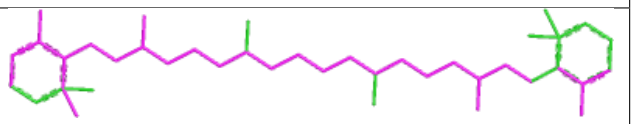


Rings

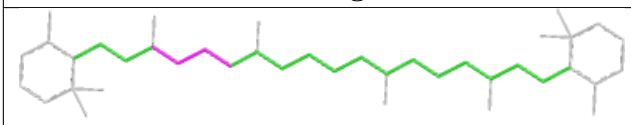
Ligand BCR H 4009



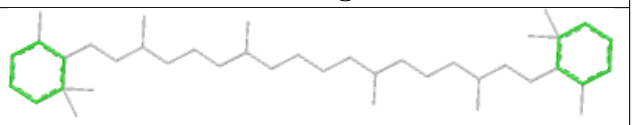
Bond lengths



Bond angles

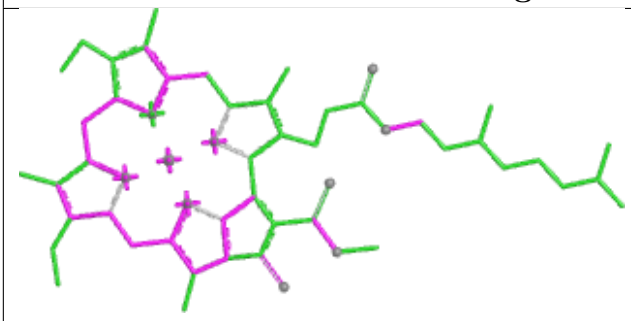


Torsions



Rings

Ligand CLA H 1216



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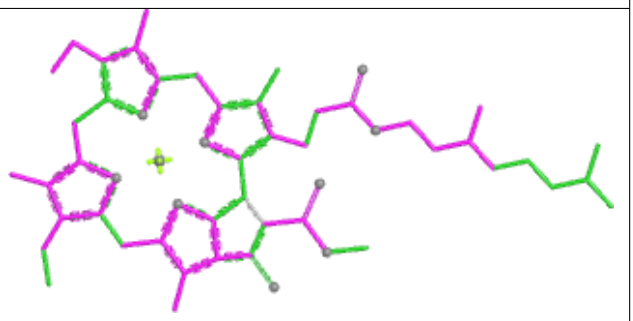
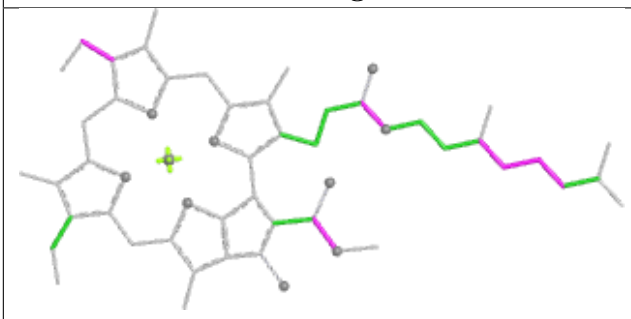


Bond angles



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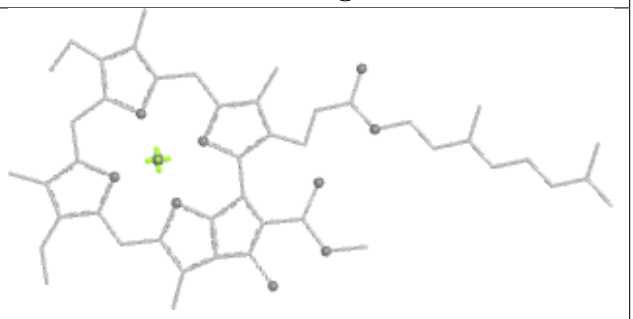
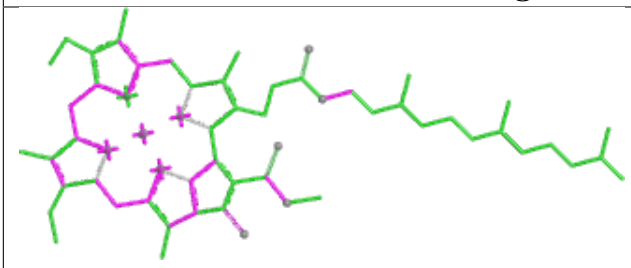


Rings

Ligand CLA G 1126



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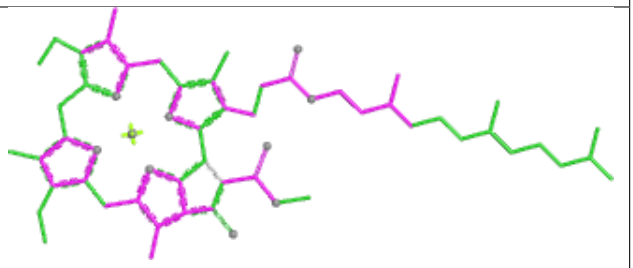
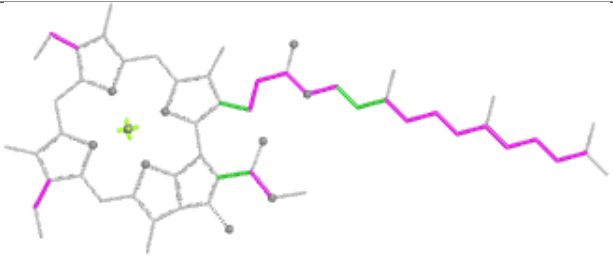


Bond angles



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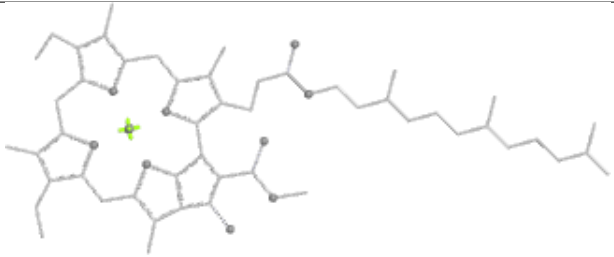
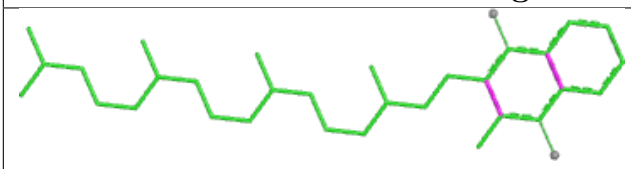


Rings

Ligand PQN H 2002



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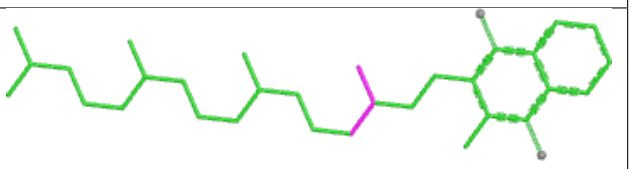
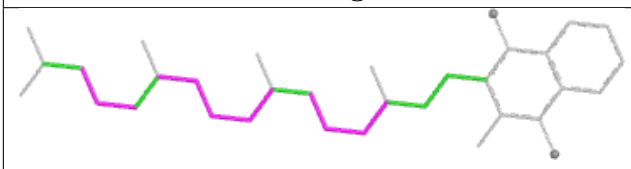


Bond angles



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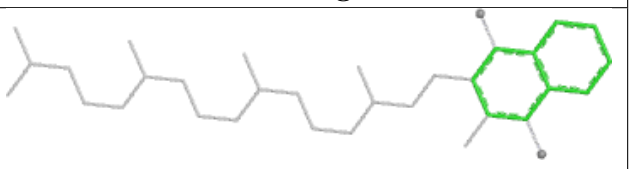
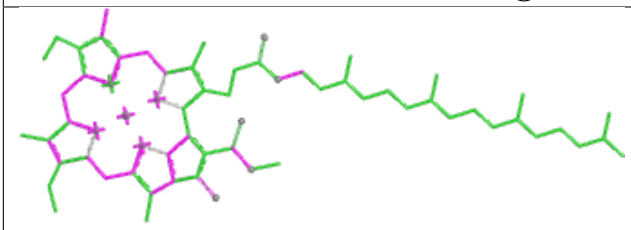


Rings

Ligand CLA B 1226



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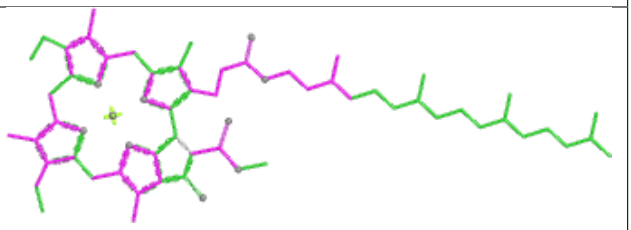
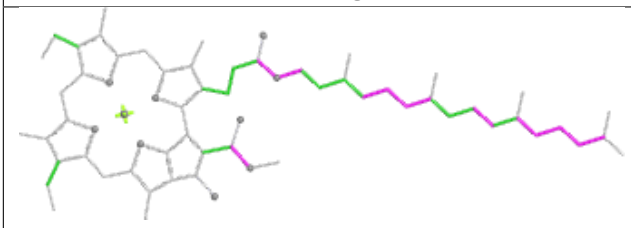
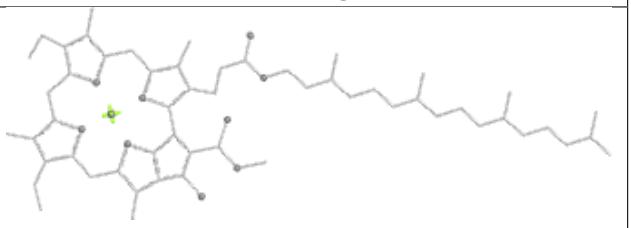


Bond angles

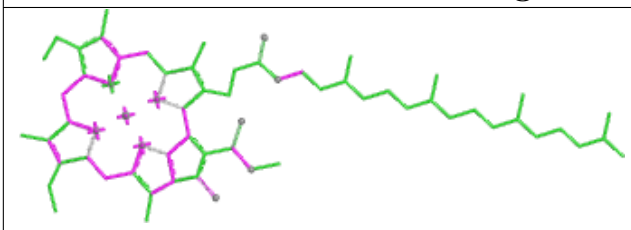


Torsions



Rings

Ligand CLA G 1127



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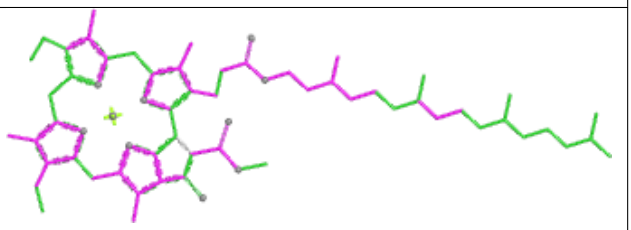

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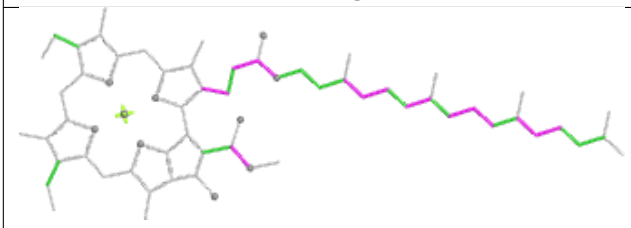

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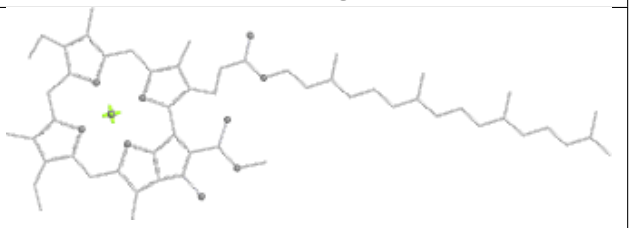
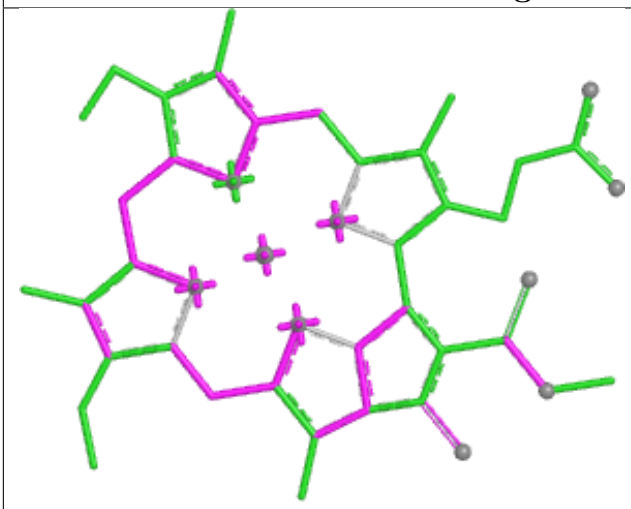


Rings

Ligand CLA G 1137



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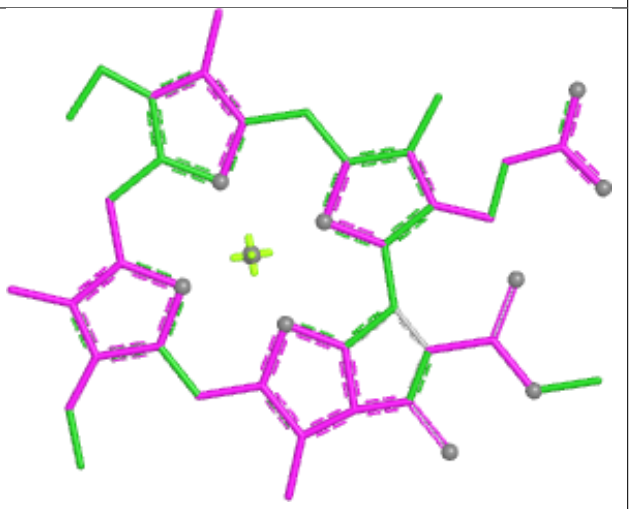
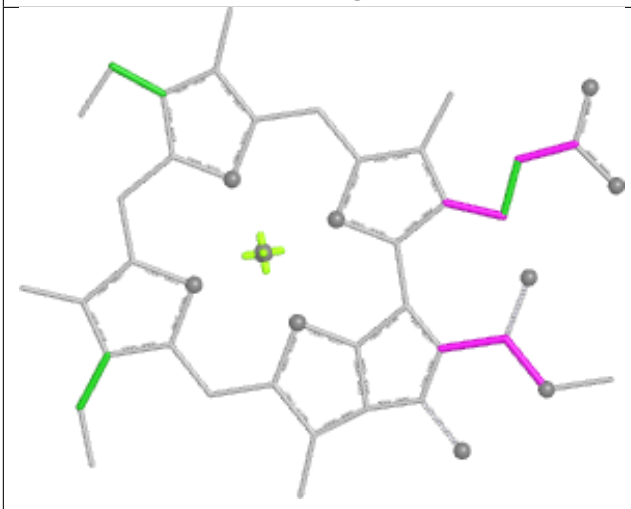


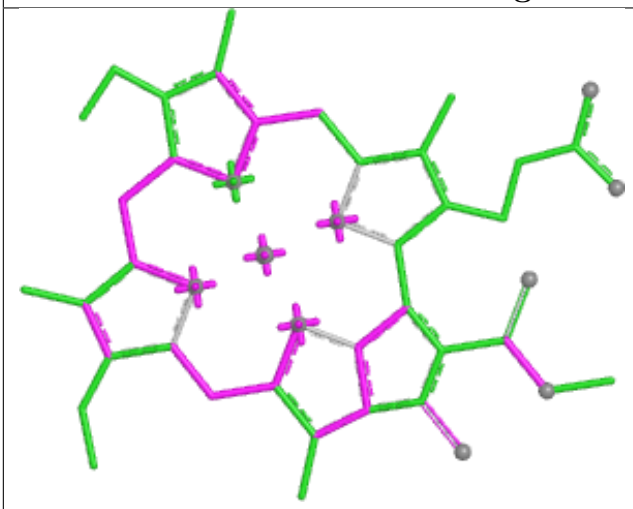
Bond angles



Torsions

Rings

Ligand CLA G 1107



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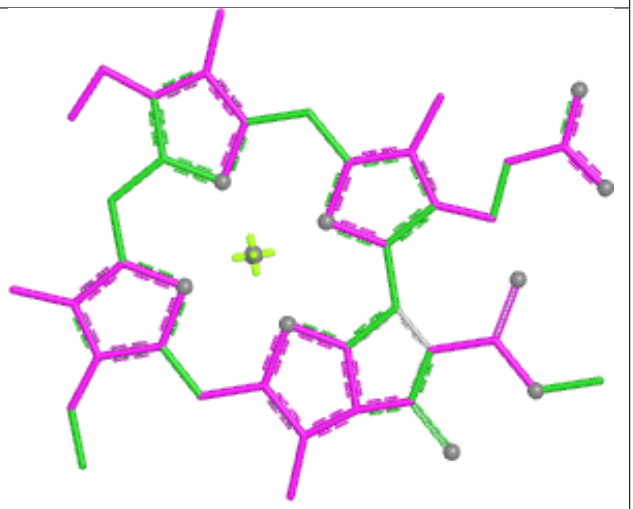
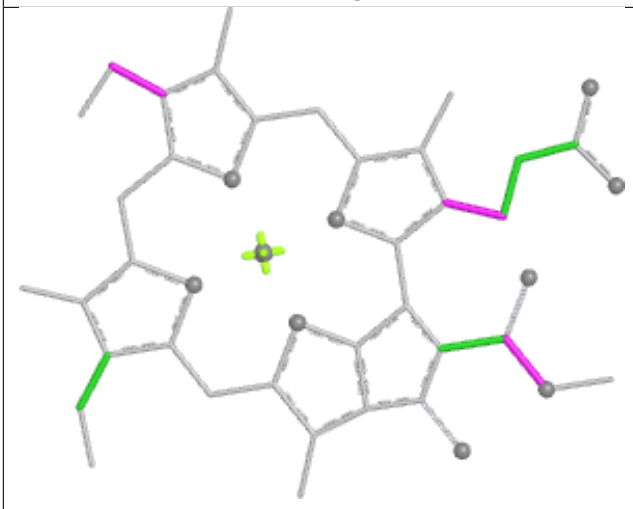


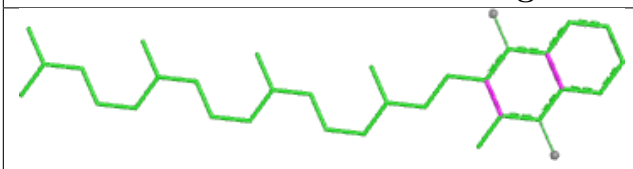
Bond angles



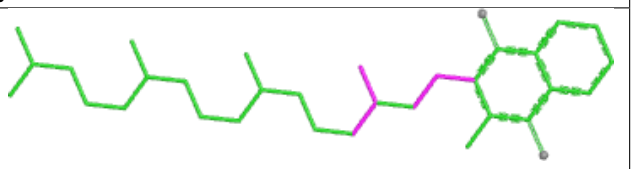
Torsions

Rings

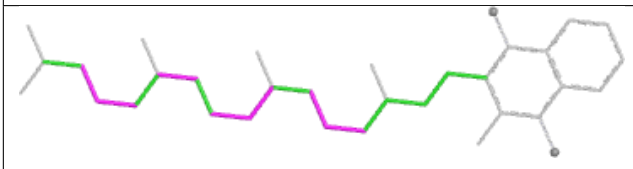
Ligand PQN a 2001



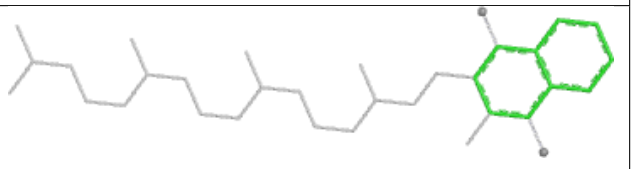
Bond lengths



Bond angles

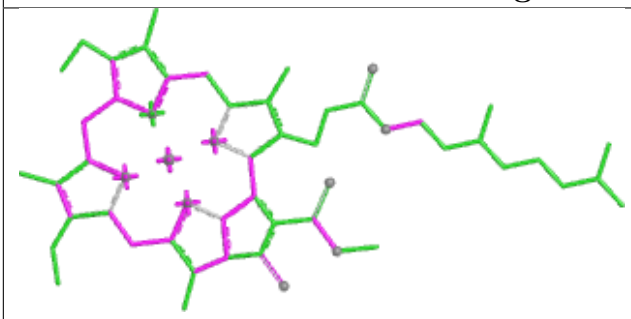


Torsions

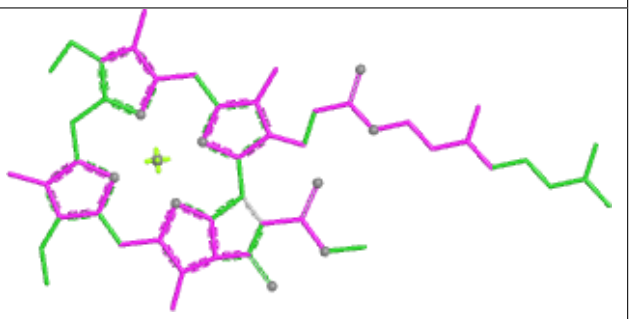


Rings

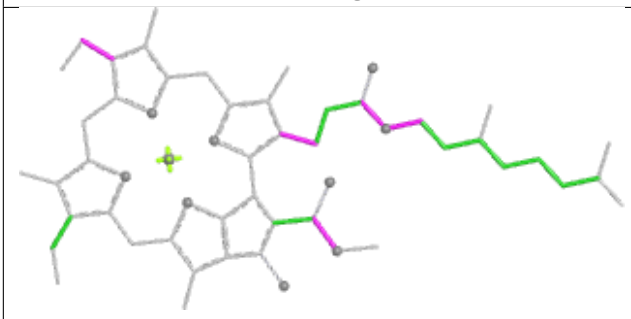
Ligand CLA G 1124



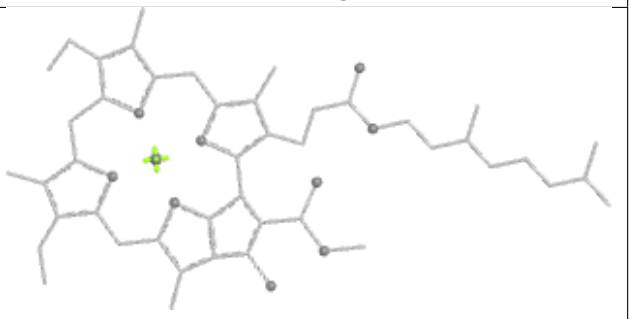
Bond lengths



Bond angles

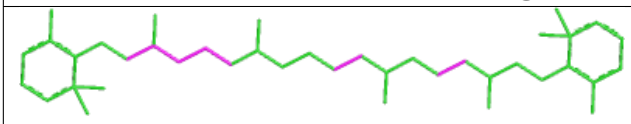


Torsions

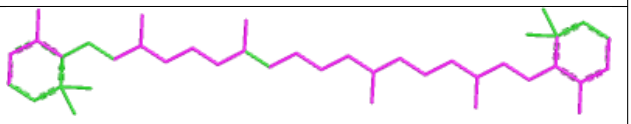


Rings

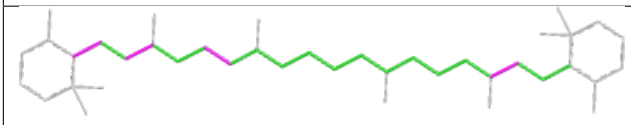
Ligand BCR a 4002



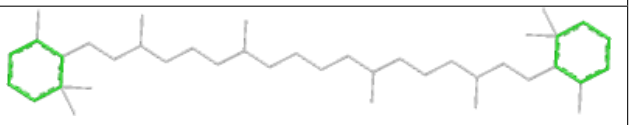
Bond lengths



Bond angles

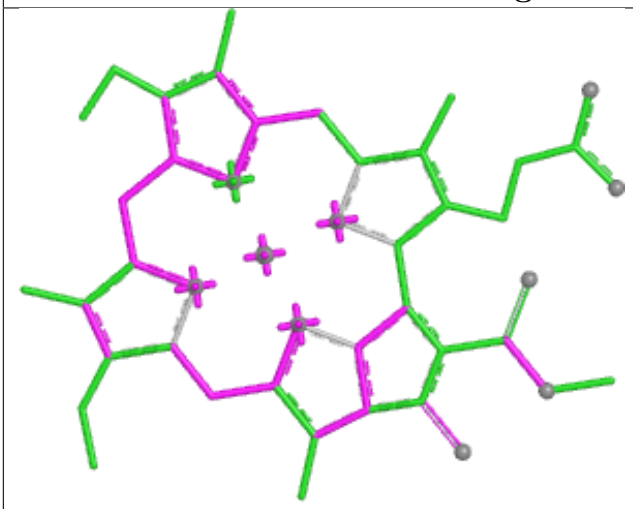


Torsions

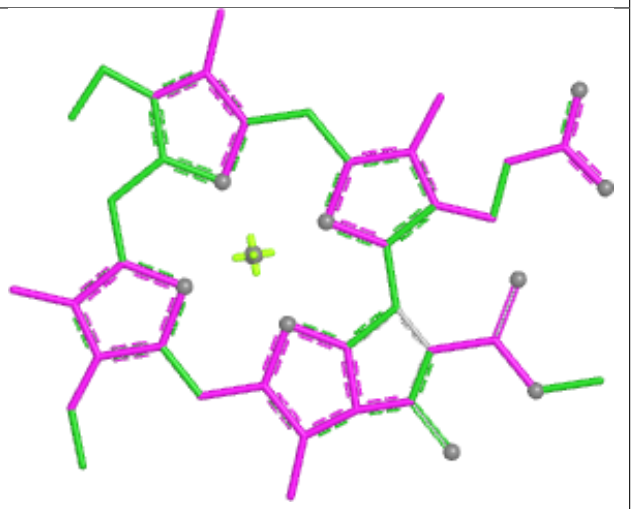


Rings

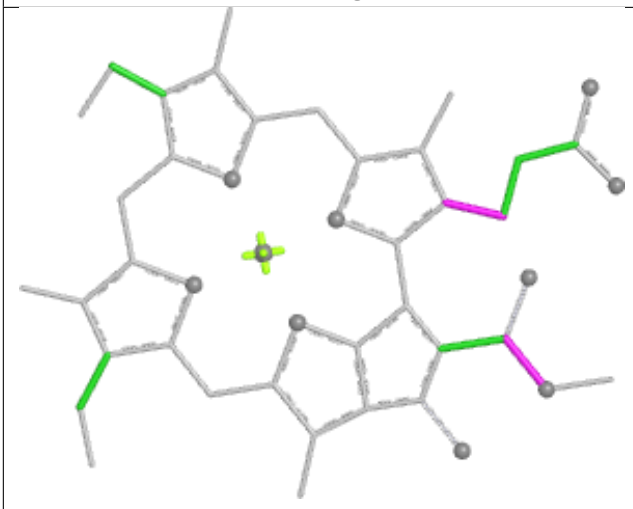
Ligand CLA A 1139



Bond lengths



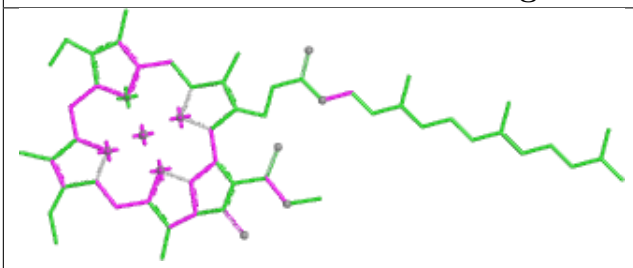
Bond angles



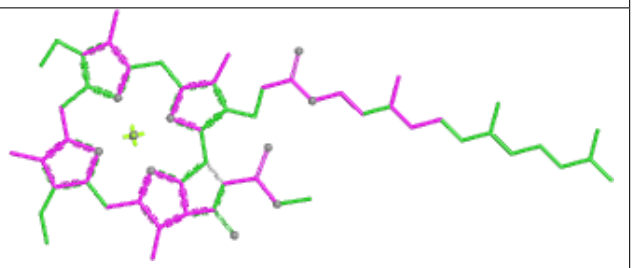
Torsions

Rings

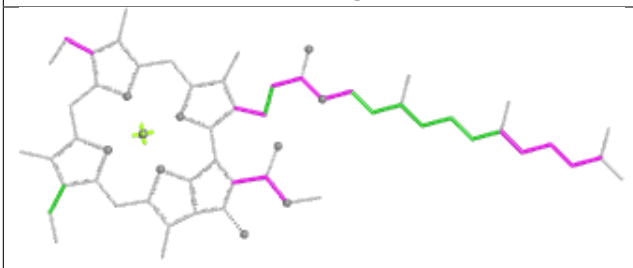
Ligand CLA a 1133



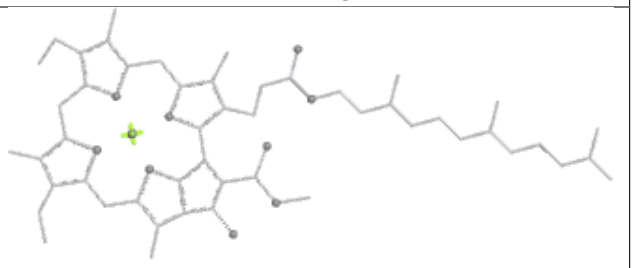
Bond lengths



Bond angles

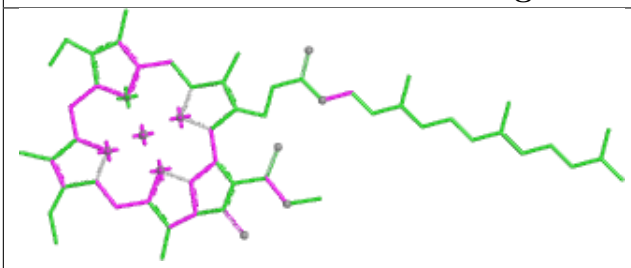


Torsions

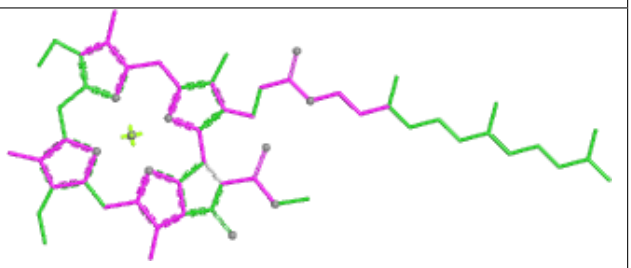


Rings

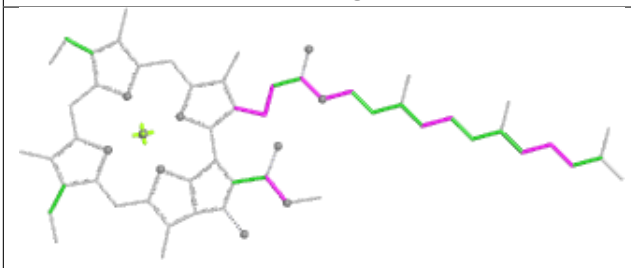
Ligand CLA A 1102



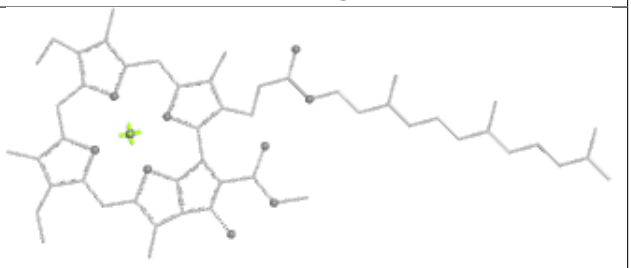
Bond lengths



Bond angles

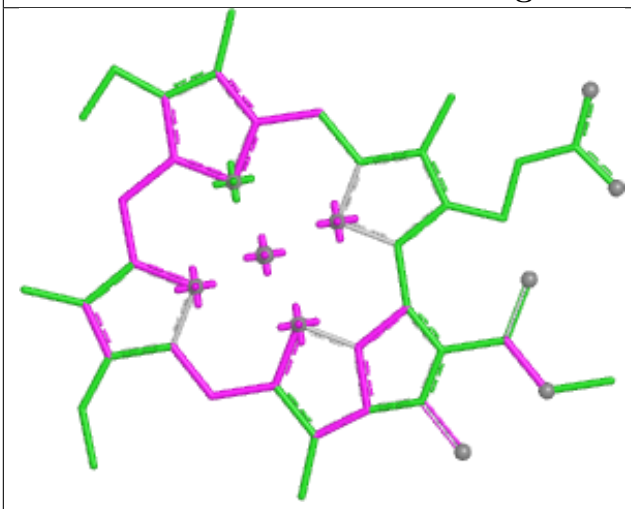


Torsions

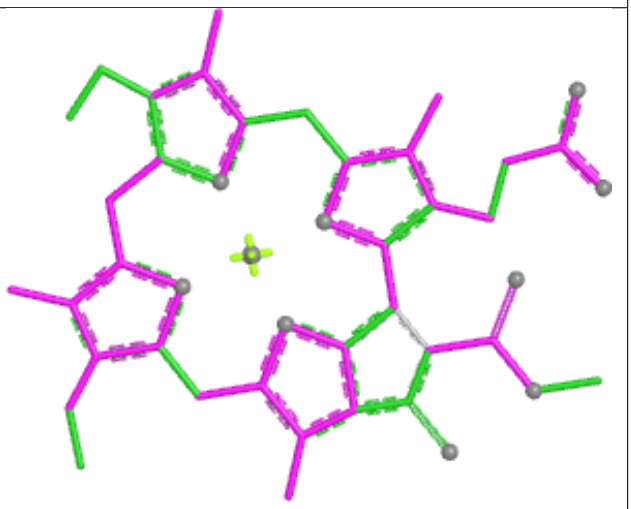


Rings

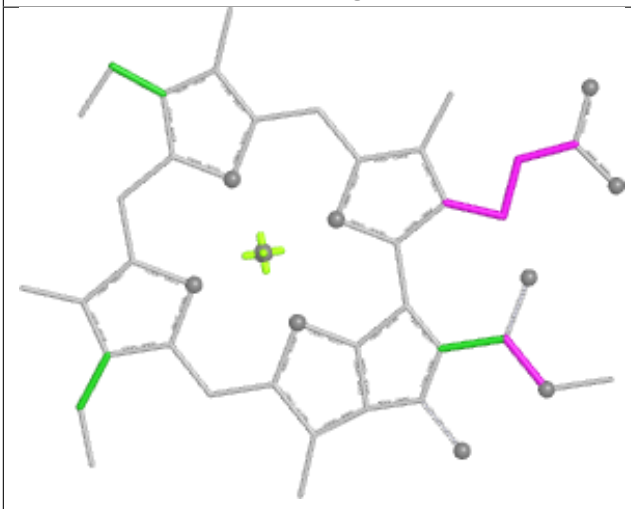
Ligand CLA B 1207



Bond lengths

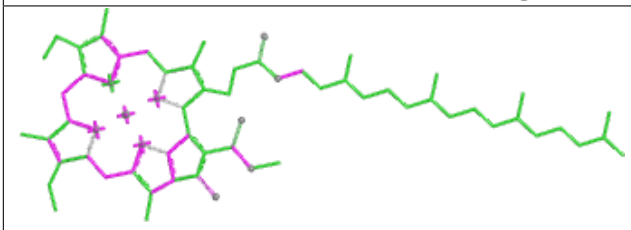
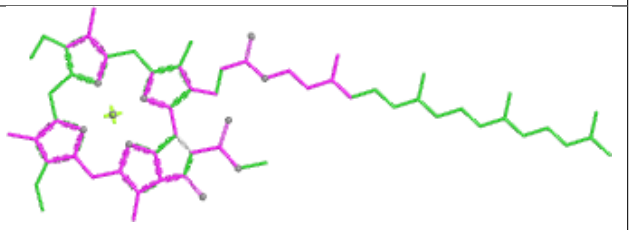
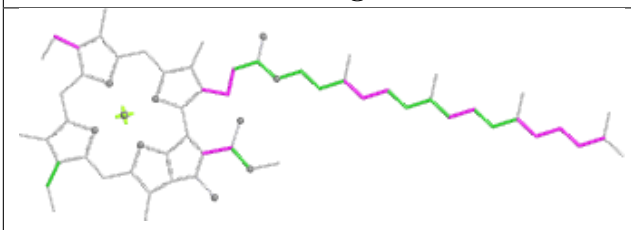
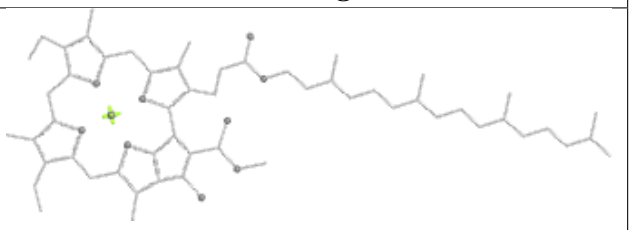


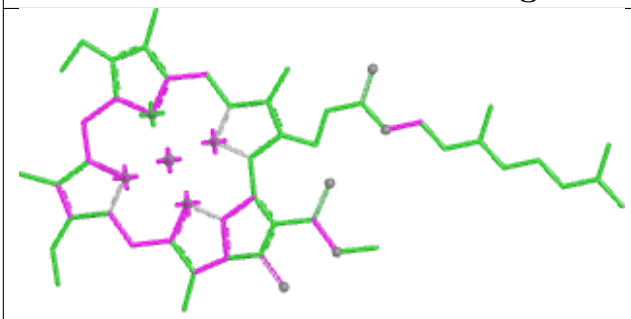
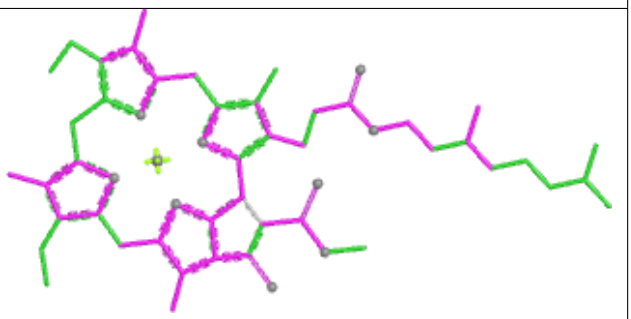
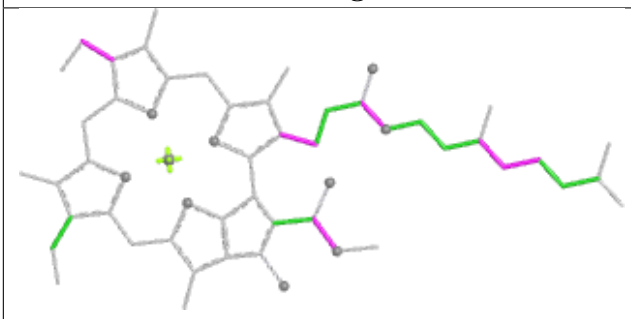
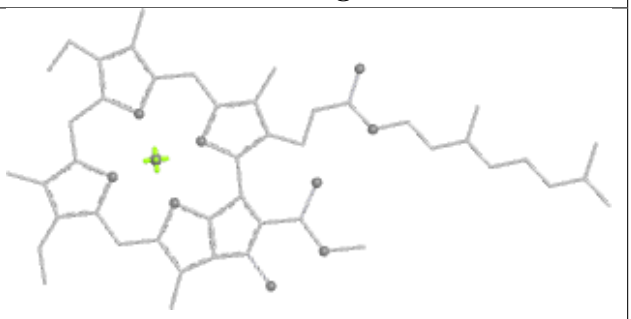
Bond angles



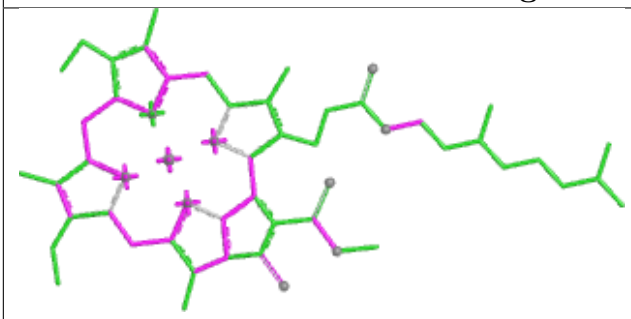
Torsions

Rings

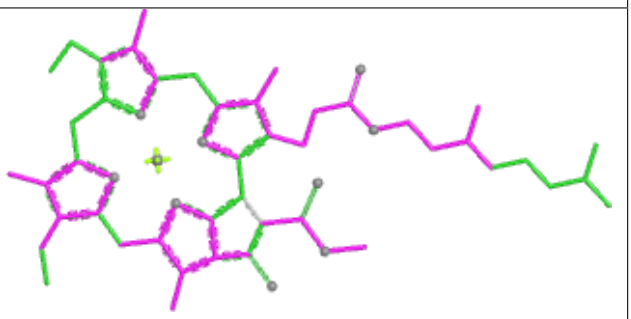
Ligand CLA B 1022	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 1130	
 Bond lengths	 Bond angles
 Torsions	 Rings

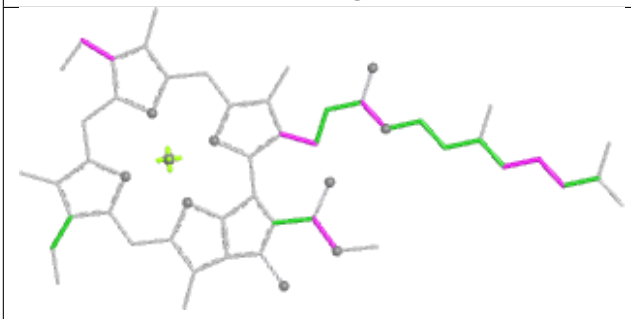
Ligand CLA a 1122



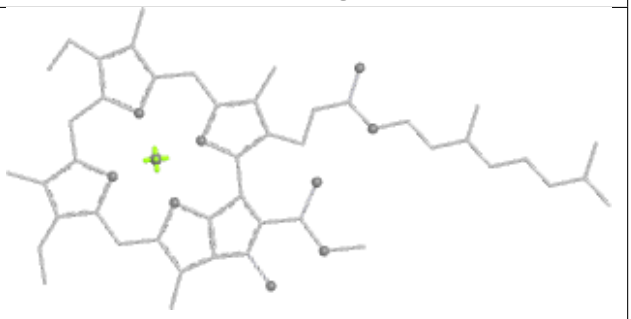
Bond lengths



Bond angles

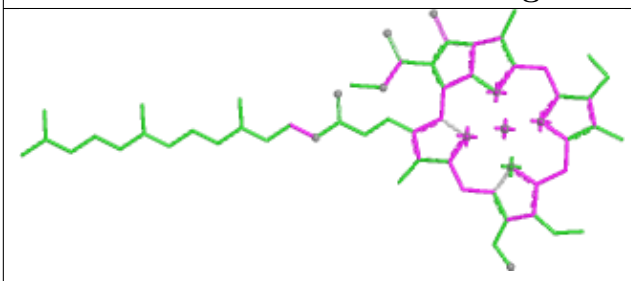


Torsions

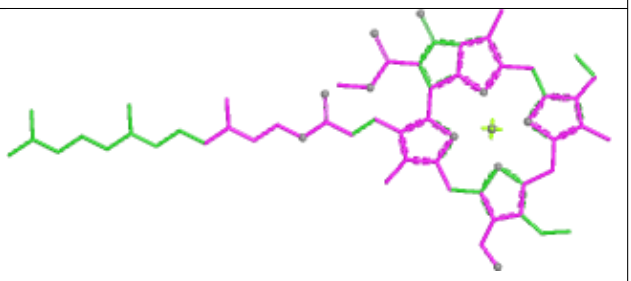


Rings

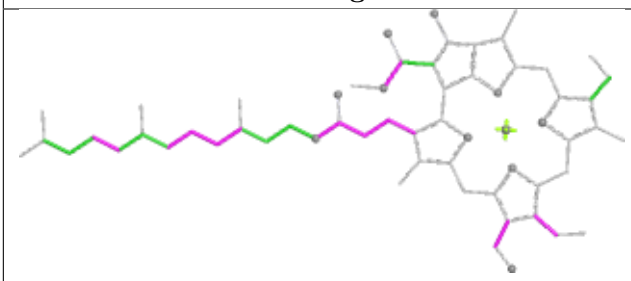
Ligand F6C b 1237



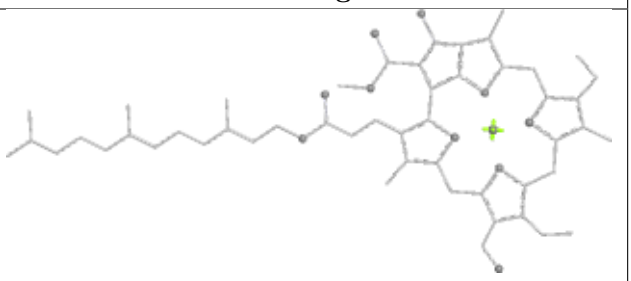
Bond lengths



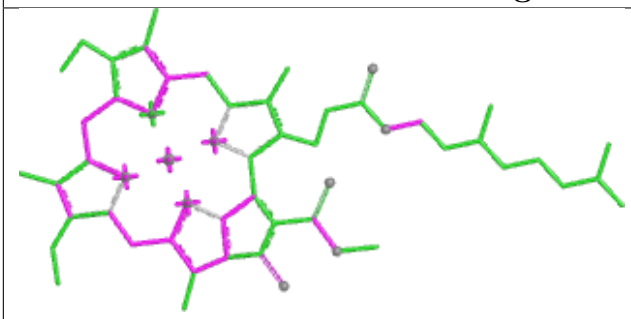
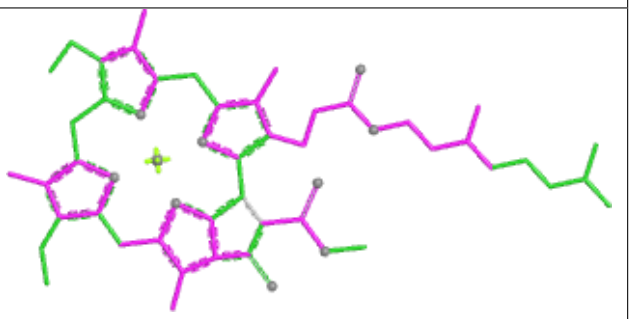
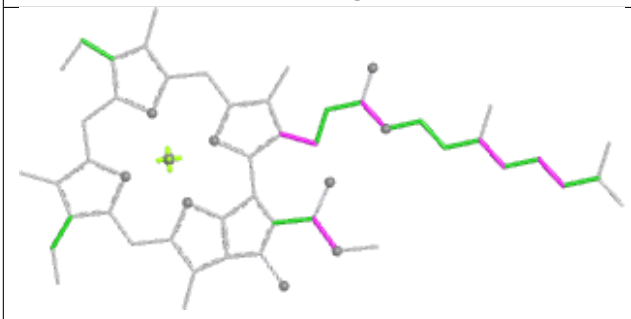
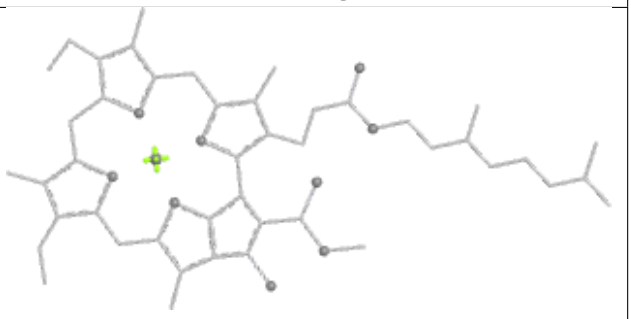
Bond angles

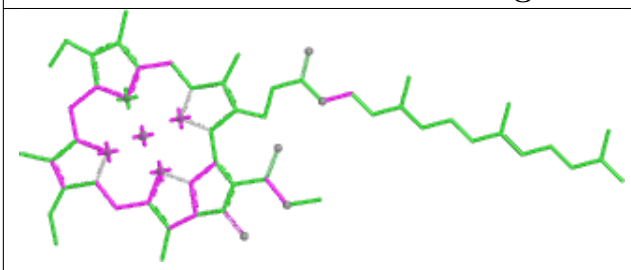
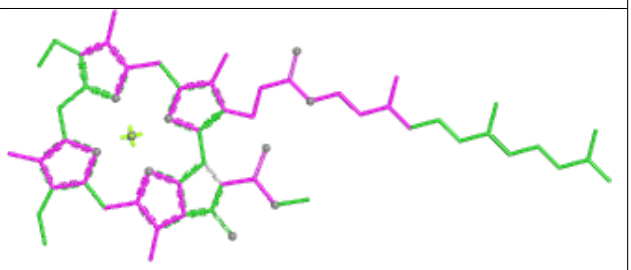
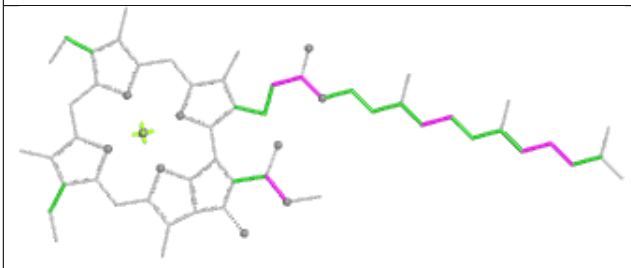
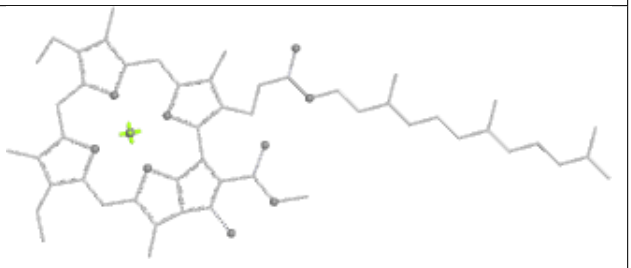


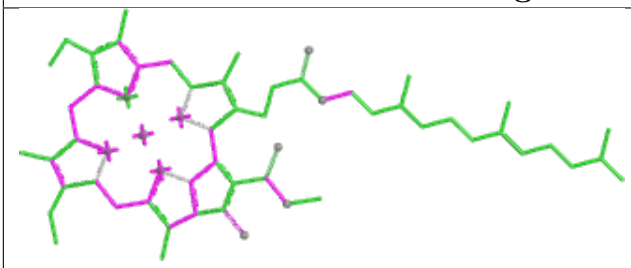
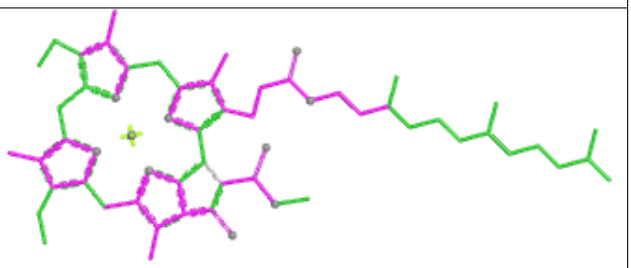
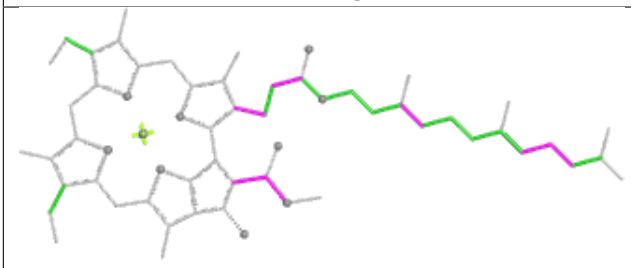
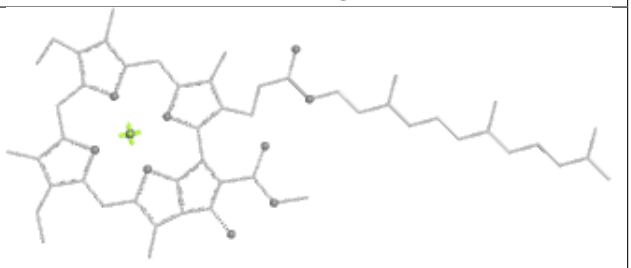
Torsions

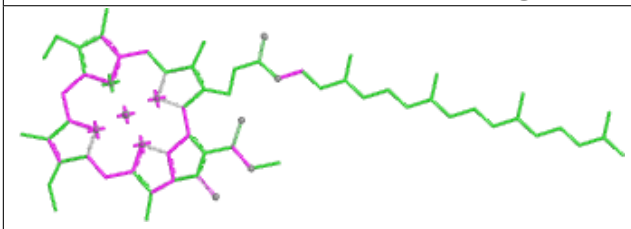
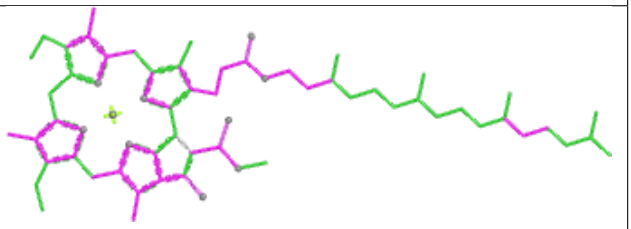
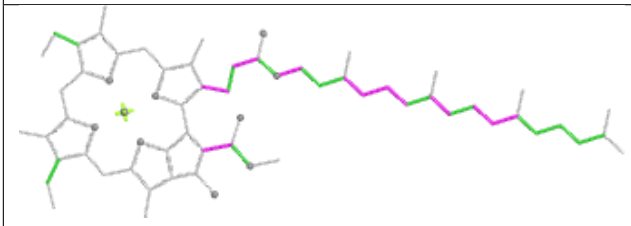
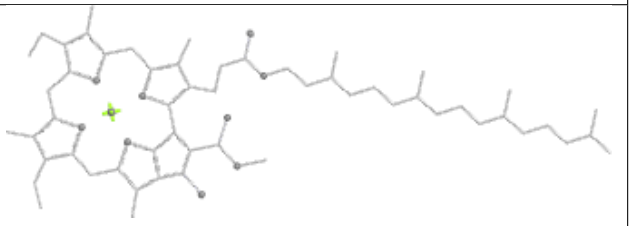


Rings

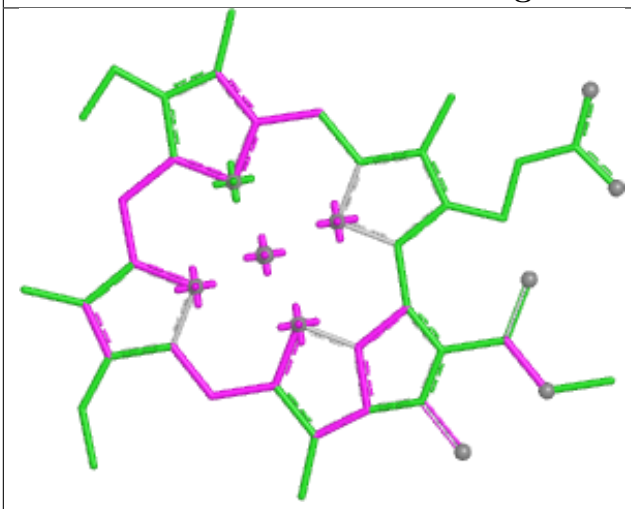
Ligand CLA G 1115	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1235	
	
Bond lengths	Bond angles
	
Torsions	Rings

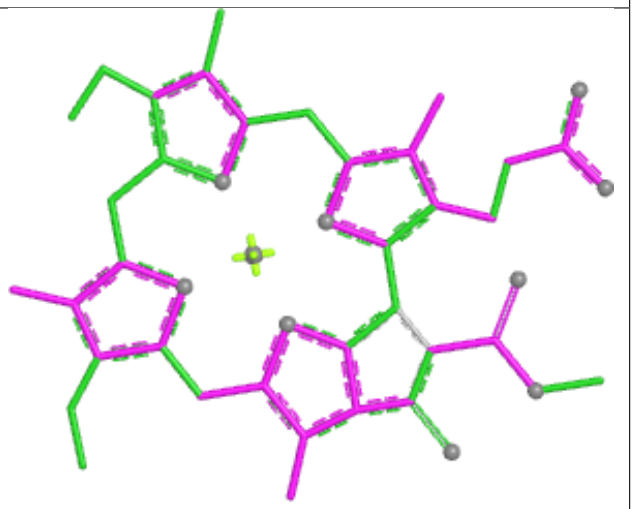
Ligand CLA U 1501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 1205	
 Bond lengths	 Bond angles
 Torsions	 Rings

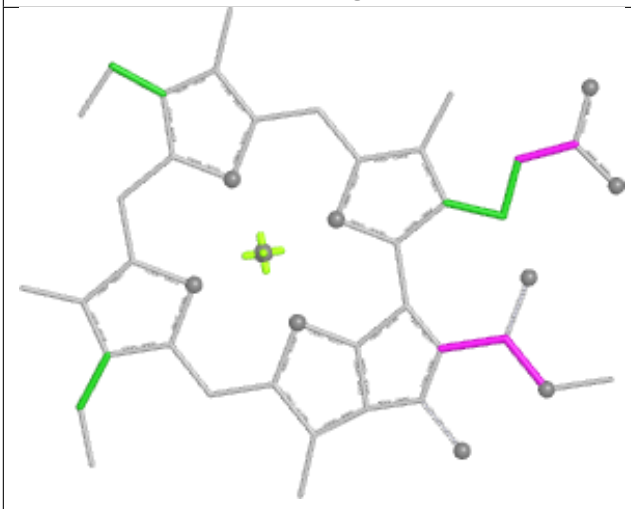
Ligand CLA H 1218



Bond lengths

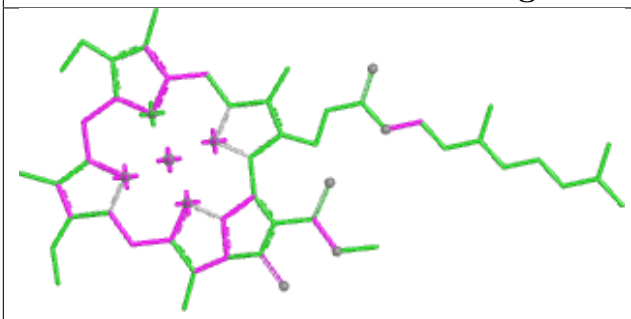
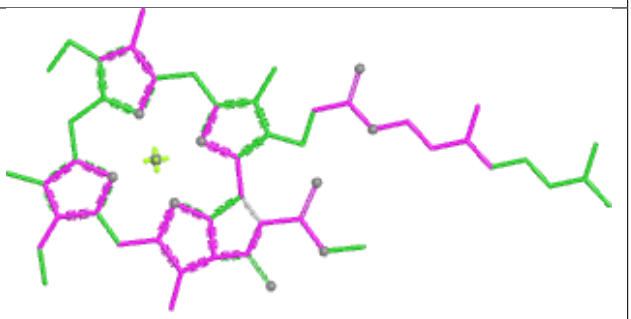
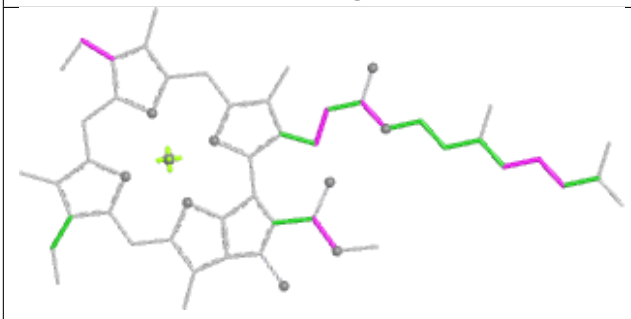
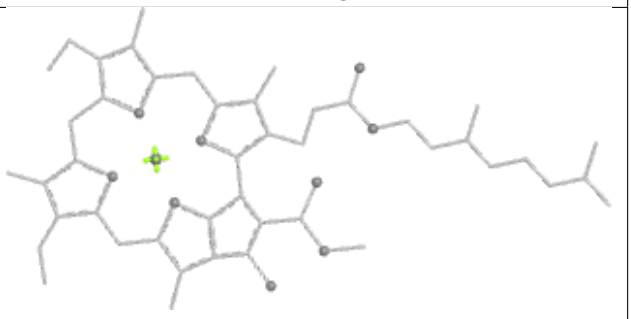


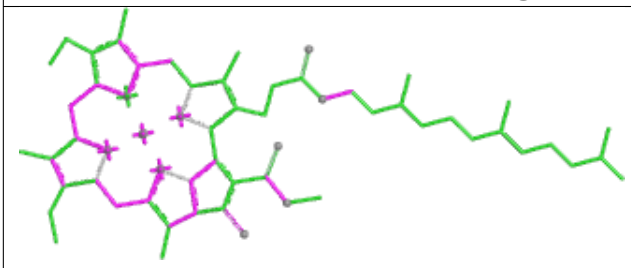
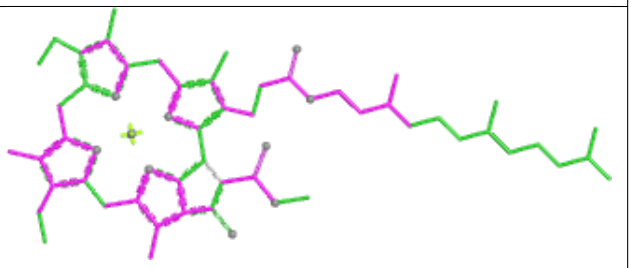
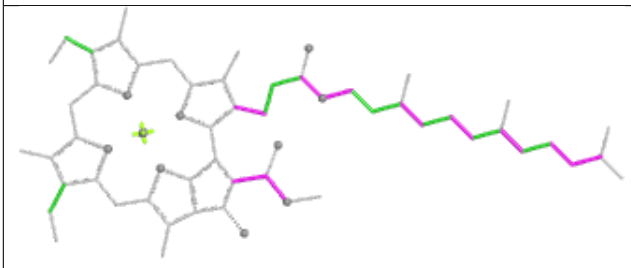
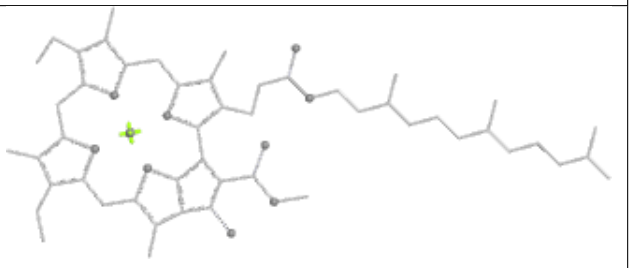
Bond angles



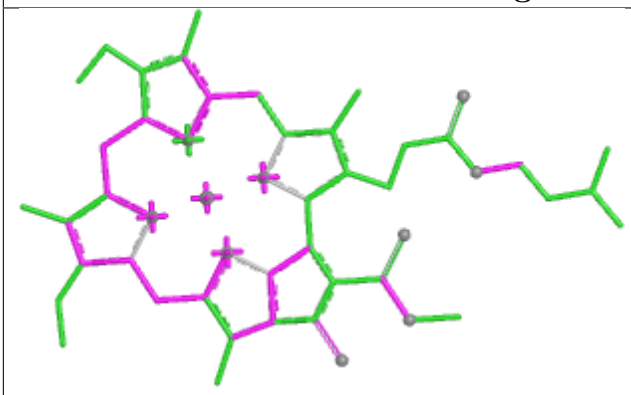
Torsions

Rings

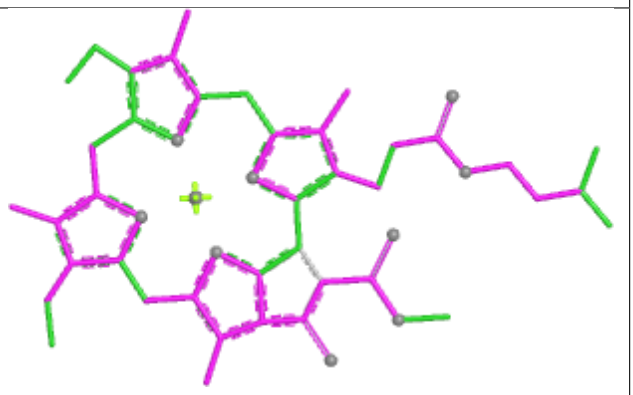
Ligand CLA b 1234	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1103	
	
Bond lengths	Bond angles
	
Torsions	Rings

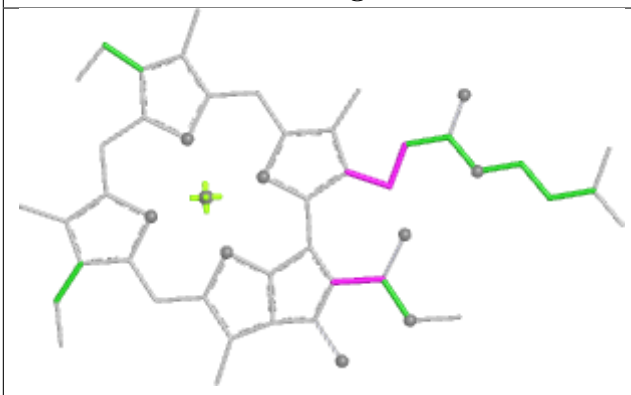
Ligand CLA G 1135



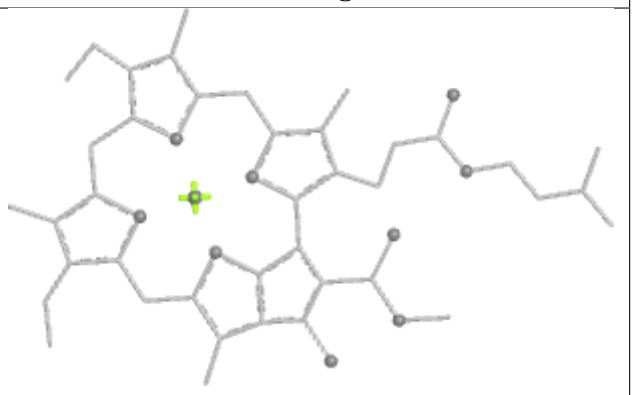
Bond lengths



Bond angles

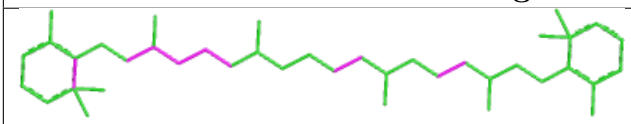


Torsions

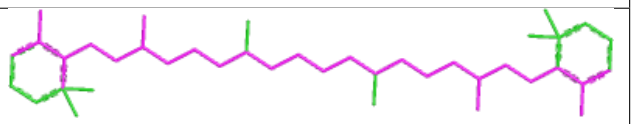


Rings

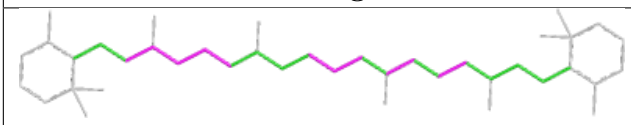
Ligand BCR R 4018



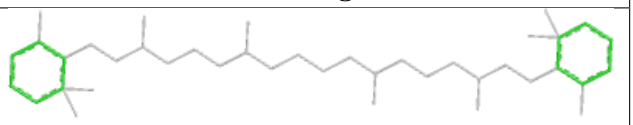
Bond lengths



Bond angles

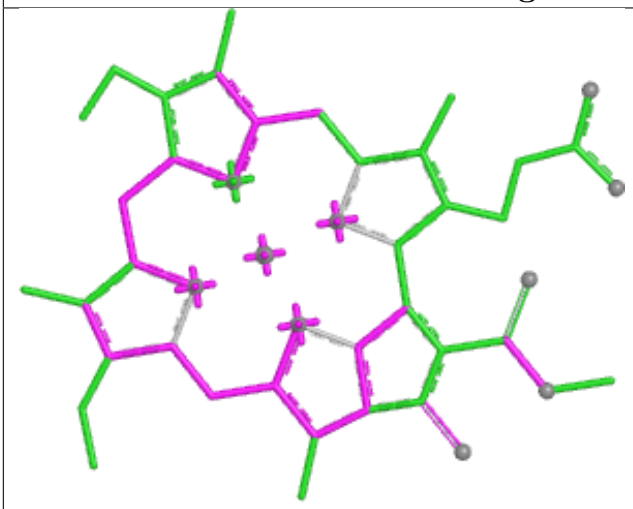


Torsions



Rings

Ligand CLA b 1233



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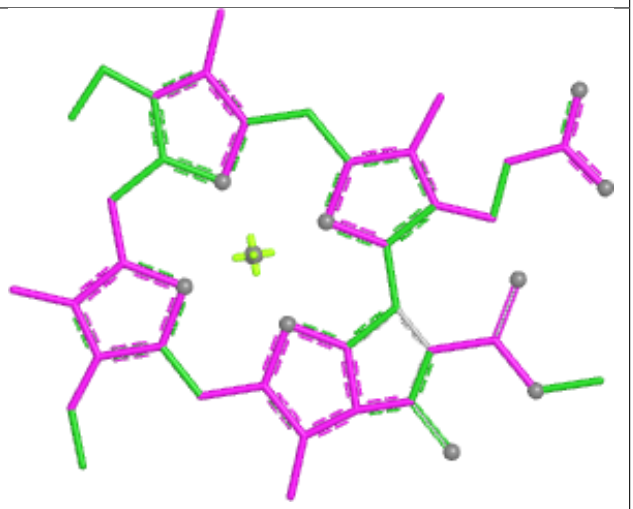
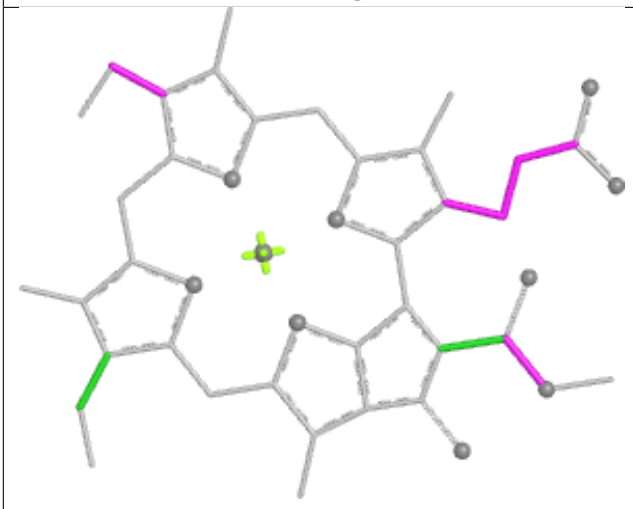


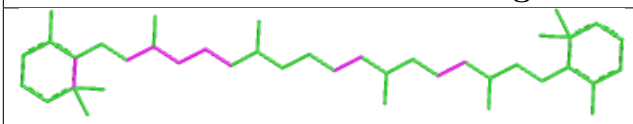
Bond angles



Torsions

Rings

Ligand BCR A 4011



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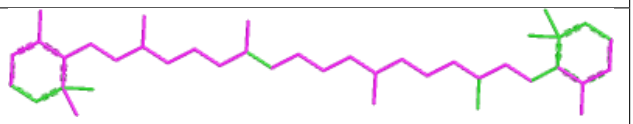
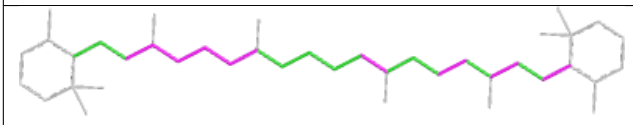
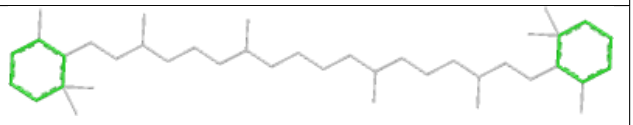


Bond angles

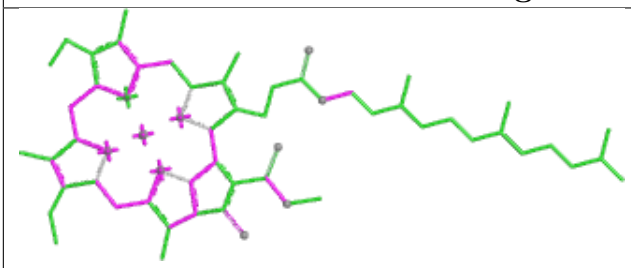


Torsions



Rings

Ligand CLA A 1133



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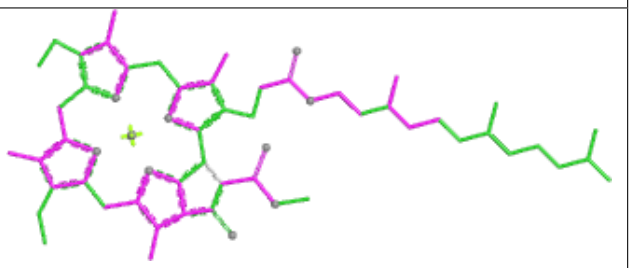
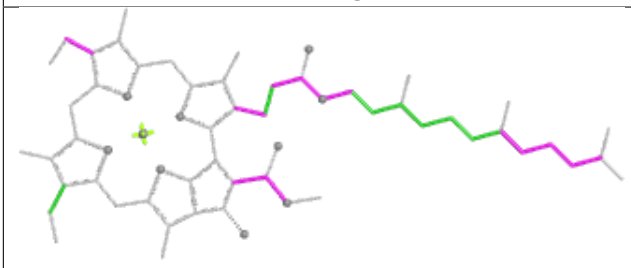
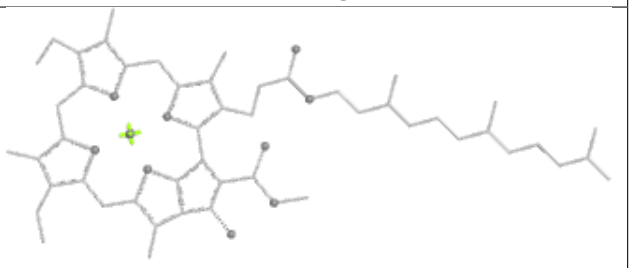


Bond angles

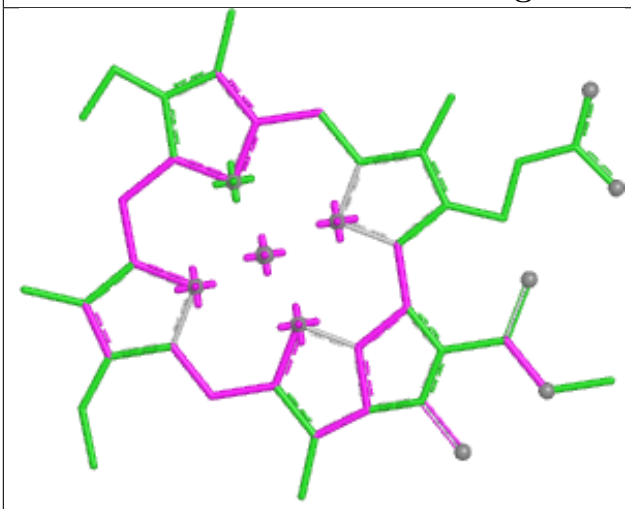


Torsions



Rings

Ligand CLA A 1106



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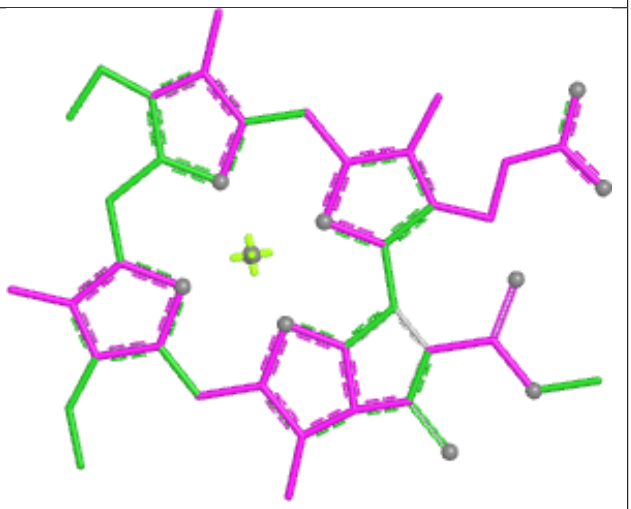

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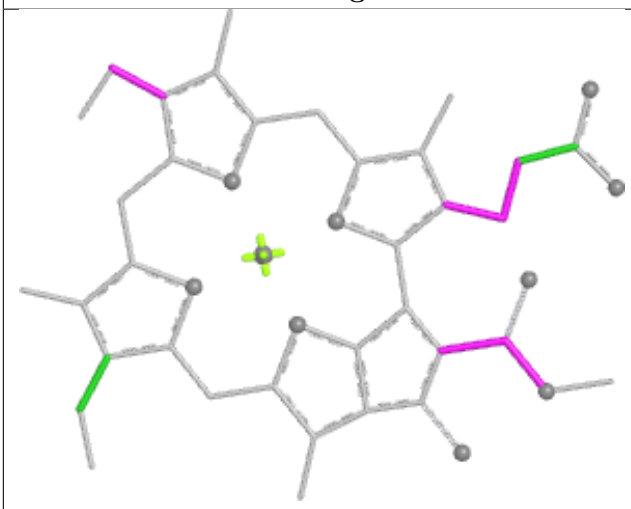
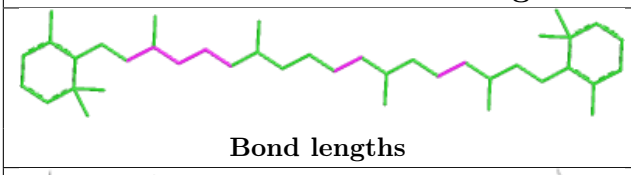


Torsions

Rings

Ligand BCR H 4017



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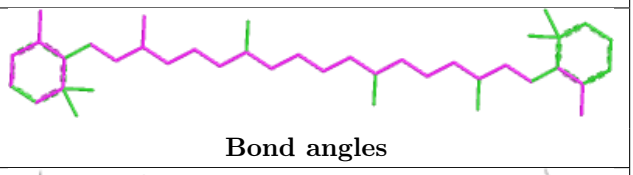
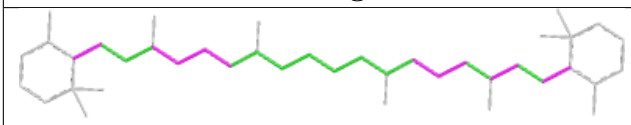
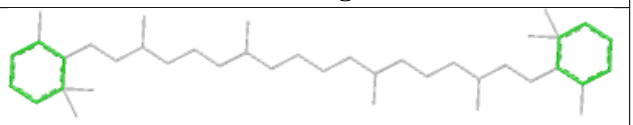


Bond angles

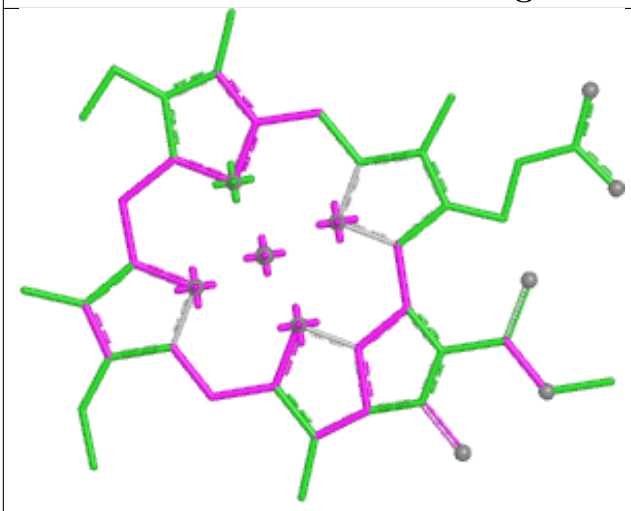


Torsions



Rings

Ligand CLA B 1219



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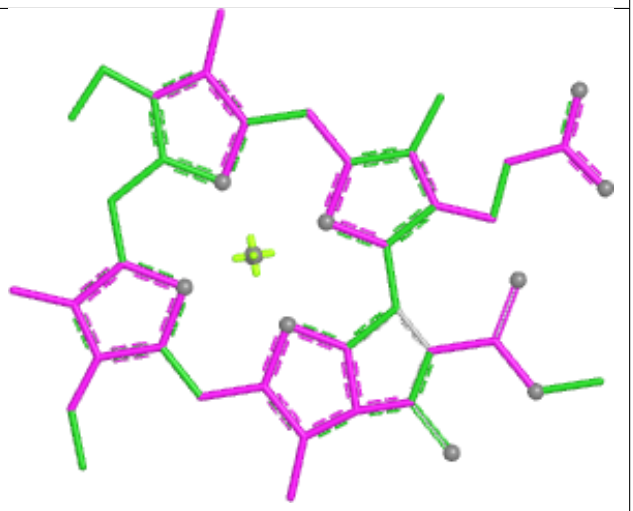
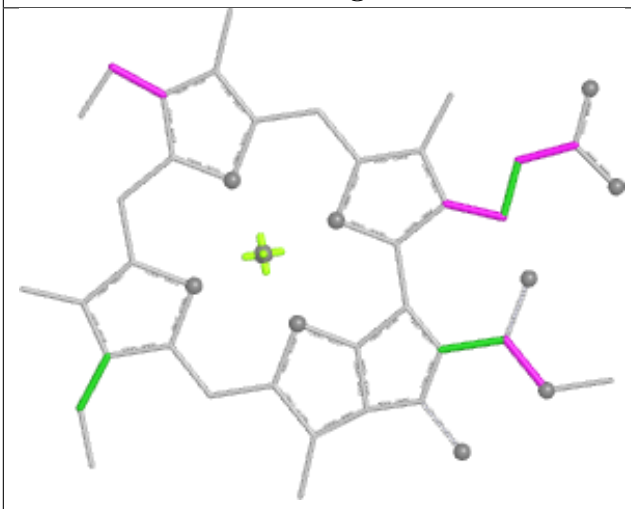


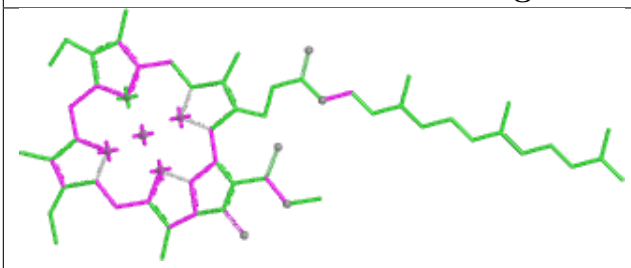
Bond angles



Torsions

Rings

Ligand CLA G 1133



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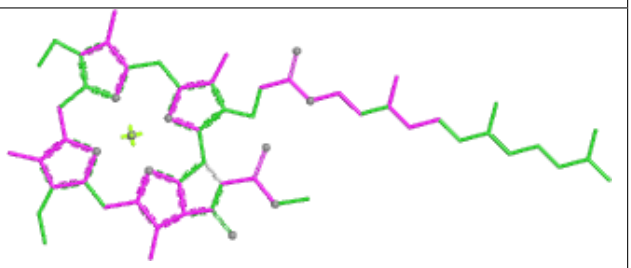
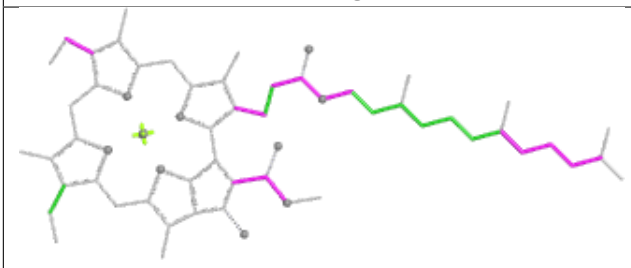
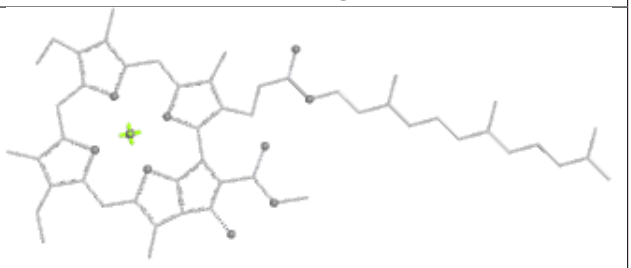


Bond angles

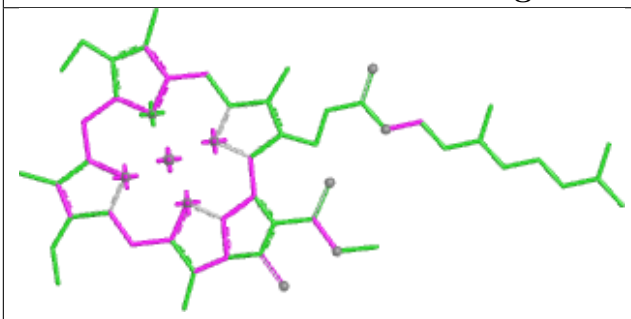


Torsions



Rings

Ligand CLA H 1201



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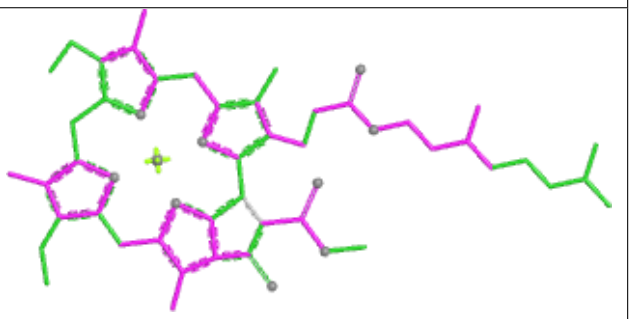
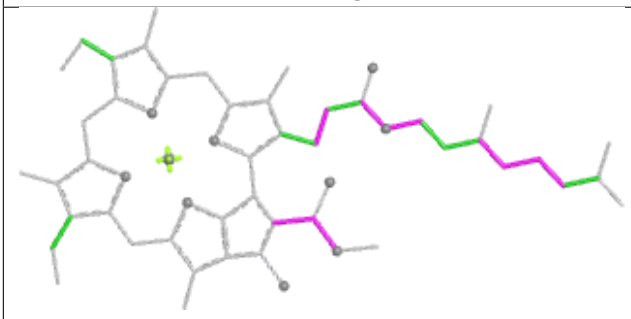


Bond angles



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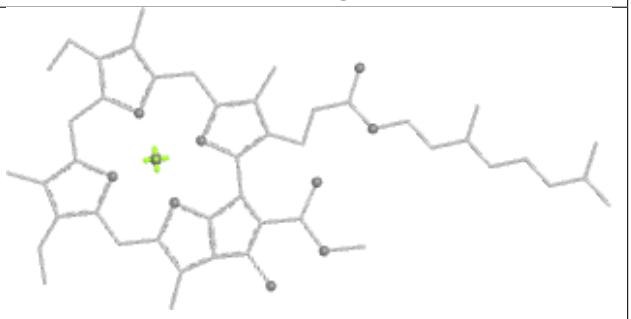
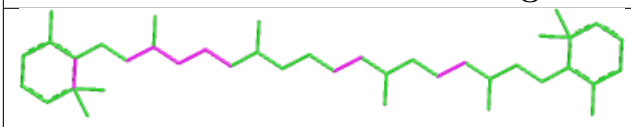


Rings

Ligand BCR i 4020



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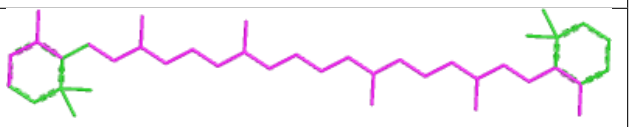
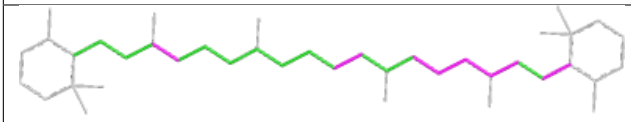


Bond angles



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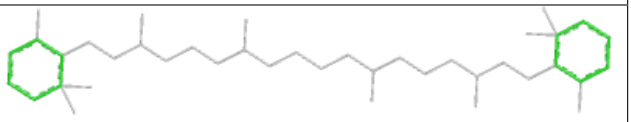
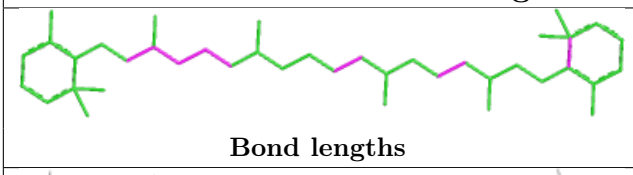


Rings

Ligand BCR H 4005



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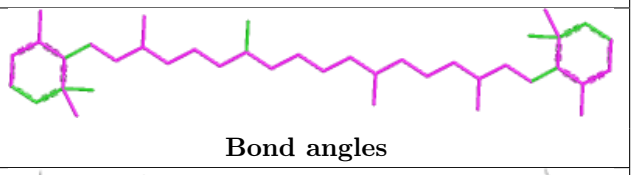
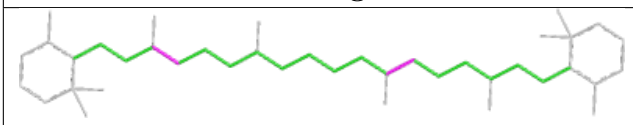


Bond angles



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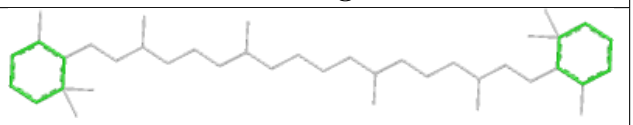
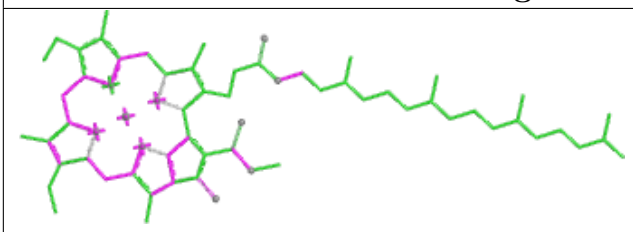


Rings

Ligand CLA G 1119



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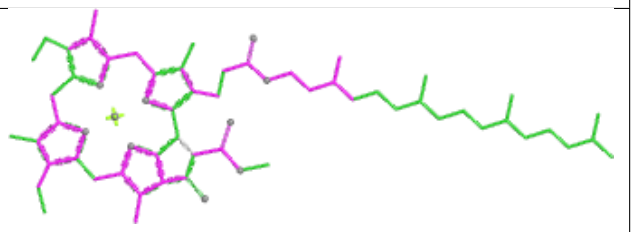
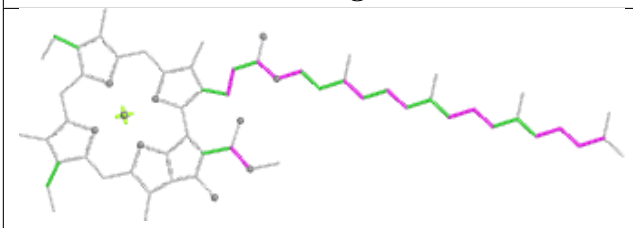
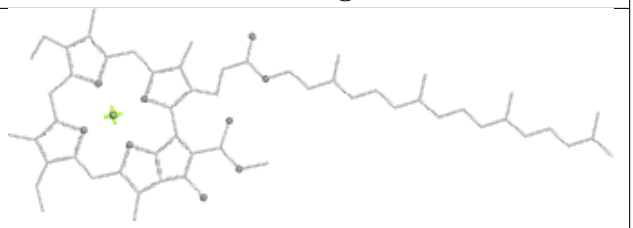


Bond angles

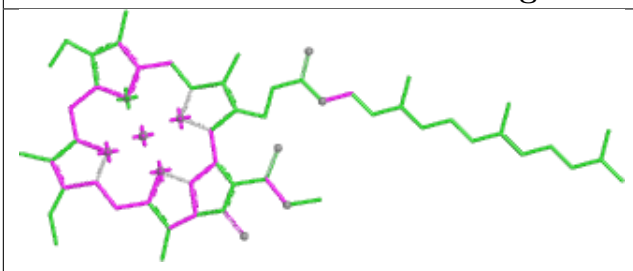


Torsions

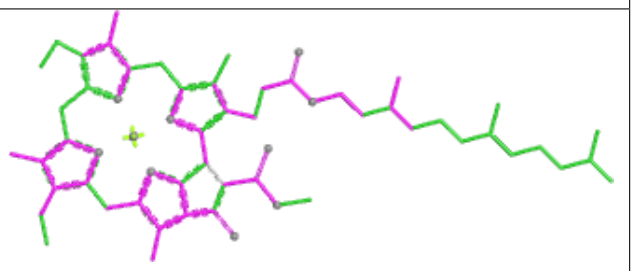


Rings

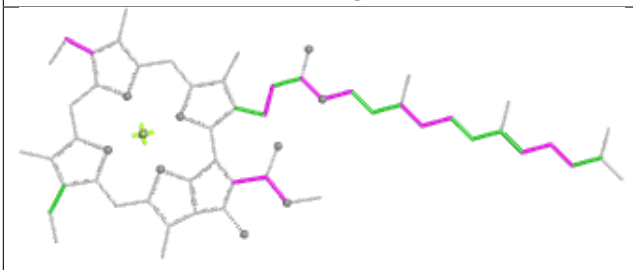
Ligand CLA a 1111



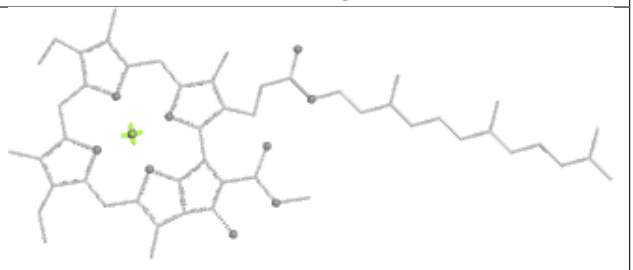
Bond lengths



Bond angles

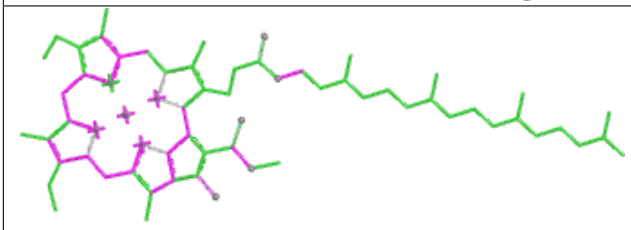


Torsions



Rings

Ligand CLA b 1023



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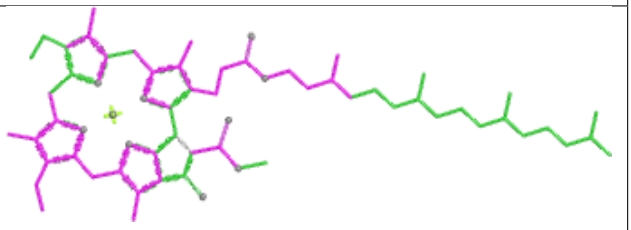
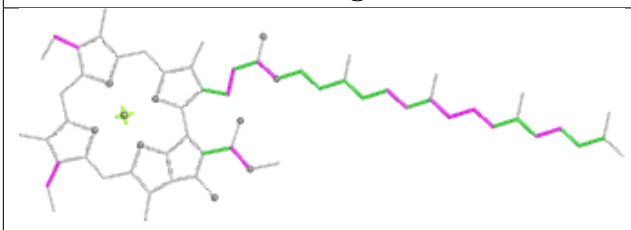
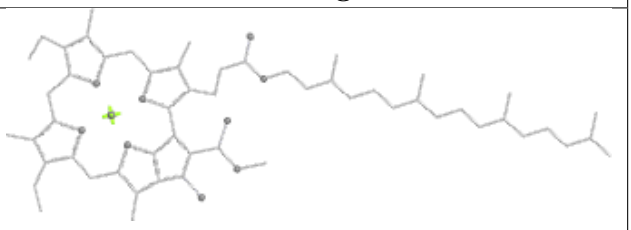


Bond angles

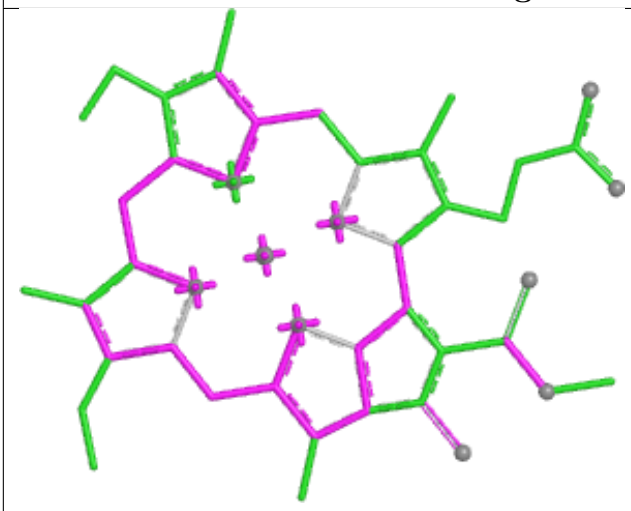


Torsions

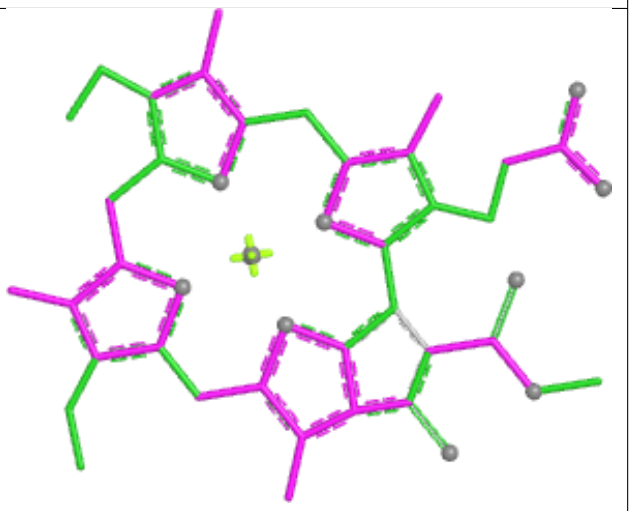


Rings

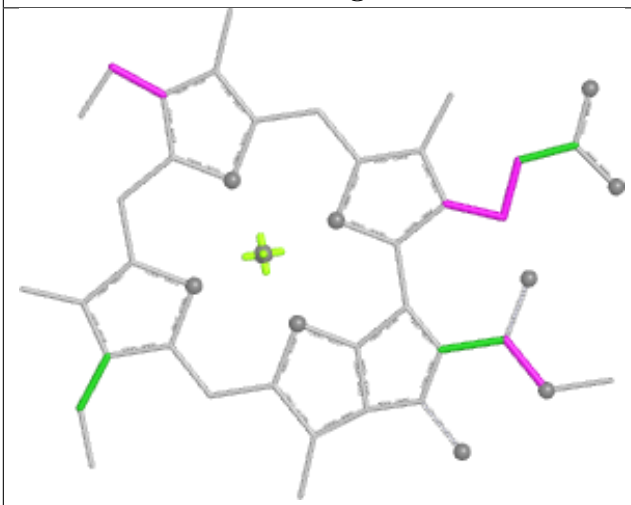
Ligand CLA K 1401



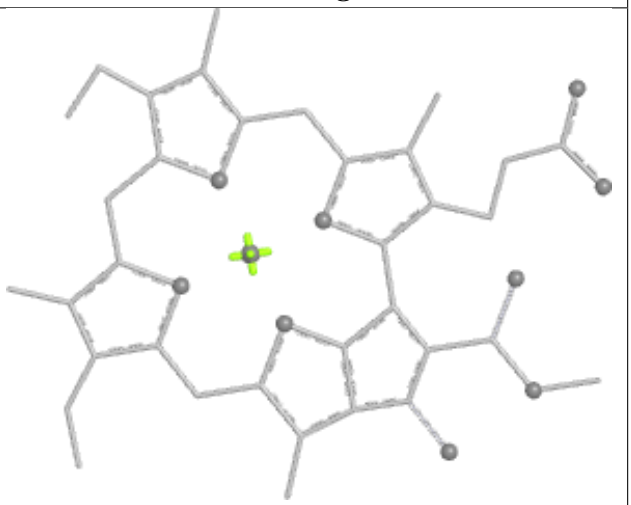
Bond lengths



Bond angles

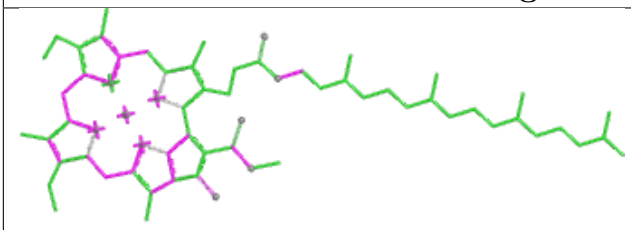


Torsions



Rings

Ligand CLA a 1104



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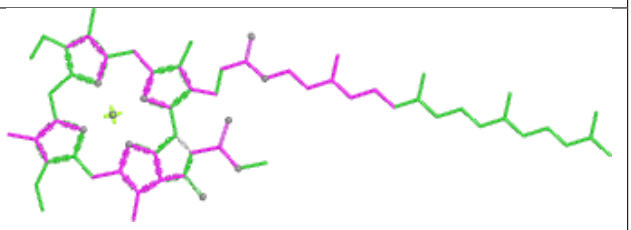
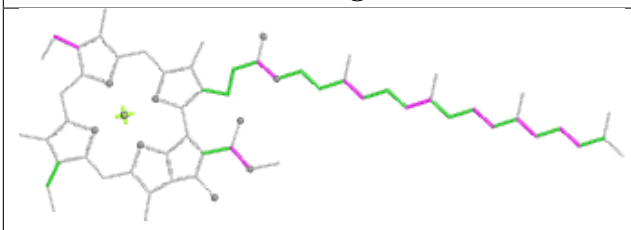


Bond angles



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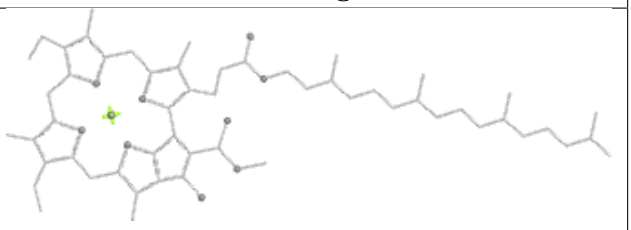
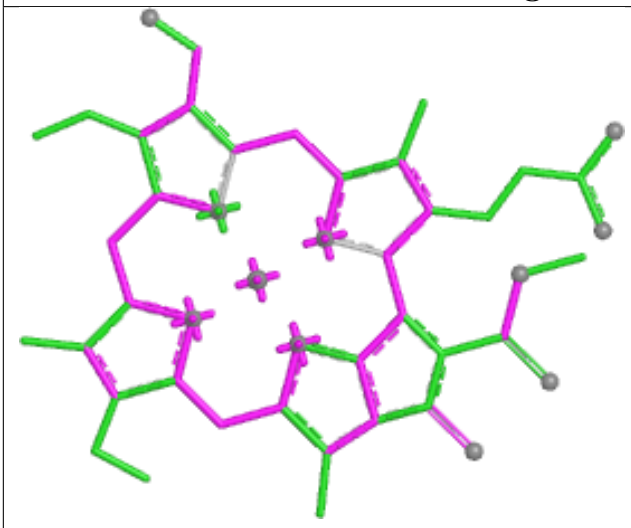


Rings

Ligand F6C a 1120



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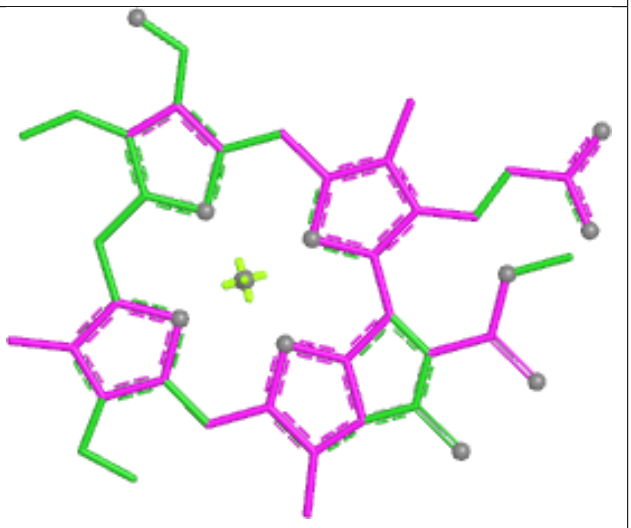

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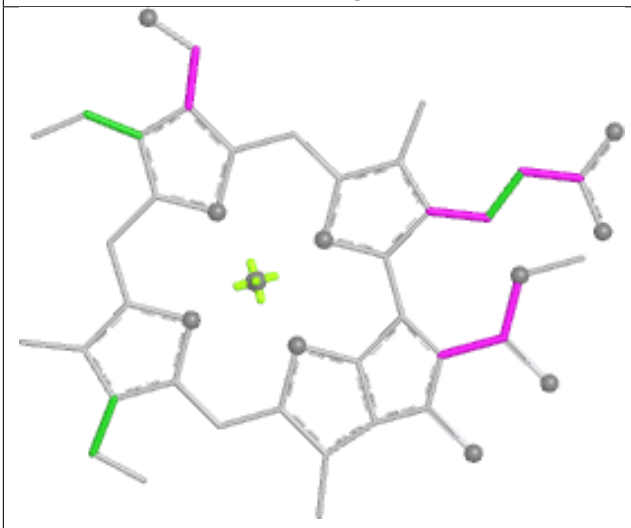

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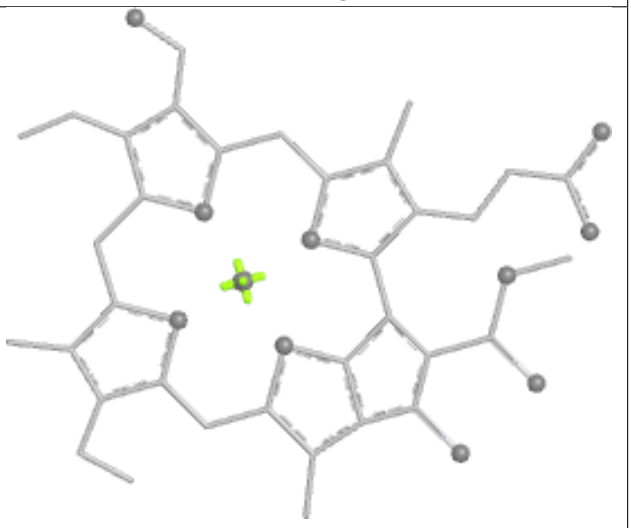
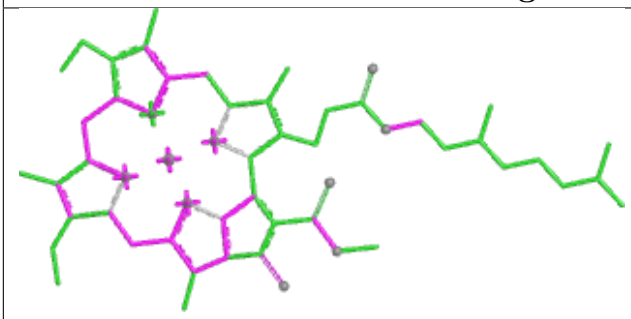


Rings

Ligand CLA b 1213



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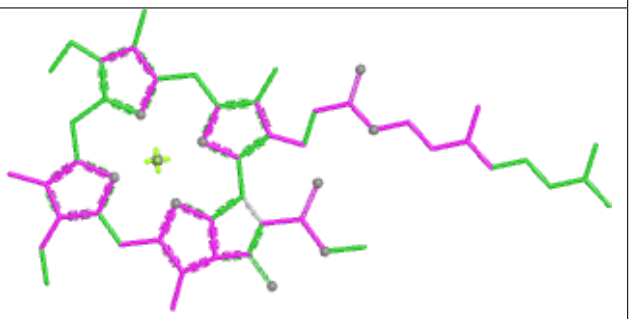
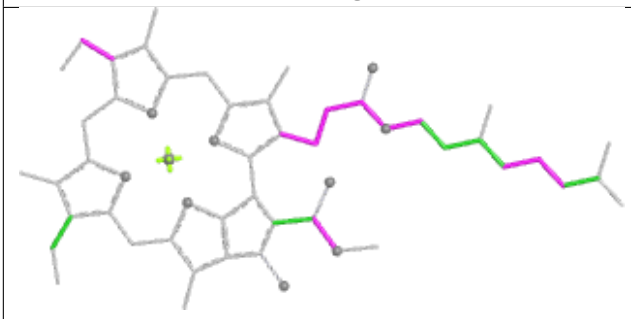


Bond angles



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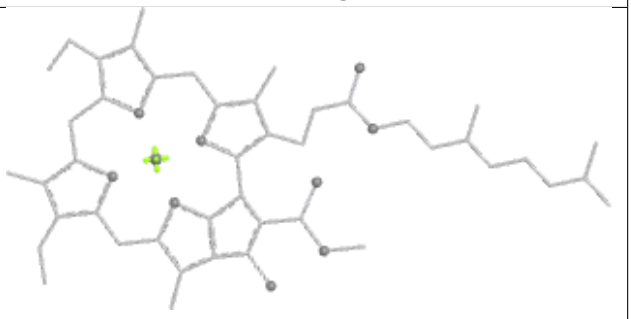
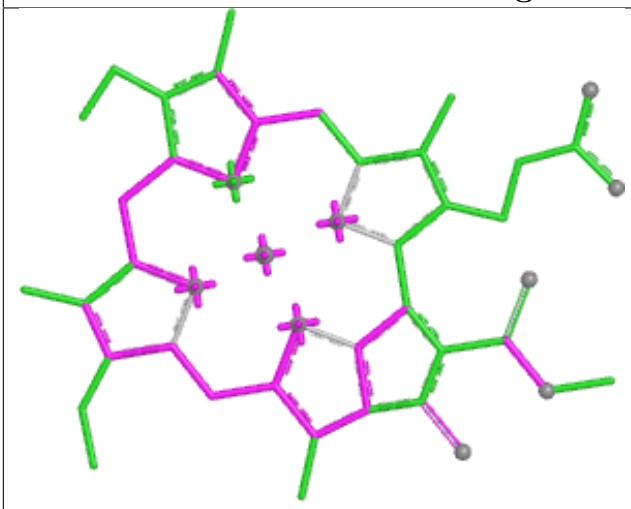


Rings

Ligand CLA B 1228



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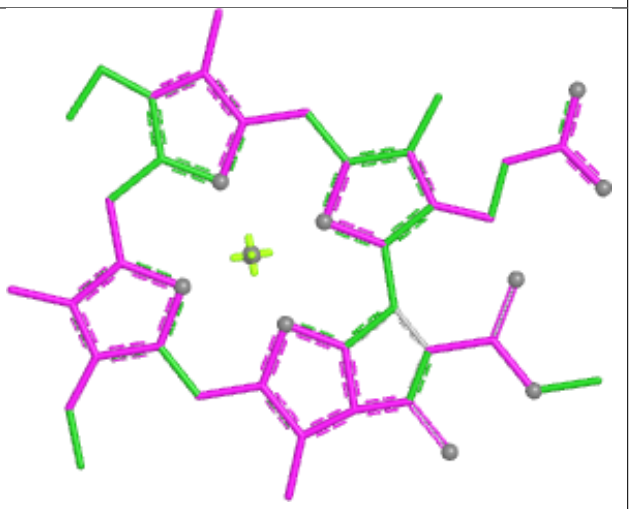
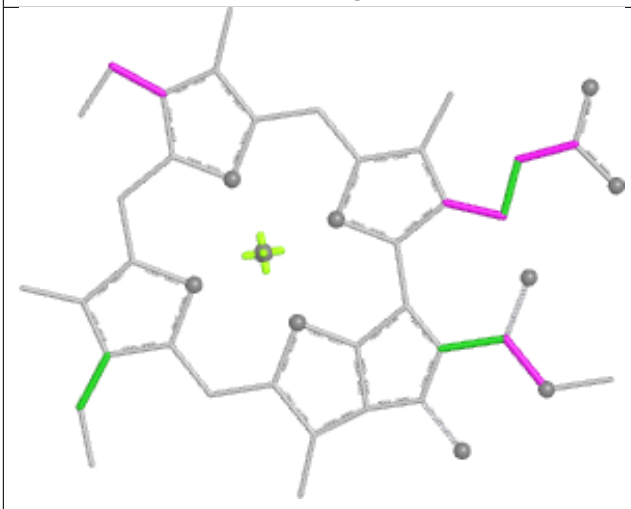


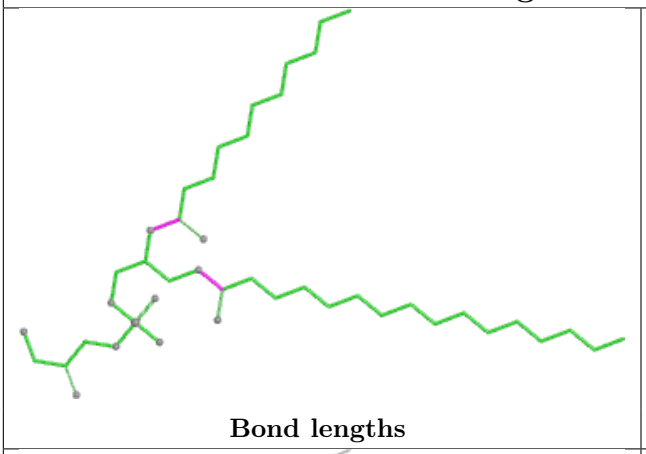
Bond angles



Torsions

Rings

Ligand LHG b 5004



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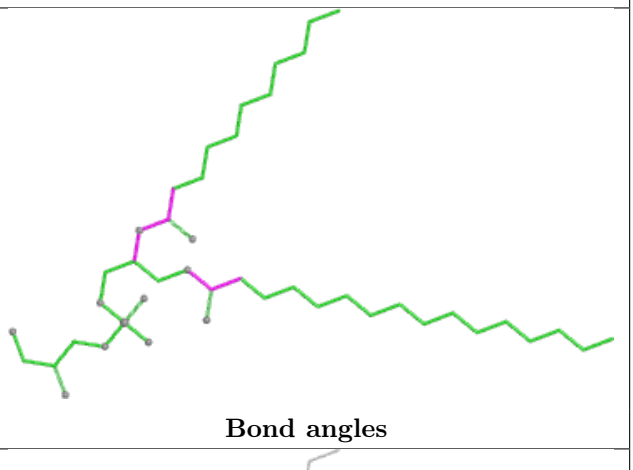

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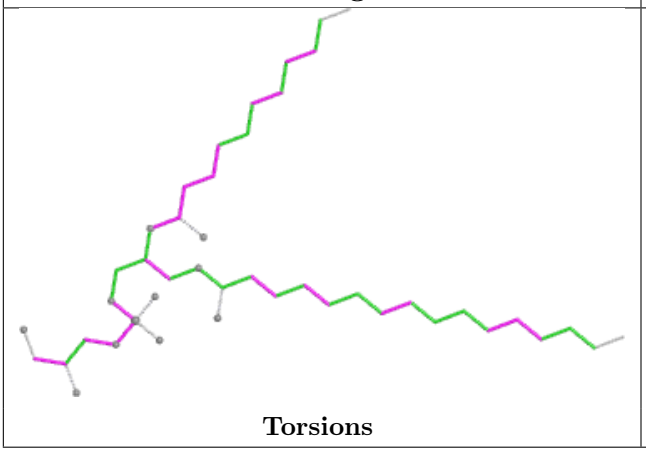

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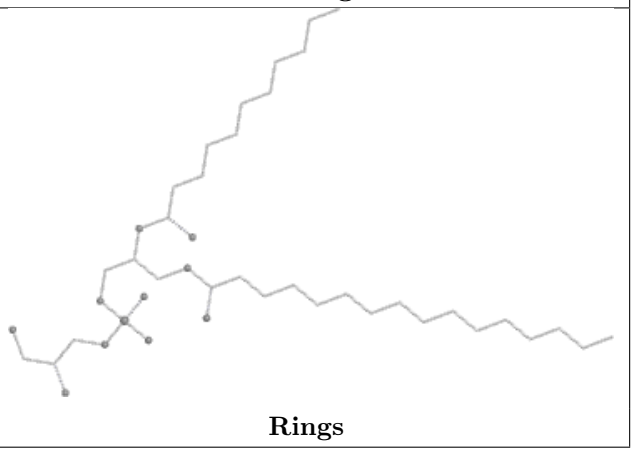
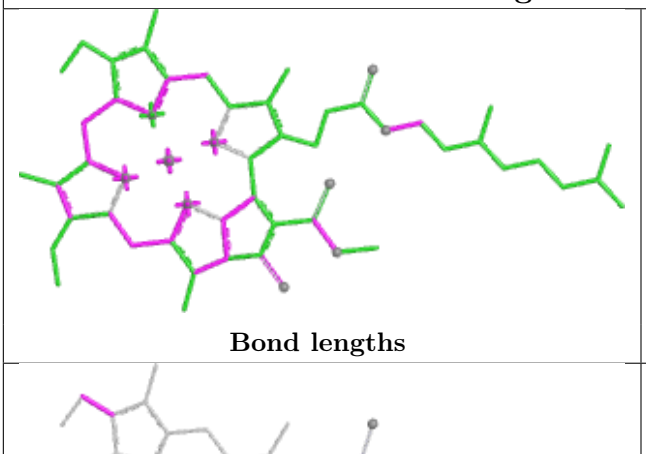


Rings

Ligand CLA A 1130



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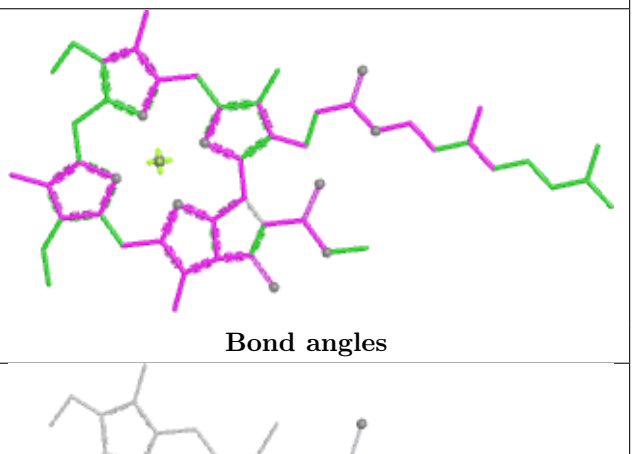
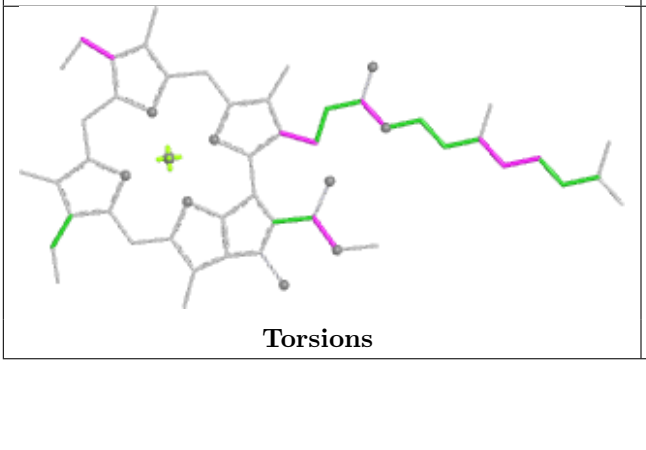


Bond angles



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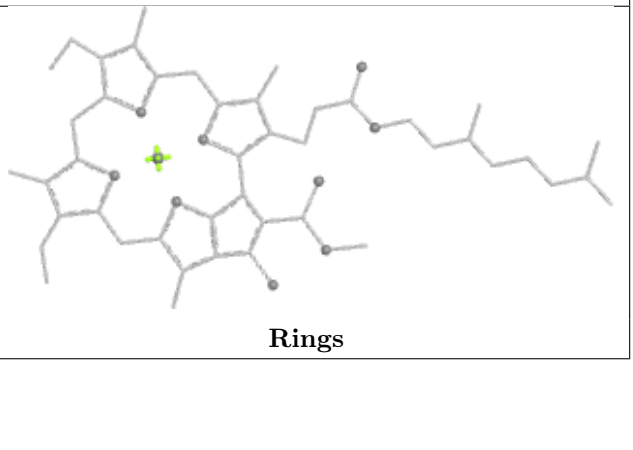
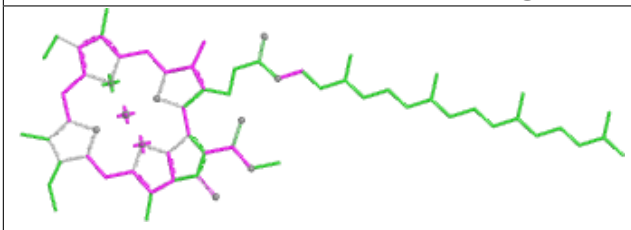


Rings

Ligand CL0 G 1011



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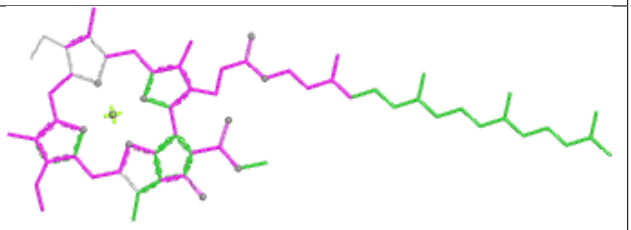

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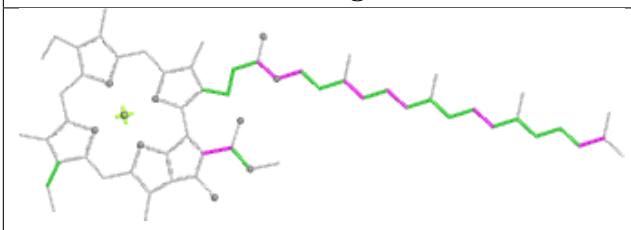

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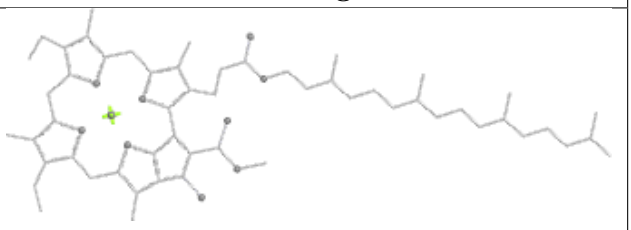
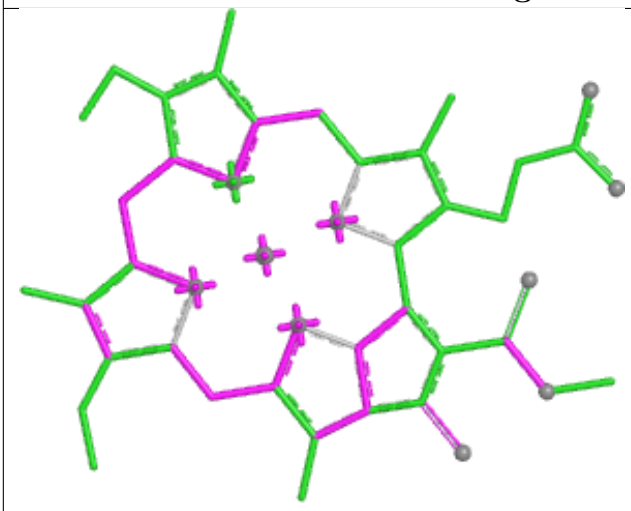


Rings

Ligand CLA G 1129



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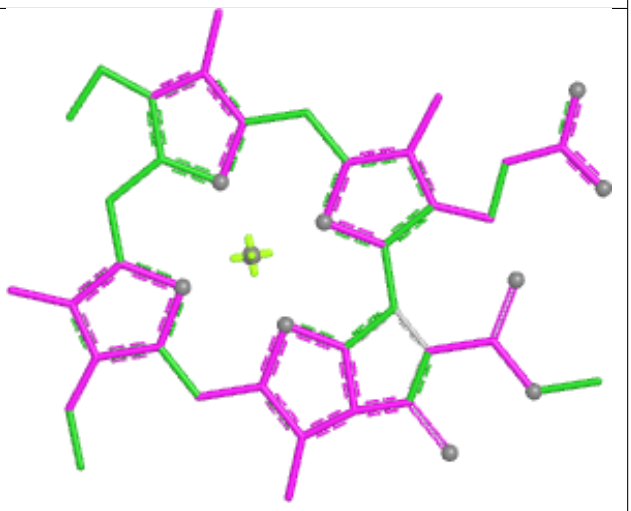

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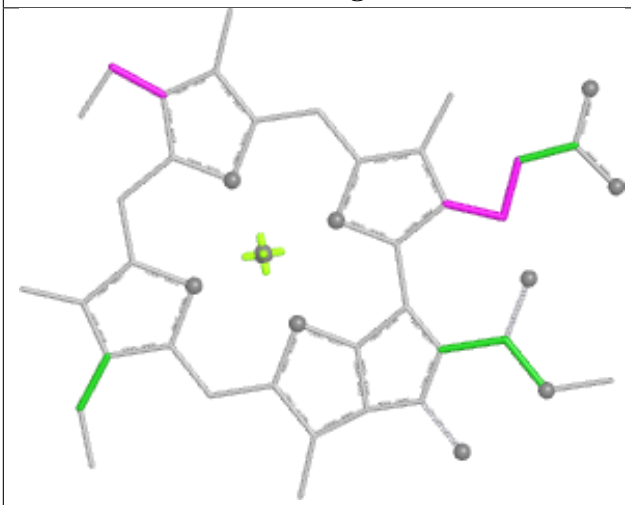

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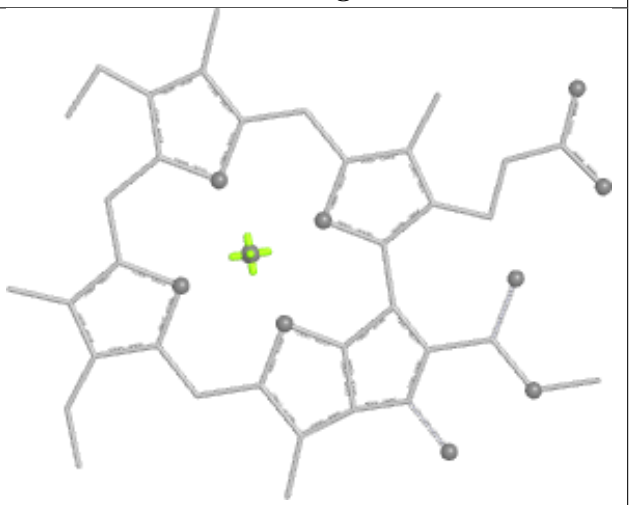
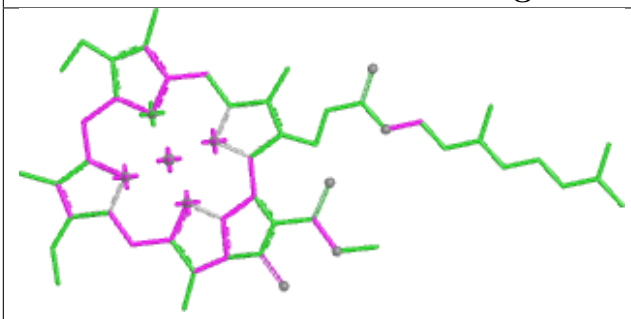


Rings

Ligand CLA G 1136



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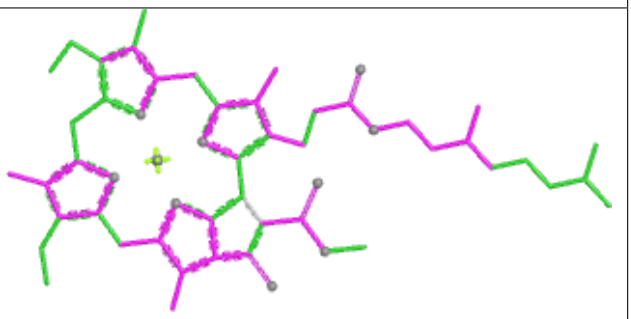
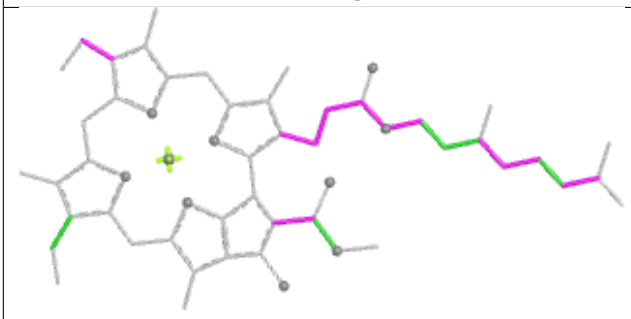
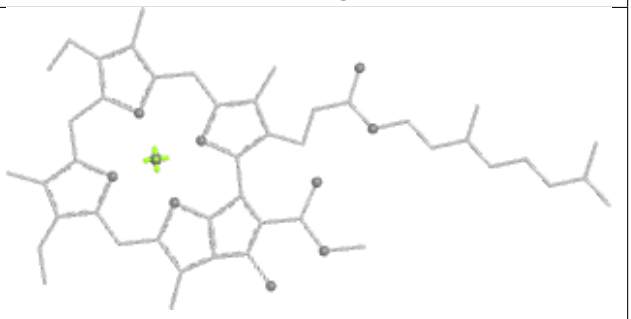


Bond angles

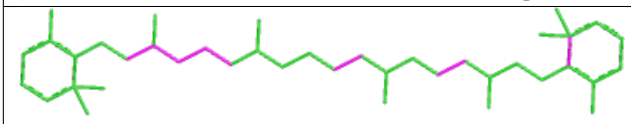


Torsions



Rings

Ligand BCR a 4008



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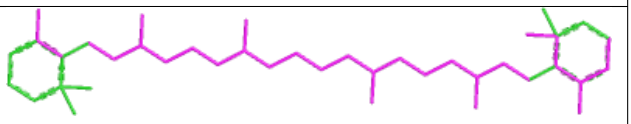
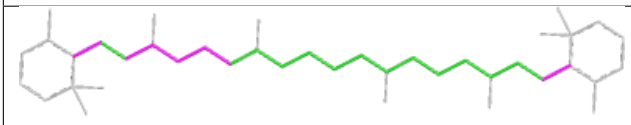


Bond angles



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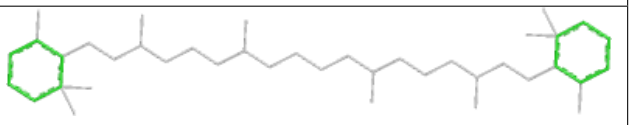
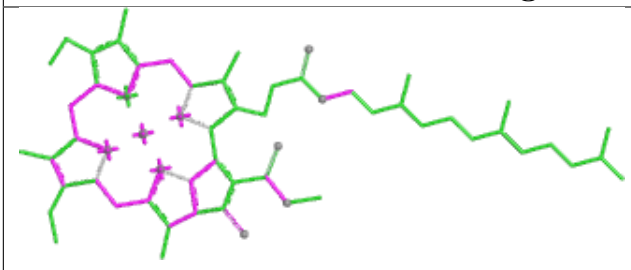


Rings

Ligand CLA a 1128



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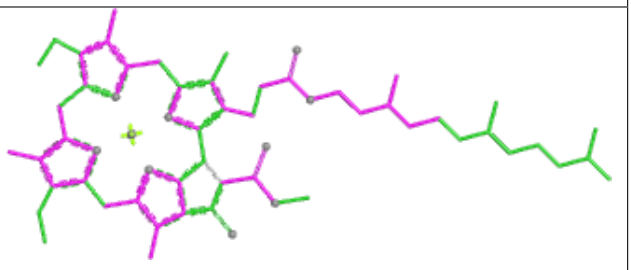
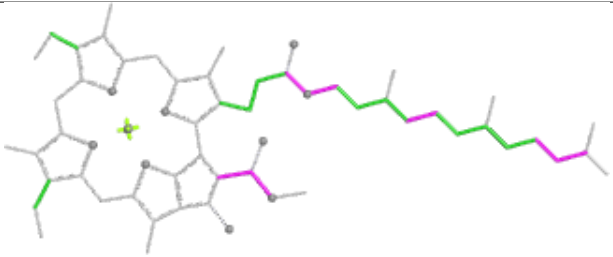
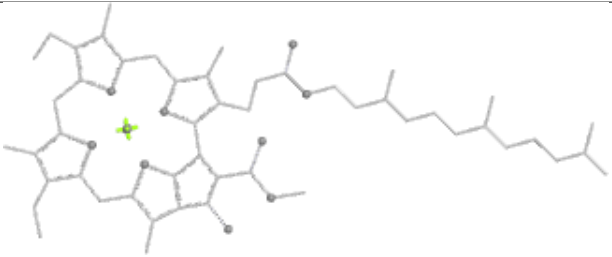


Bond angles

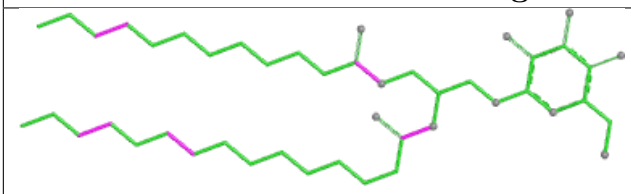


Torsions



Rings

Ligand LMG B 5002



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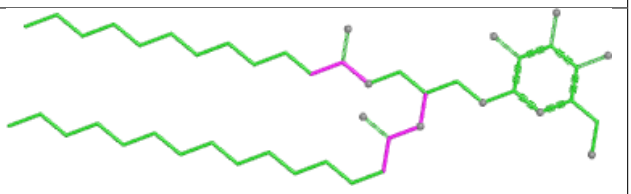
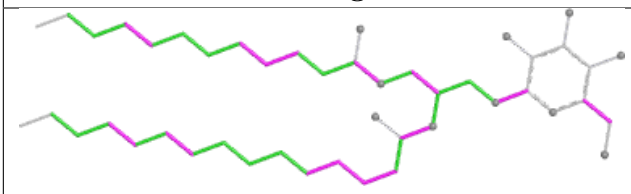
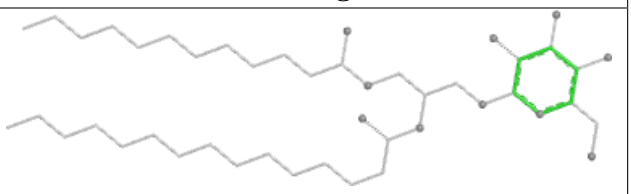


Bond angles

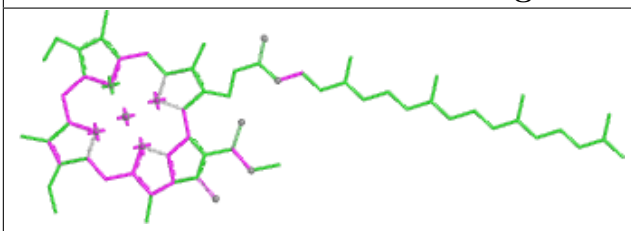


Torsions

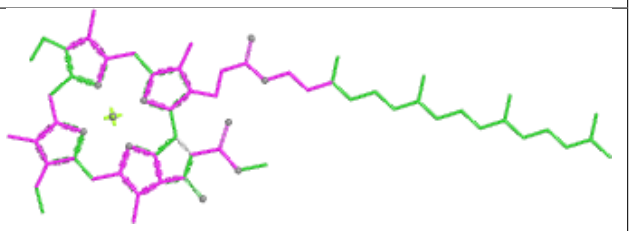


Rings

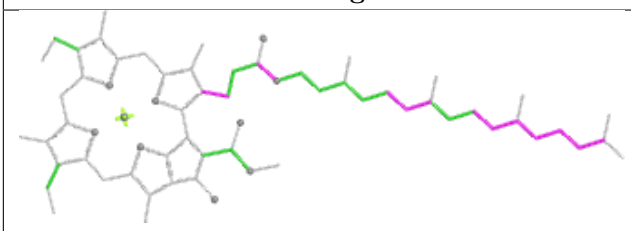
Ligand CLA A 1117



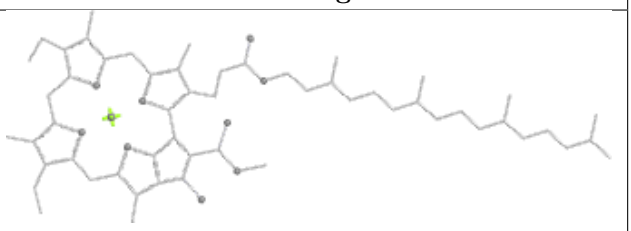
Bond lengths



Bond angles

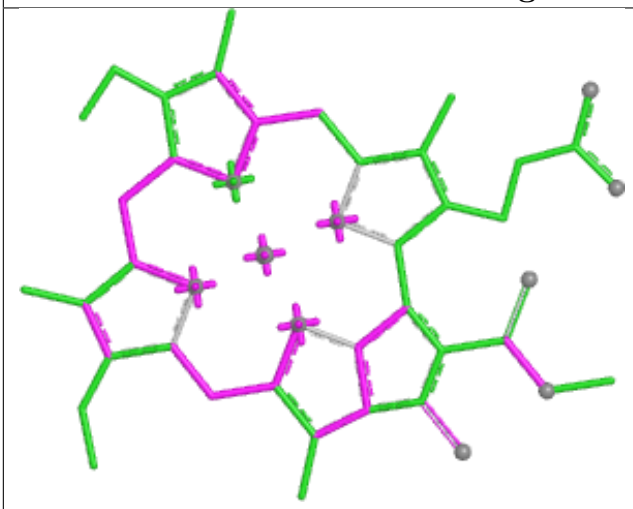


Torsions

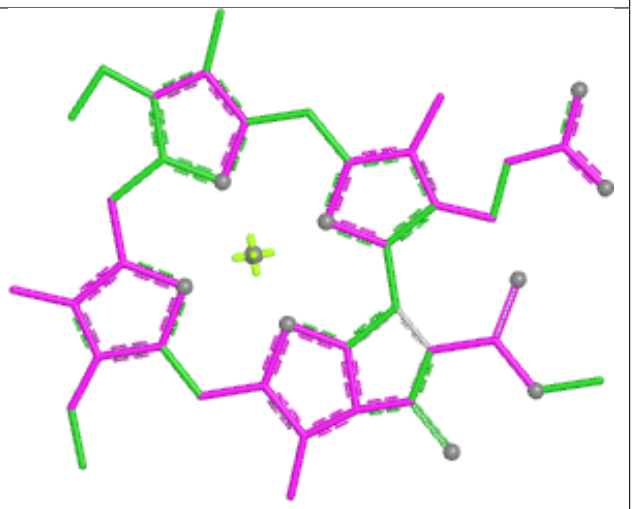


Rings

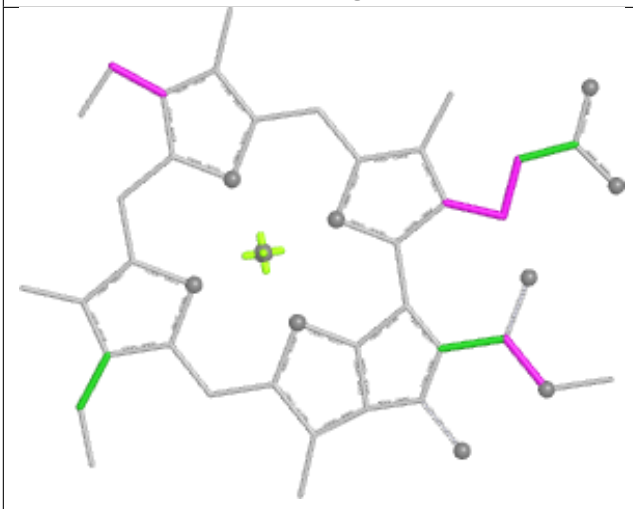
Ligand CLA b 1227



Bond lengths



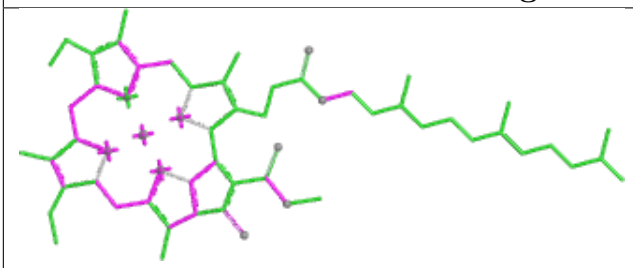
Bond angles



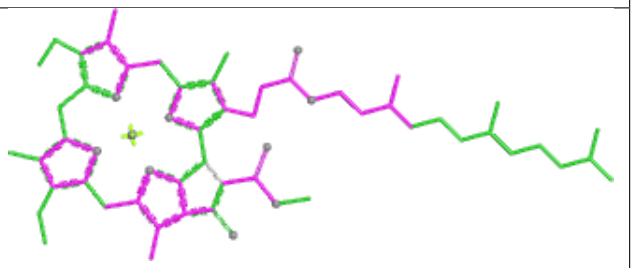
Torsions

Rings

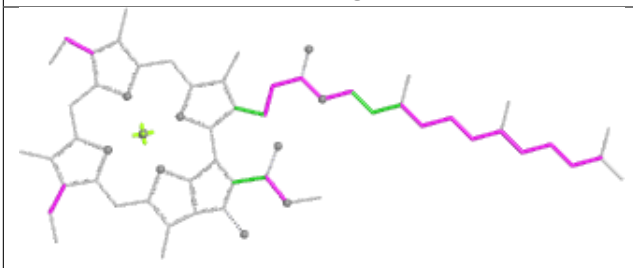
Ligand CLA a 1126



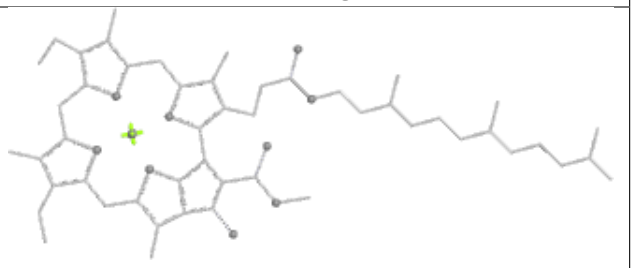
Bond lengths



Bond angles

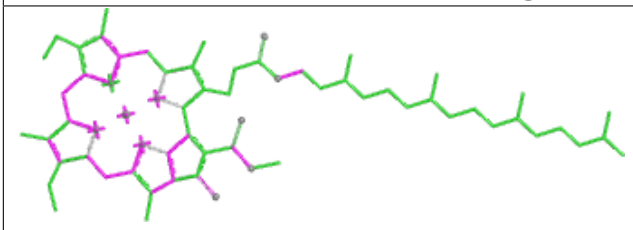


Torsions

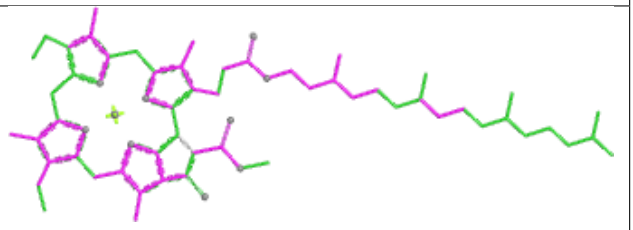


Rings

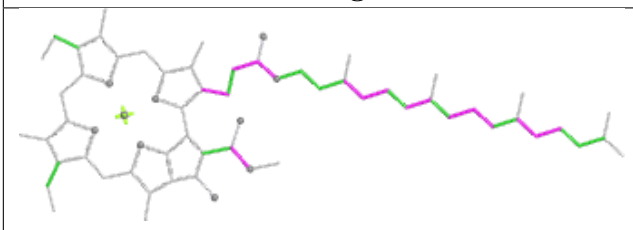
Ligand CLA a 1127



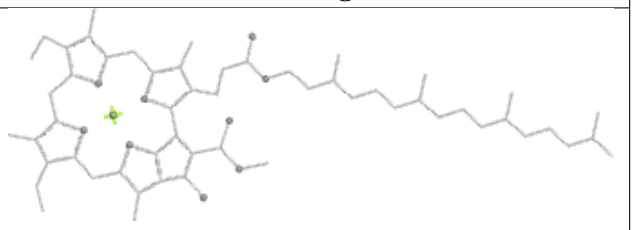
Bond lengths



Bond angles

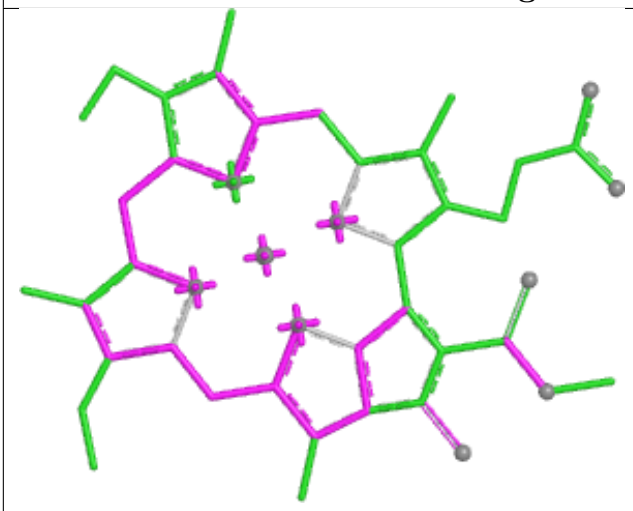


Torsions

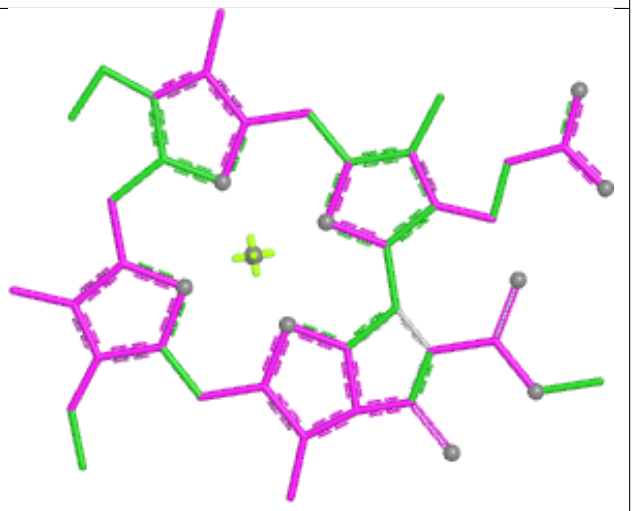


Rings

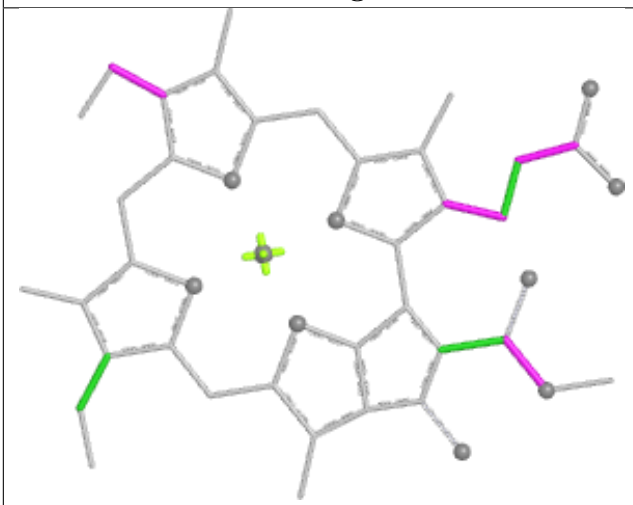
Ligand CLA b 1228



Bond lengths

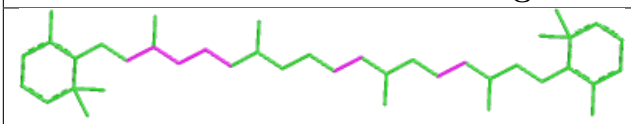
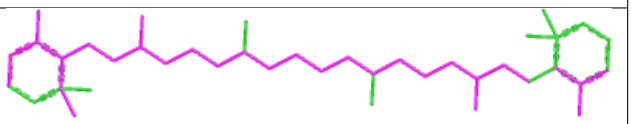
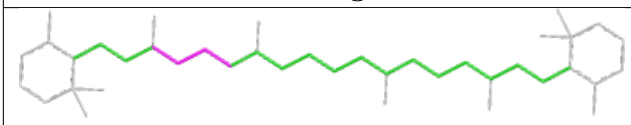
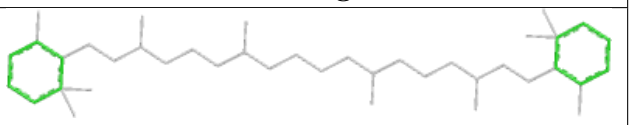


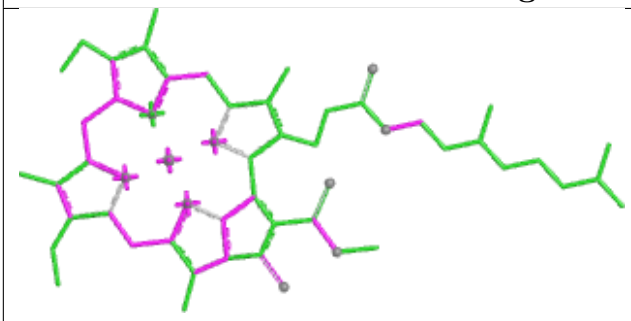
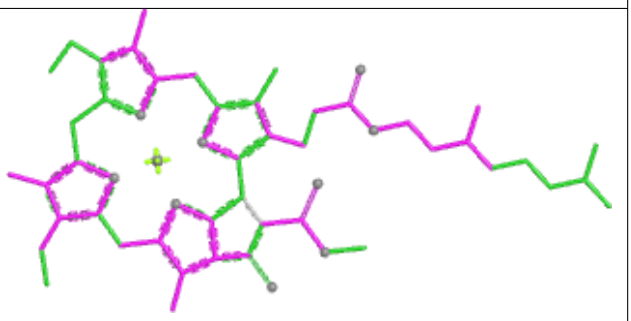
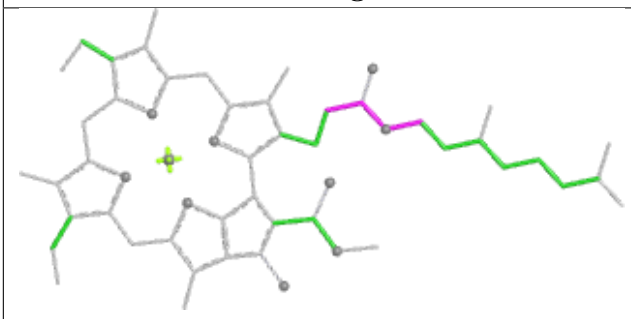
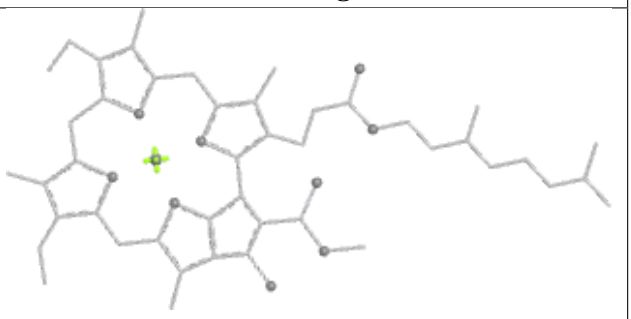
Bond angles

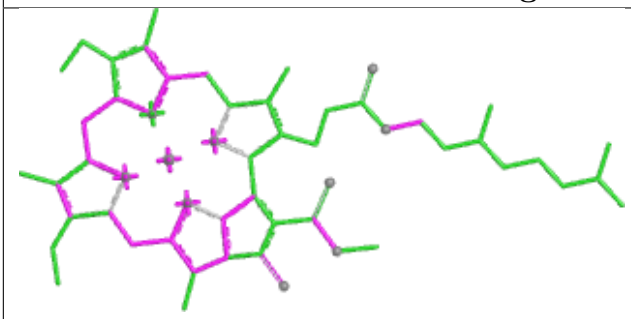
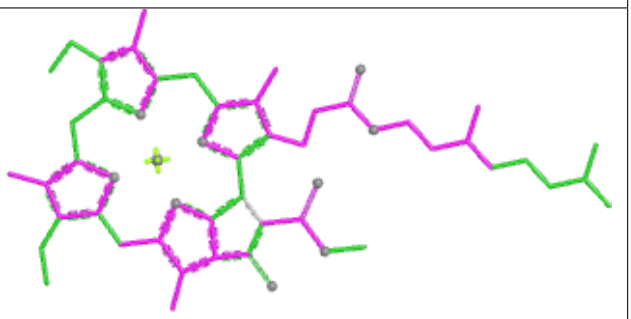
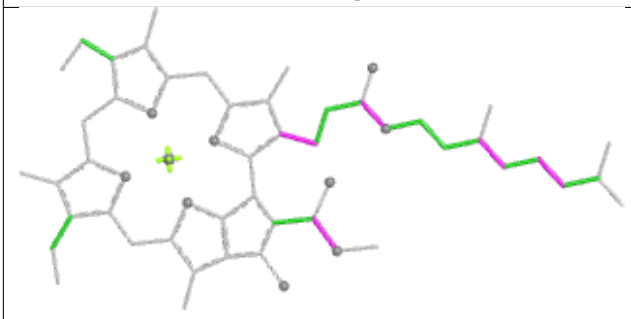
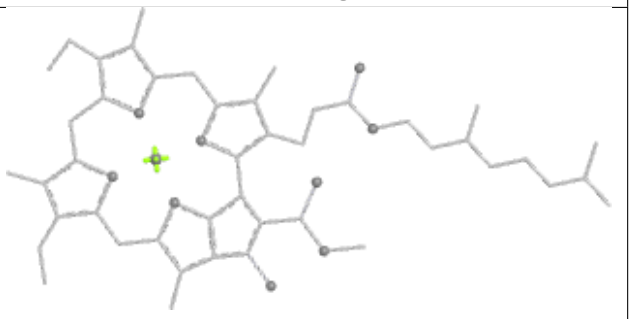


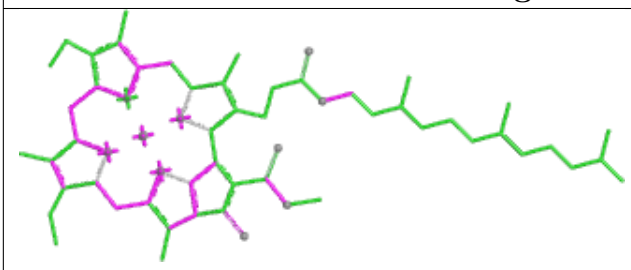
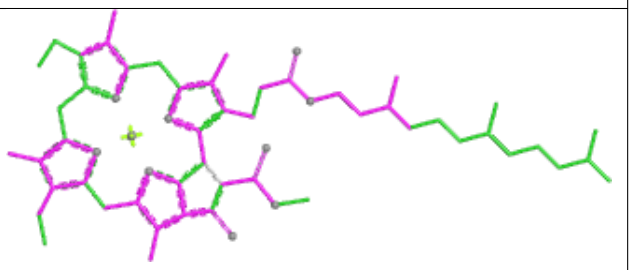
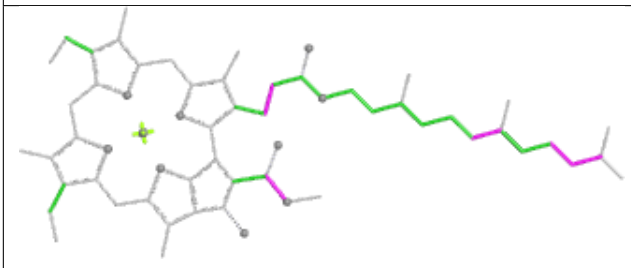
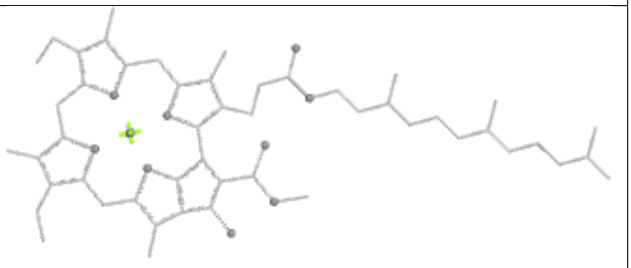
Torsions

Rings

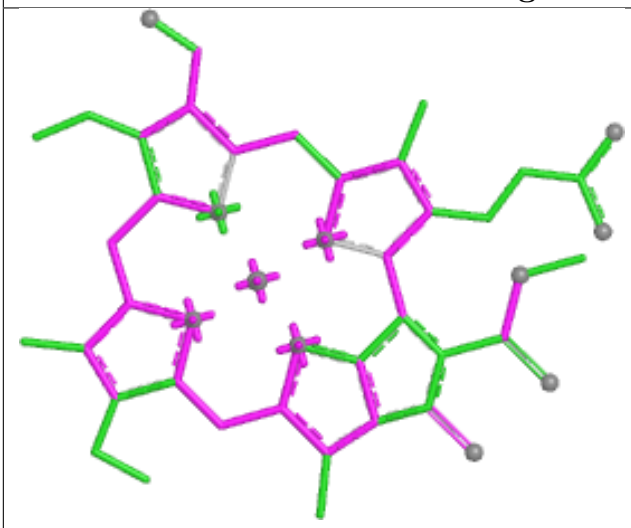
Ligand BCR B 4009	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 1231	
 Bond lengths	 Bond angles
 Torsions	 Rings

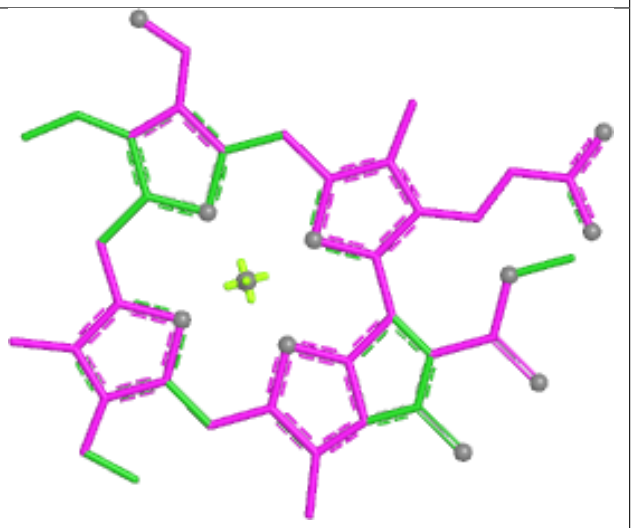
Ligand CLA a 1115	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

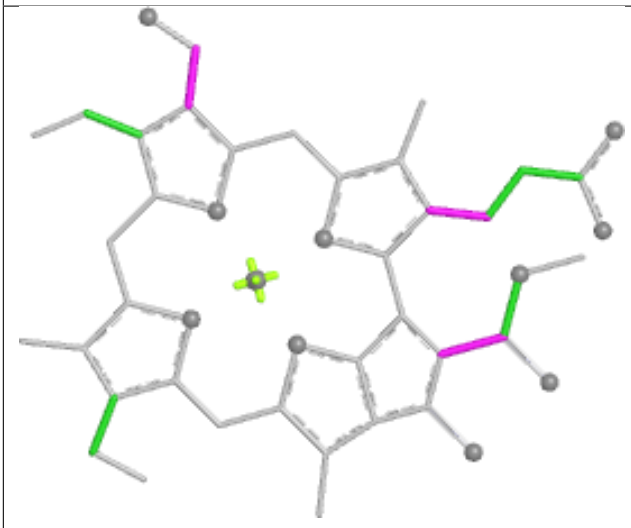
Ligand F6C H 1230



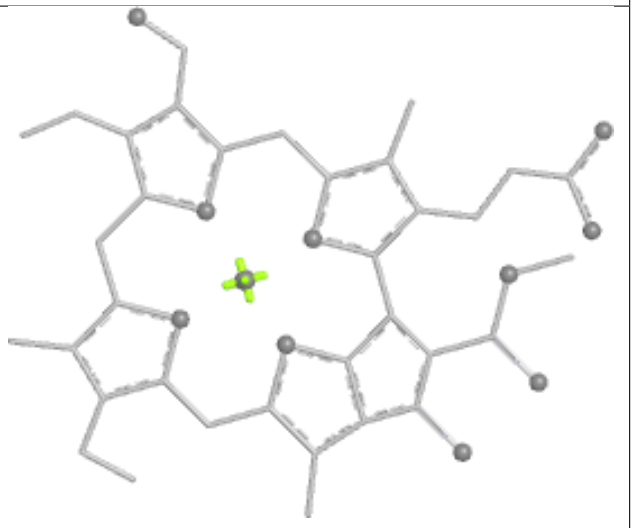
Bond lengths



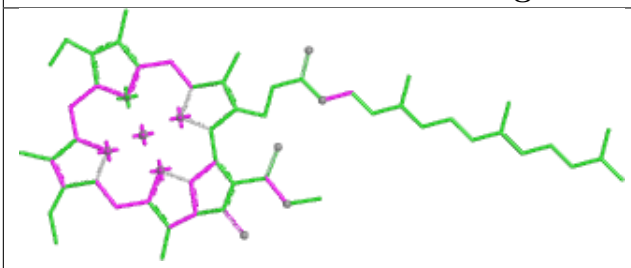
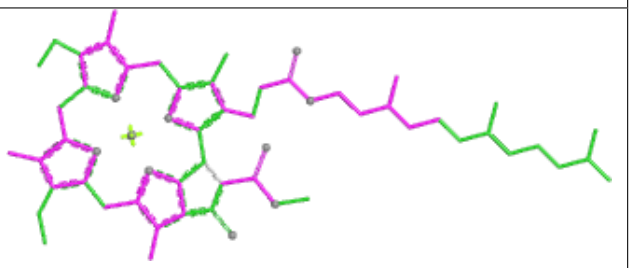
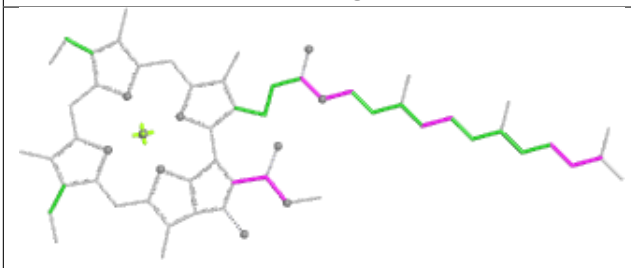
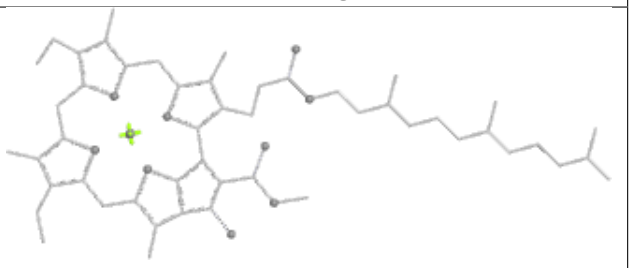
Bond angles

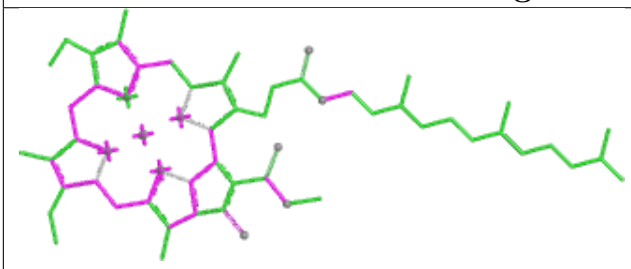
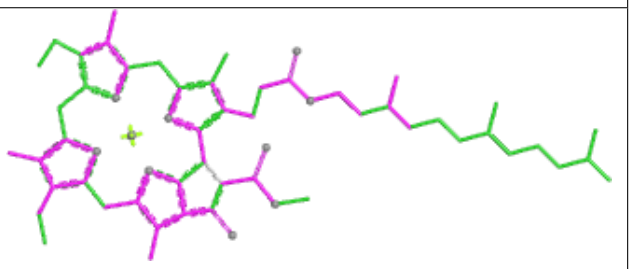
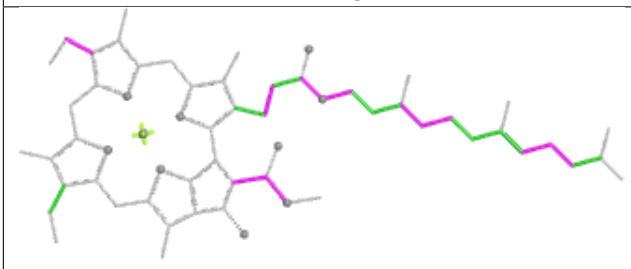
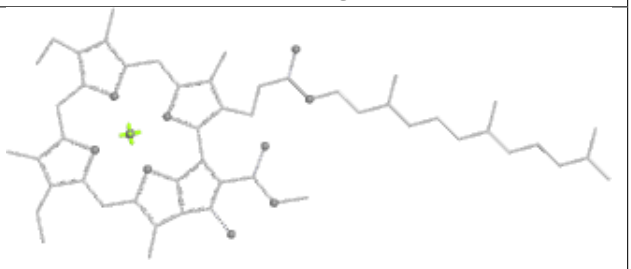


Torsions

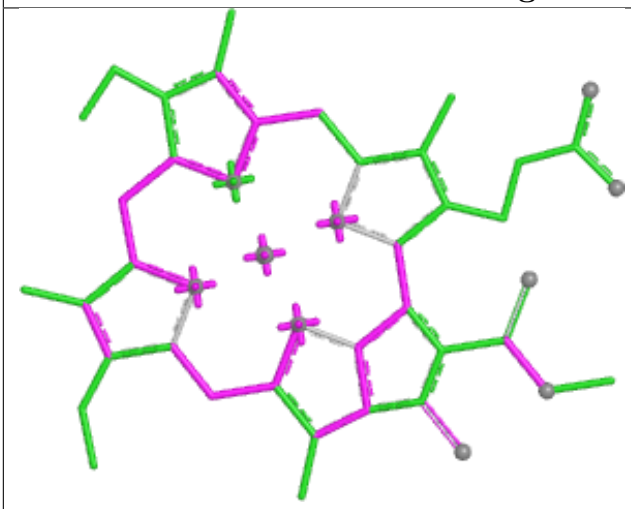


Rings

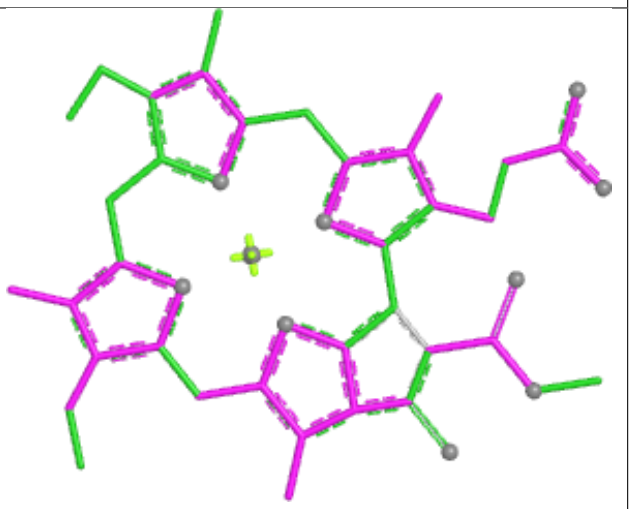
Ligand CLA G 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1111	
	
Bond lengths	Bond angles
	
Torsions	Rings

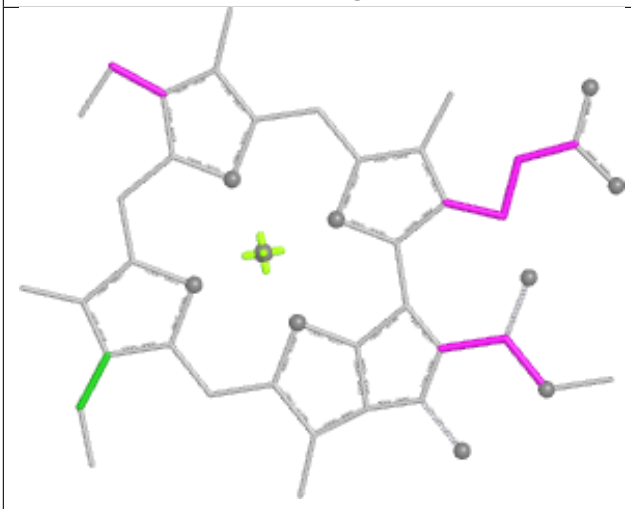
Ligand CLA b 1212



Bond lengths



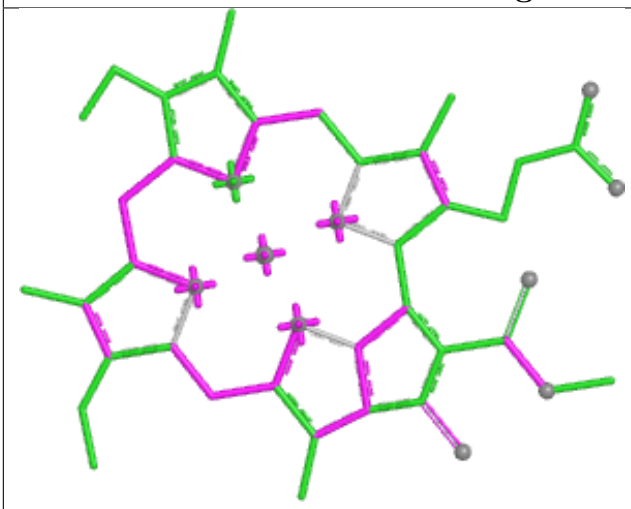
Bond angles



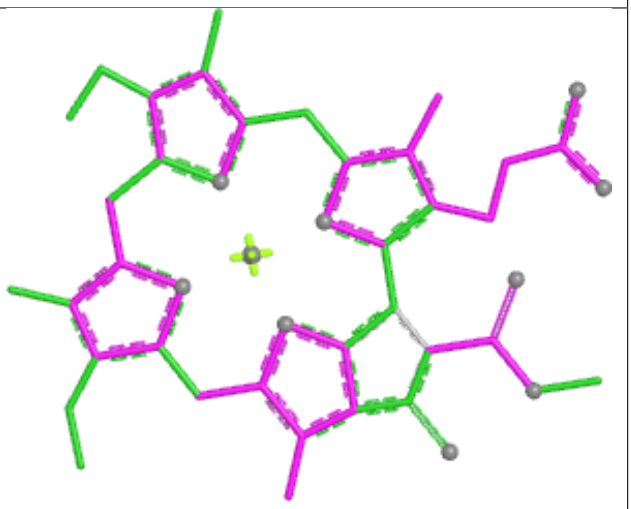
Torsions

Rings

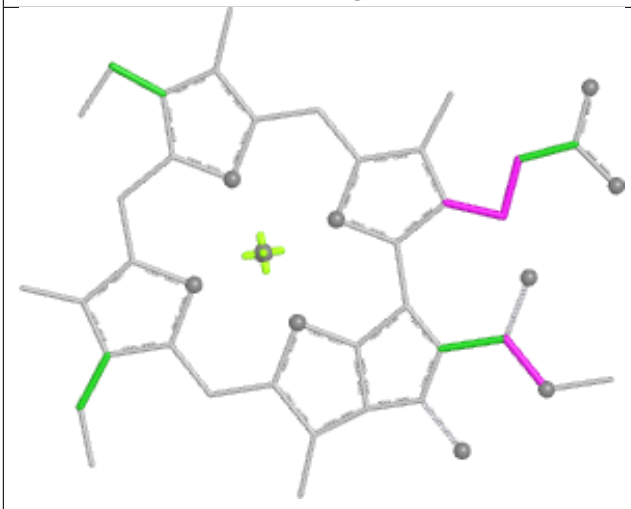
Ligand CLA B 1206



Bond lengths



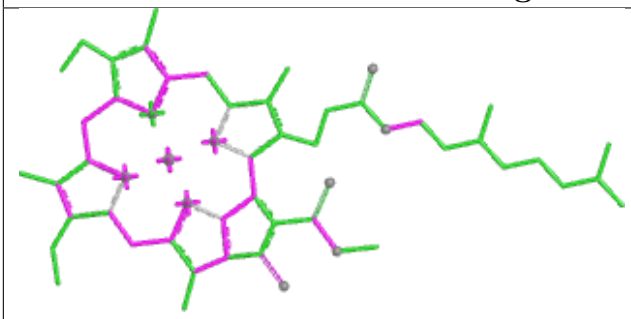
Bond angles



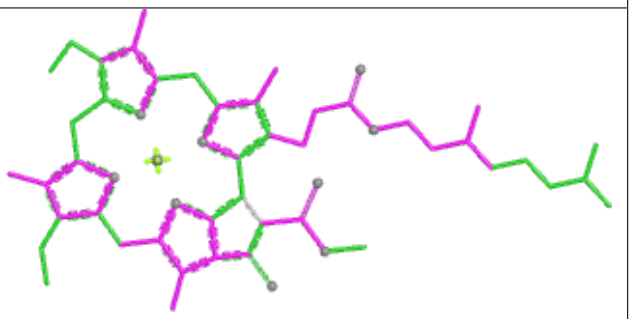
Torsions

Rings

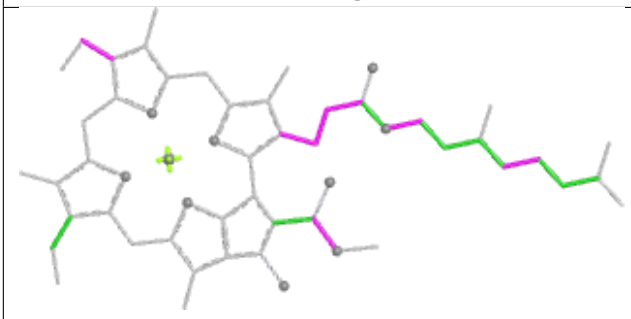
Ligand CLA H 1217



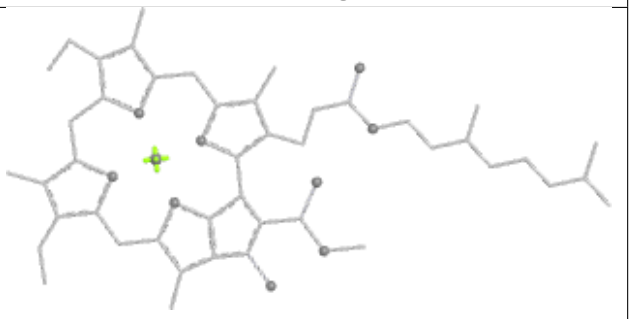
Bond lengths



Bond angles

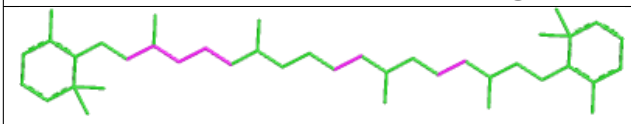


Torsions

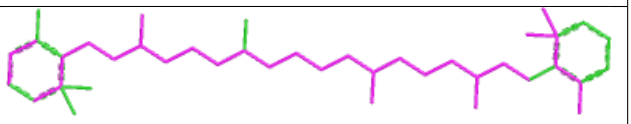


Rings

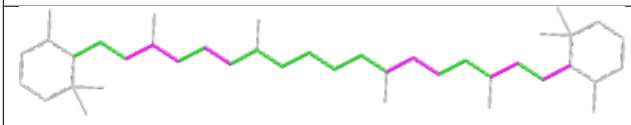
Ligand BCR M 4021



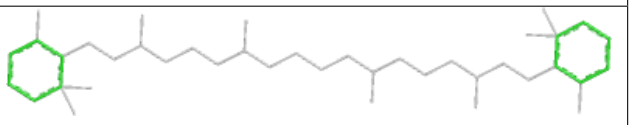
Bond lengths



Bond angles

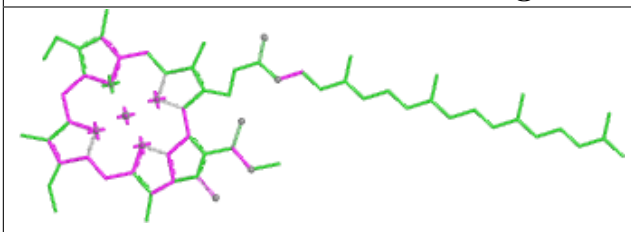


Torsions



Rings

Ligand CLA B 1239



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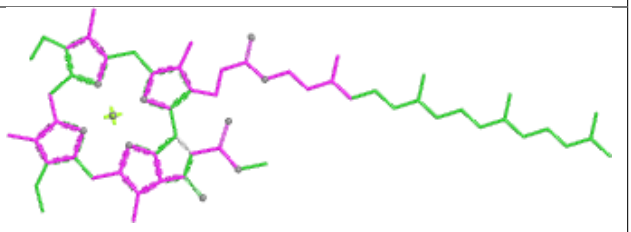
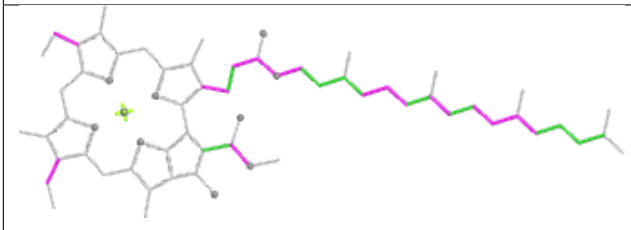


Bond angles



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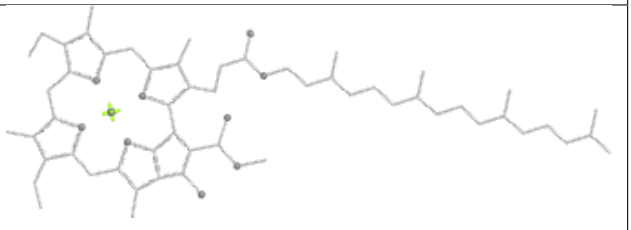
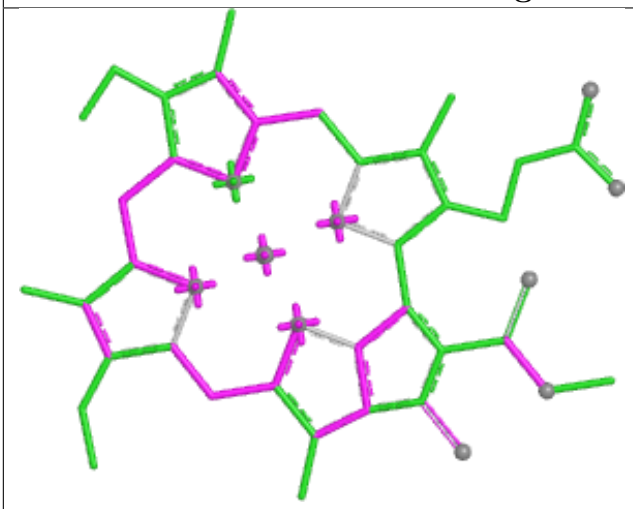


Rings

Ligand CLA A 1101



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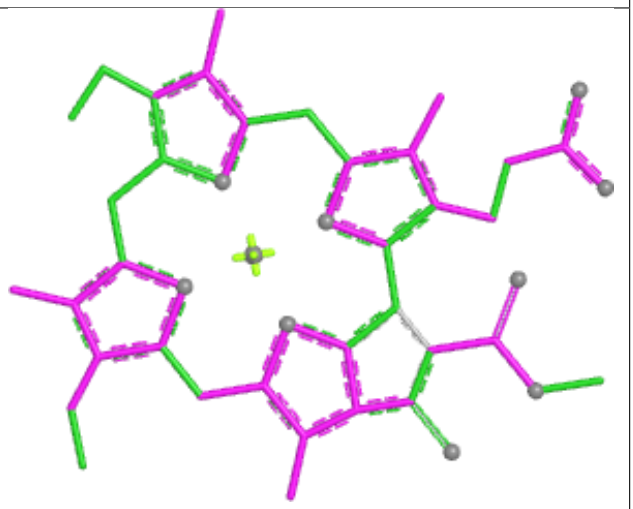

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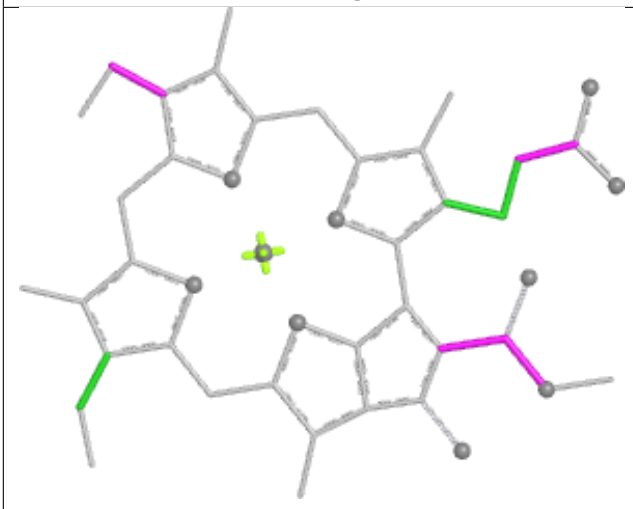
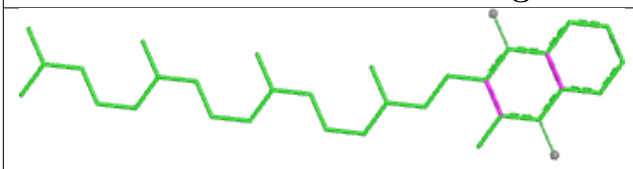


Torsions

Rings

Ligand PQN A 2001



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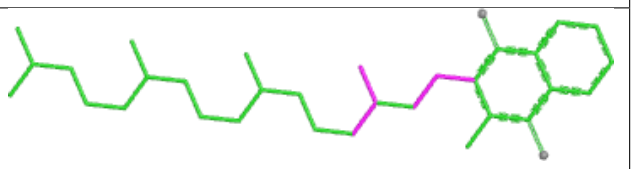

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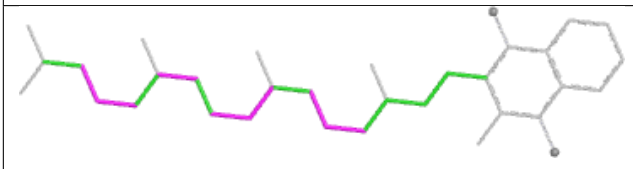
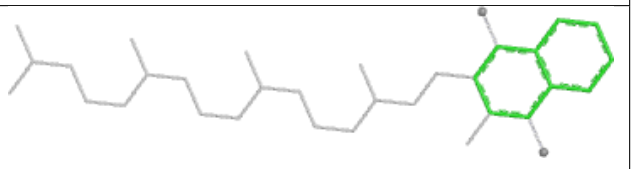
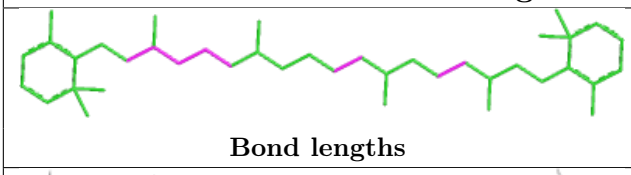


Torsions



Rings

Ligand BCR L 4022



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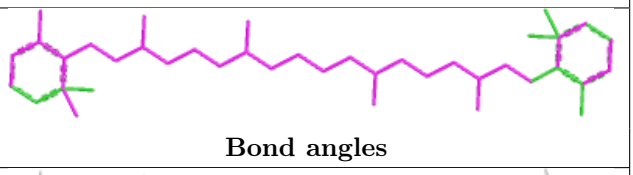
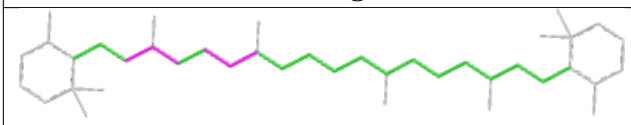
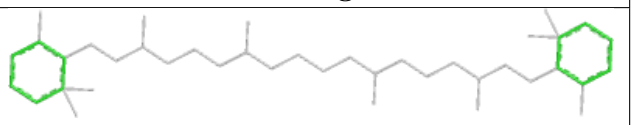


Bond angles

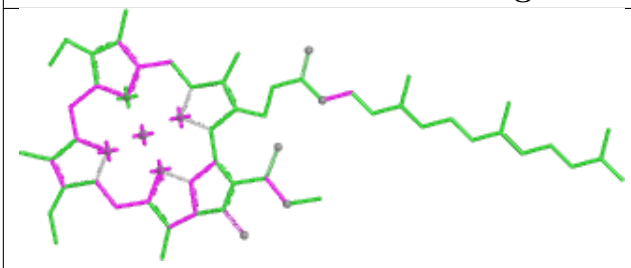


Torsions

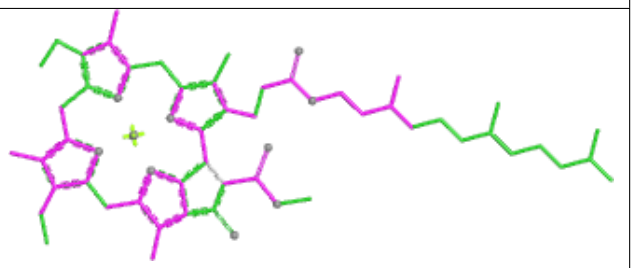


Rings

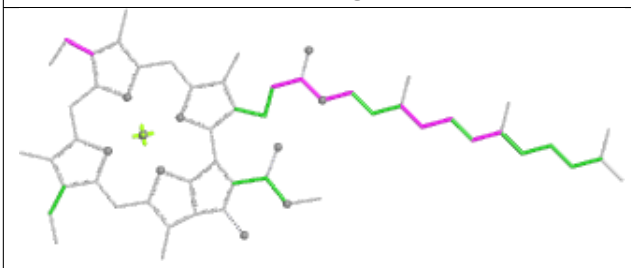
Ligand CLA H 1202



Bond lengths



Bond angles



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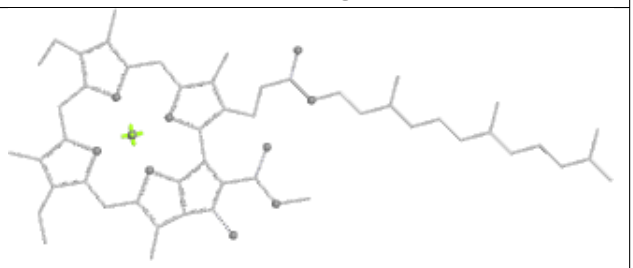
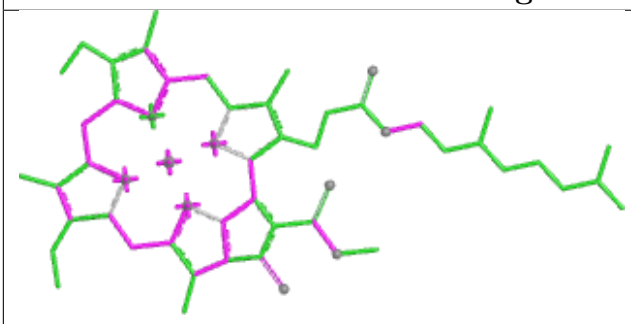
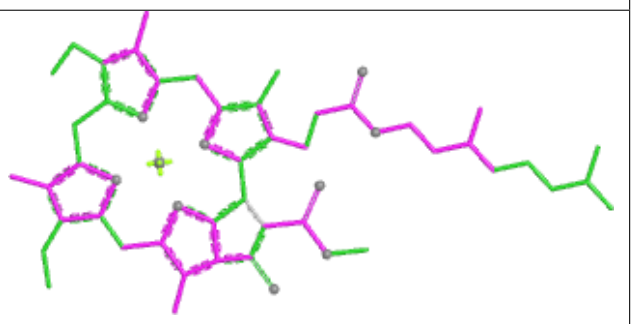


Rings

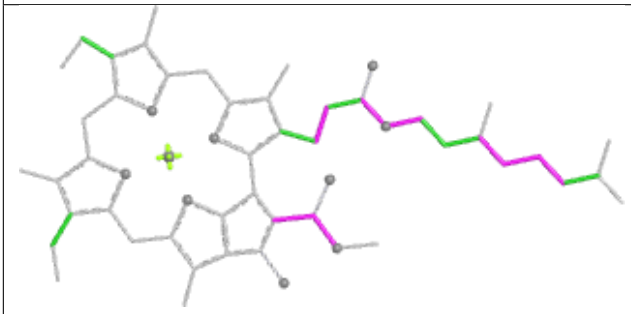
Ligand CLA B 1201



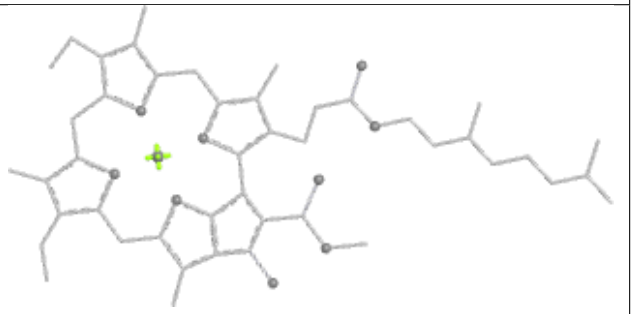
Bond lengths



Bond angles

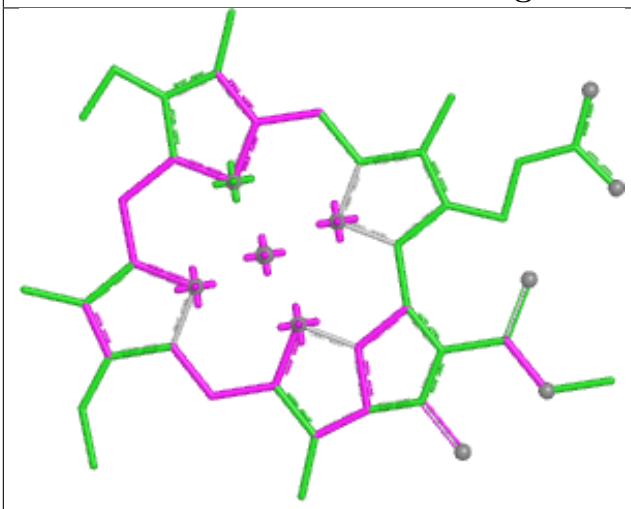


Torsions



Rings

Ligand CLA A 1137



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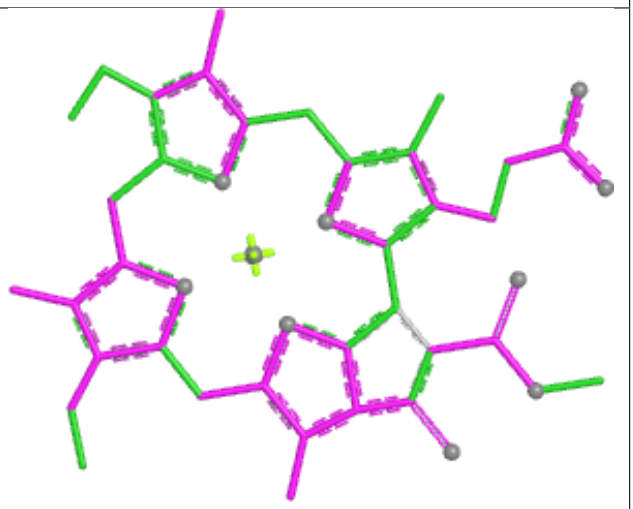
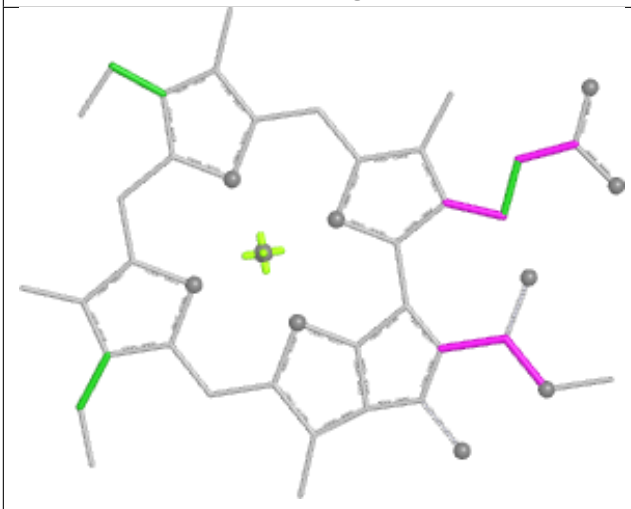


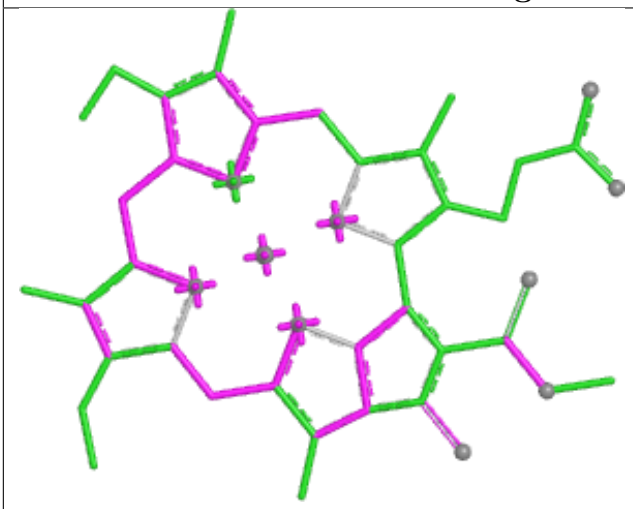
Bond angles



Torsions

Rings

Ligand CLA H 1207



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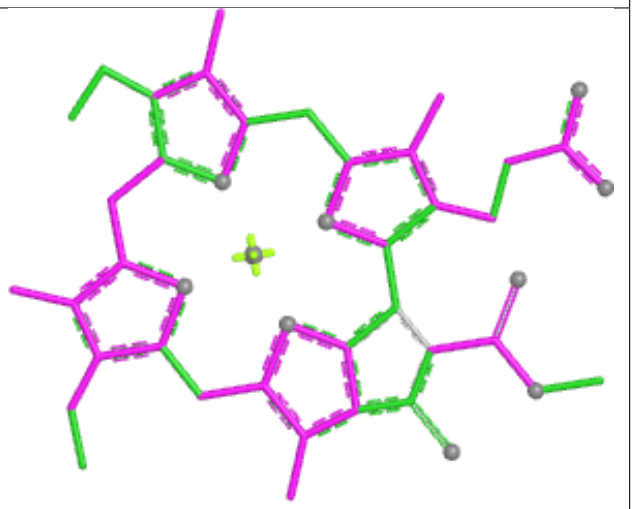
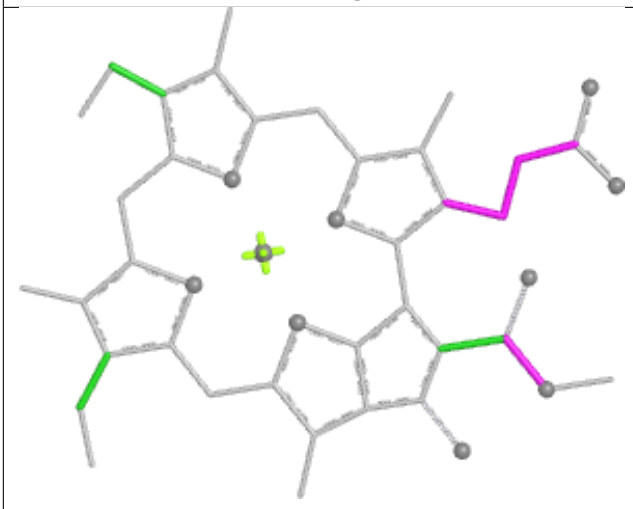


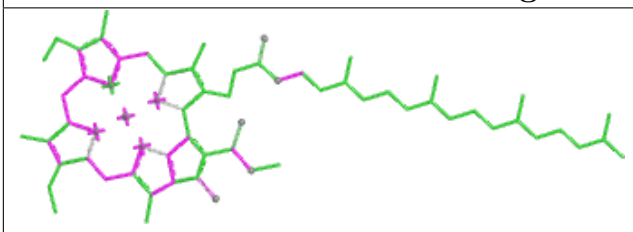
Bond angles



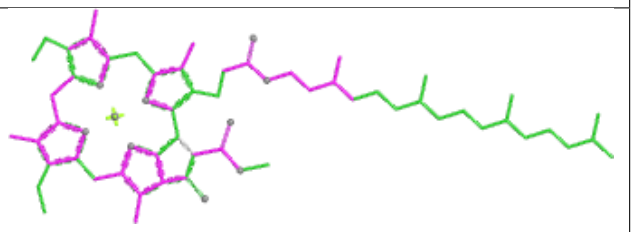
Torsions

Rings

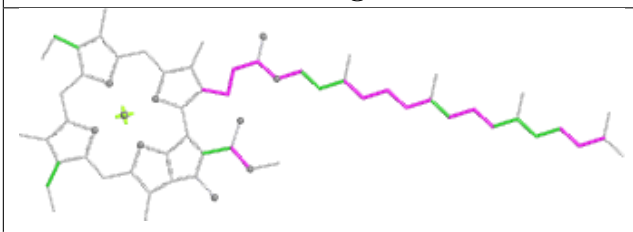
Ligand CLA a 1140



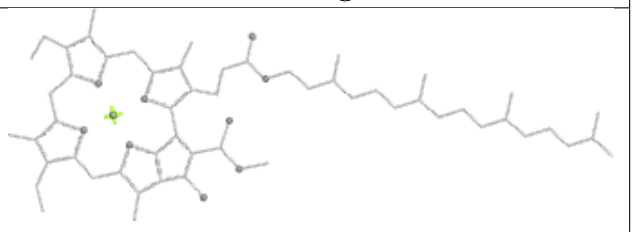
Bond lengths



Bond angles

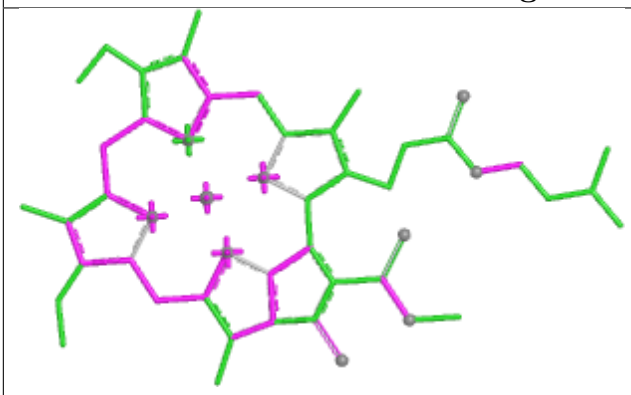


Torsions



Rings

Ligand CLA a 1135



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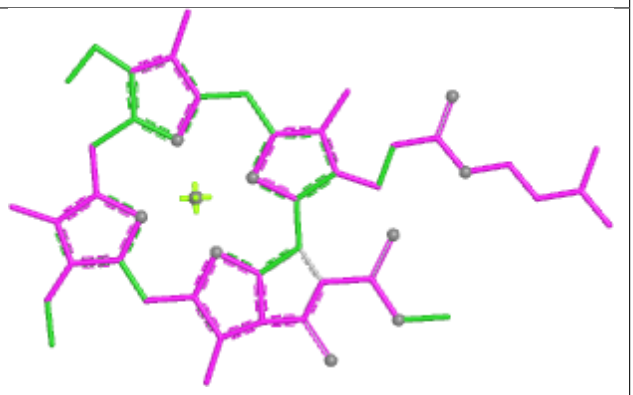
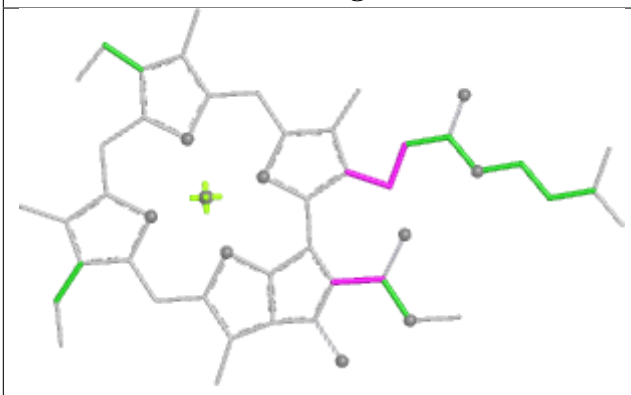


Bond angles



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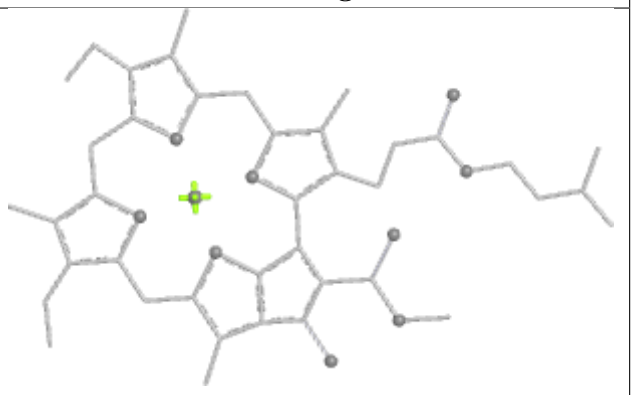
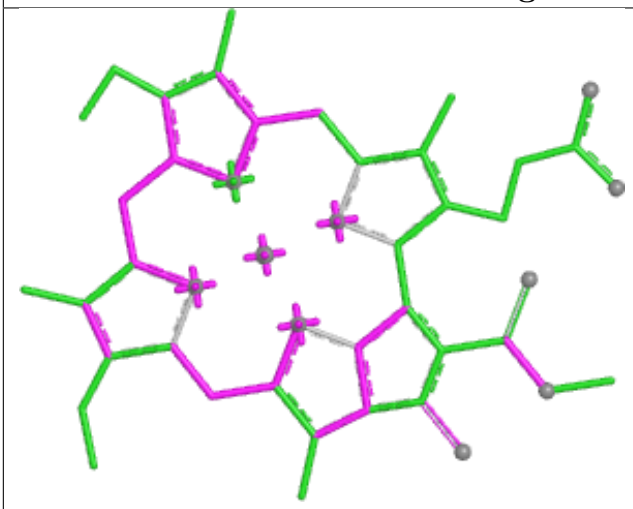


Rings

Ligand CLA b 1236



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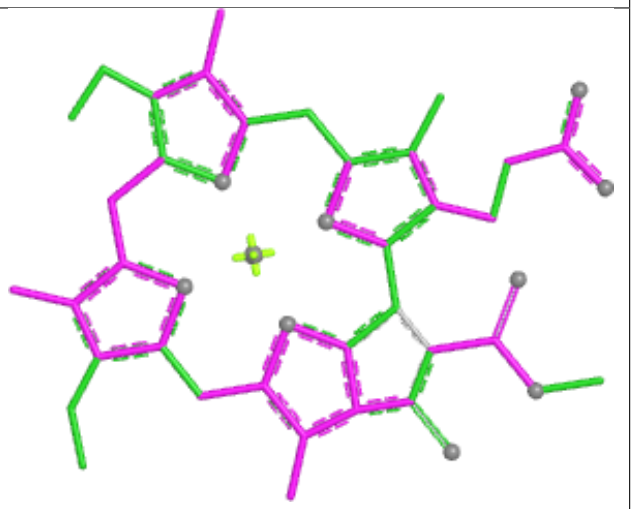
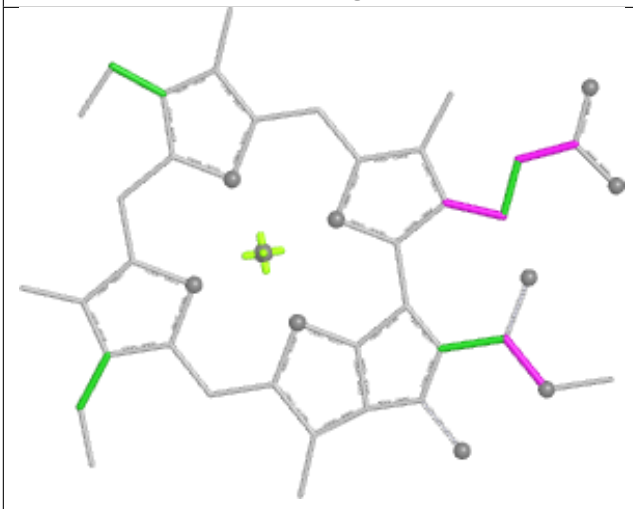


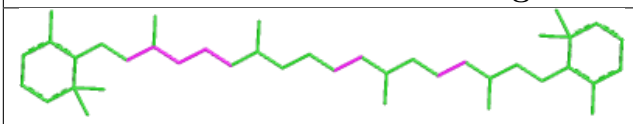
Bond angles



Torsions

Rings

Ligand BCR G 4001



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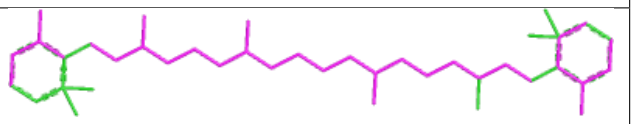

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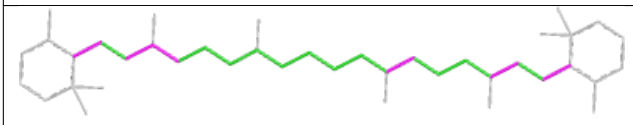
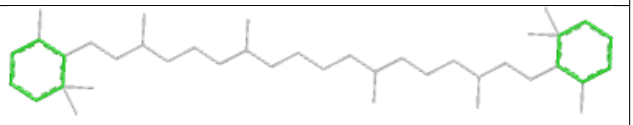
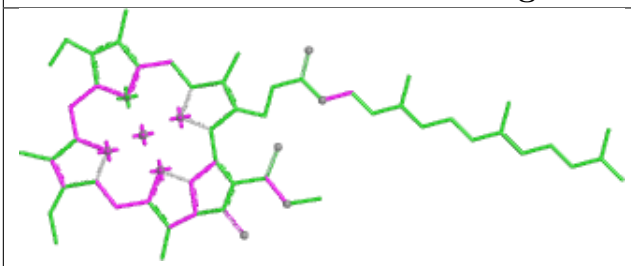


Torsions



Rings

Ligand CLA b 1235



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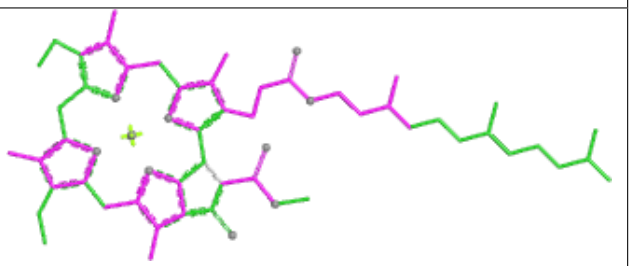
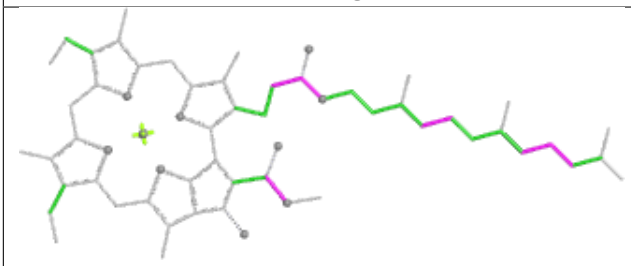
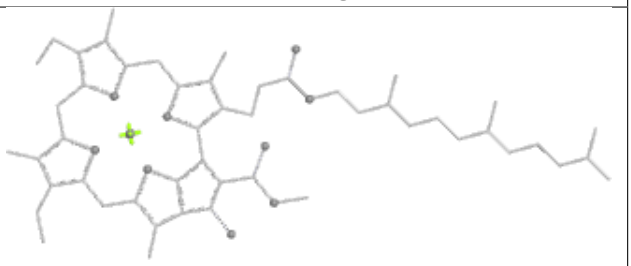


Bond angles

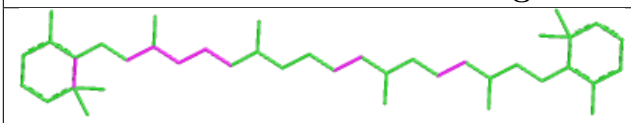


Torsions

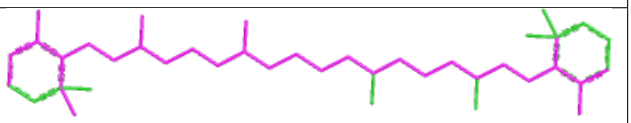


Rings

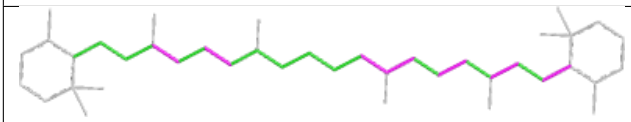
Ligand BCR A 4007



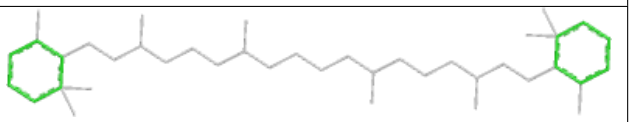
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	44:UNK	C	69:VAL	N	11.74

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Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	44:UNK	C	69:VAL	N	11.74
1	k	44:UNK	C	69:VAL	N	11.74

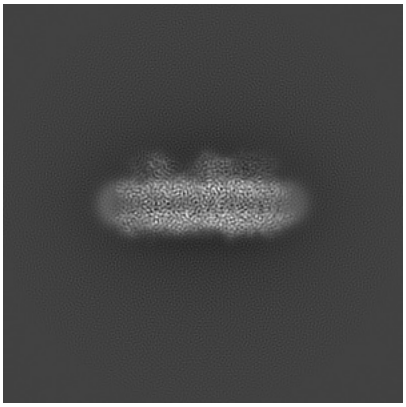
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20397. These allow visual inspection of the internal detail of the map and identification of artifacts.

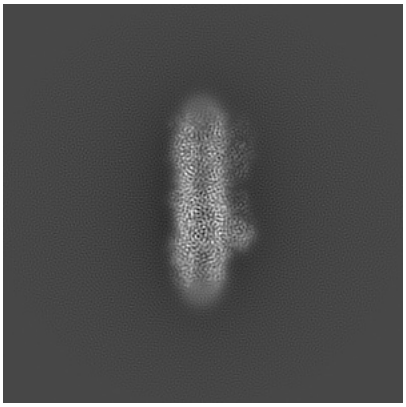
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

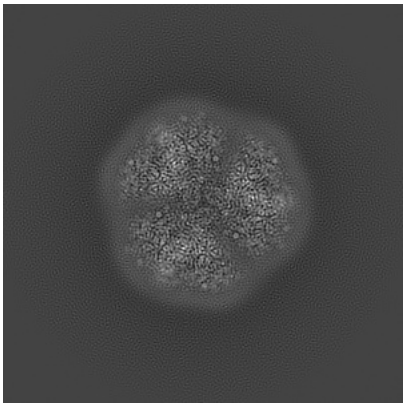
6.1.1 Primary map



X



Y

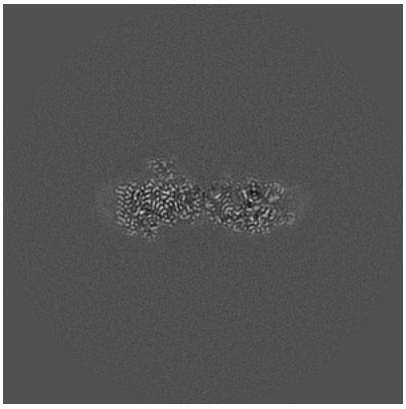


Z

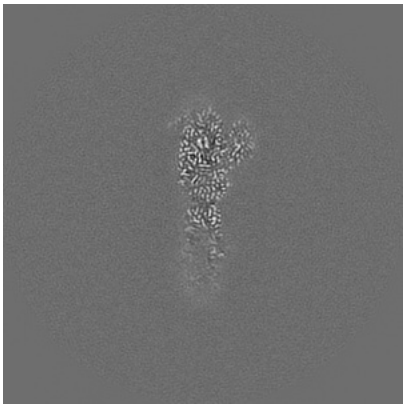
The images above show the map projected in three orthogonal directions.

6.2 Central slices

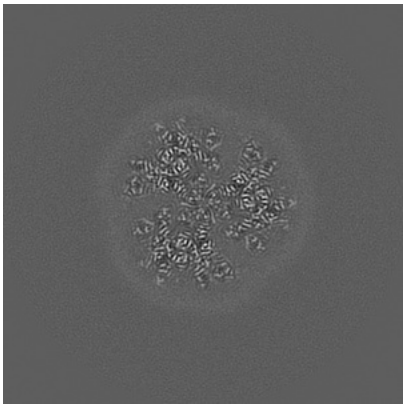
6.2.1 Primary map



X Index: 200



Y Index: 200

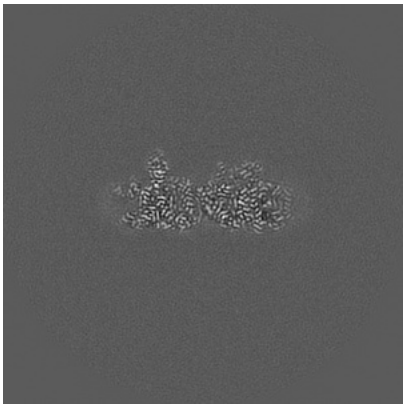


Z Index: 200

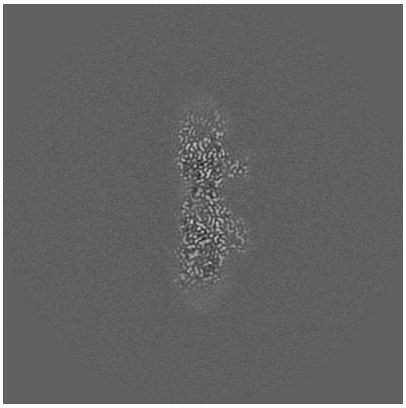
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

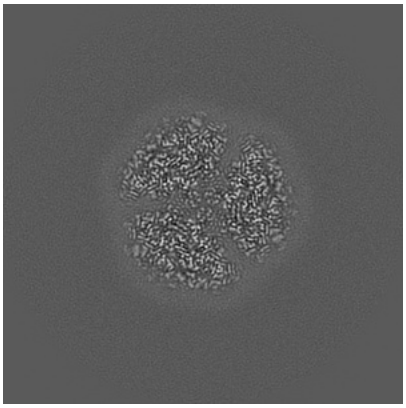
6.3.1 Primary map



X Index: 180



Y Index: 216

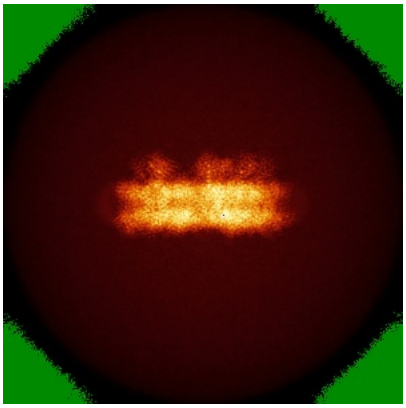


Z Index: 188

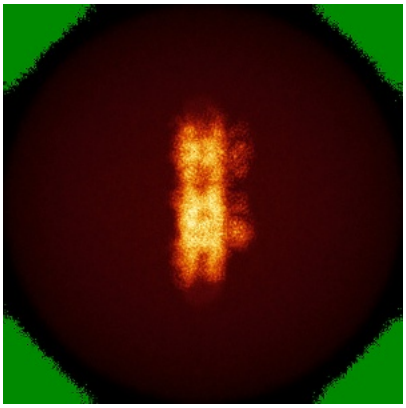
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

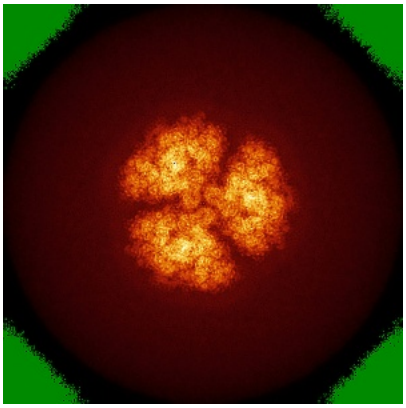
6.4.1 Primary map



X



Y

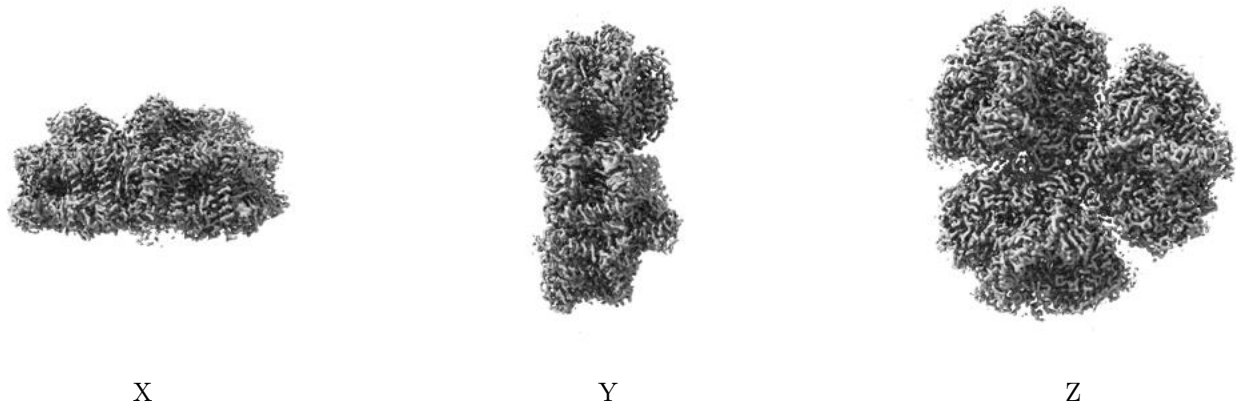


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0293. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

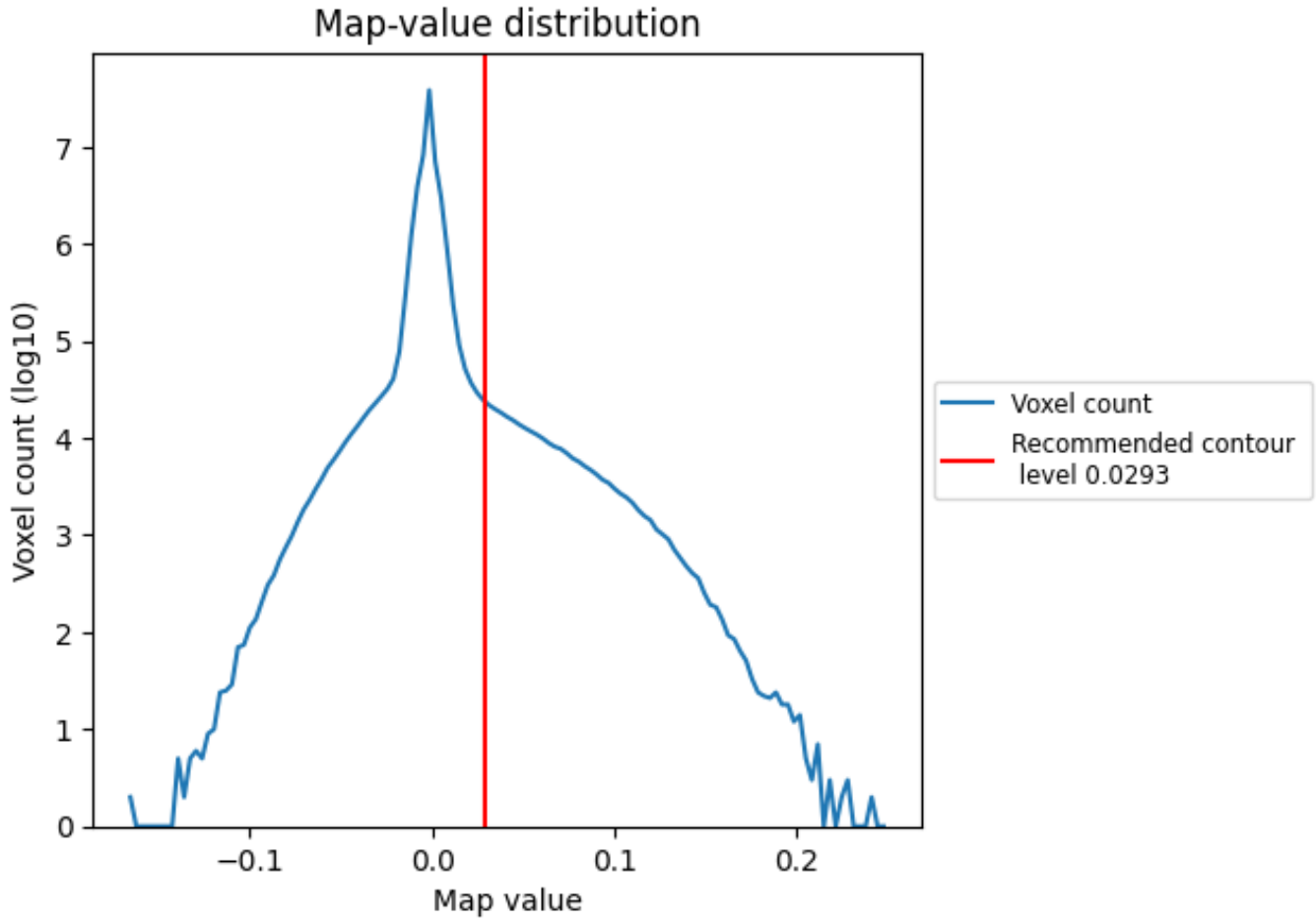
6.6 Mask visualisation (i)

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

7 Map analysis

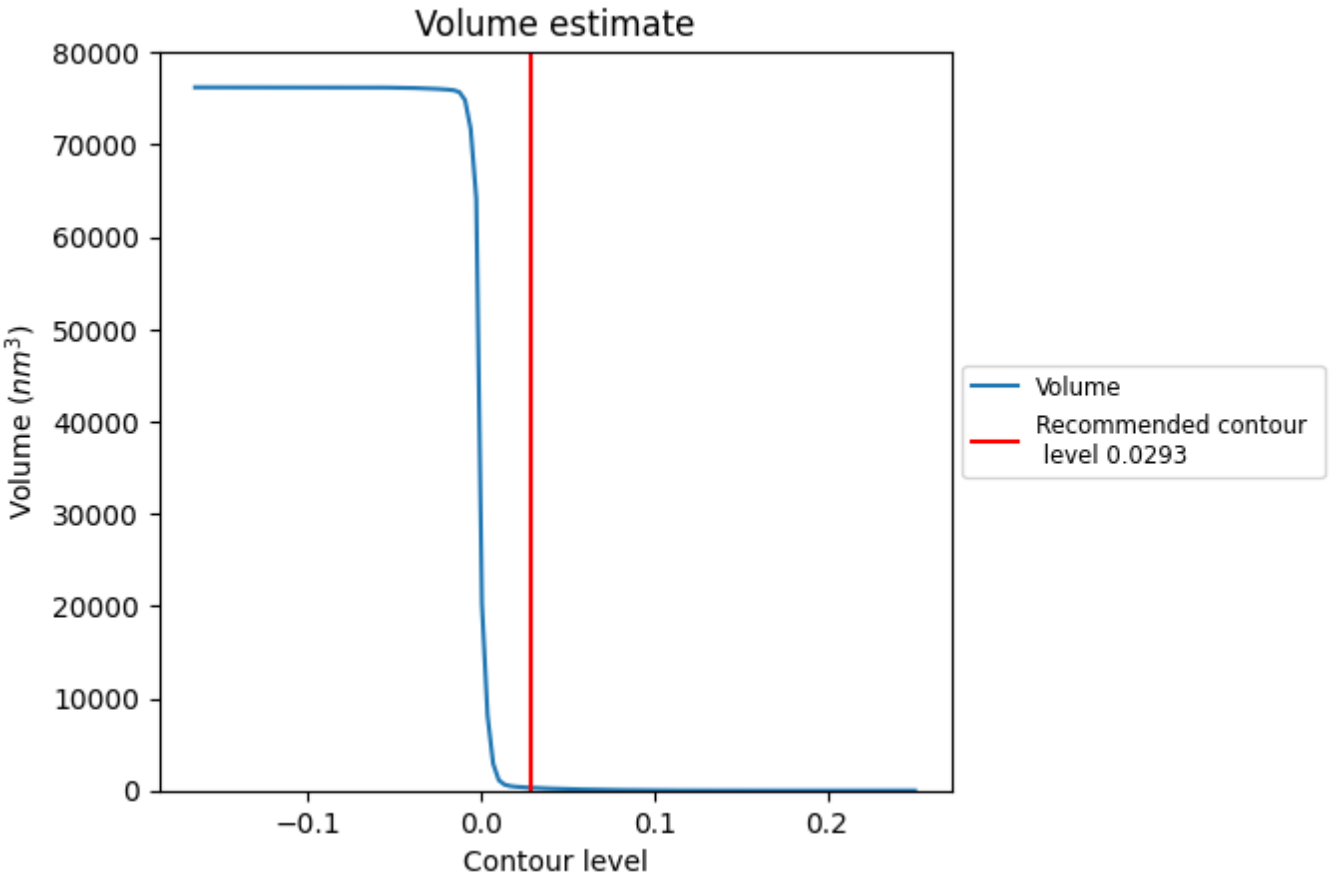
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

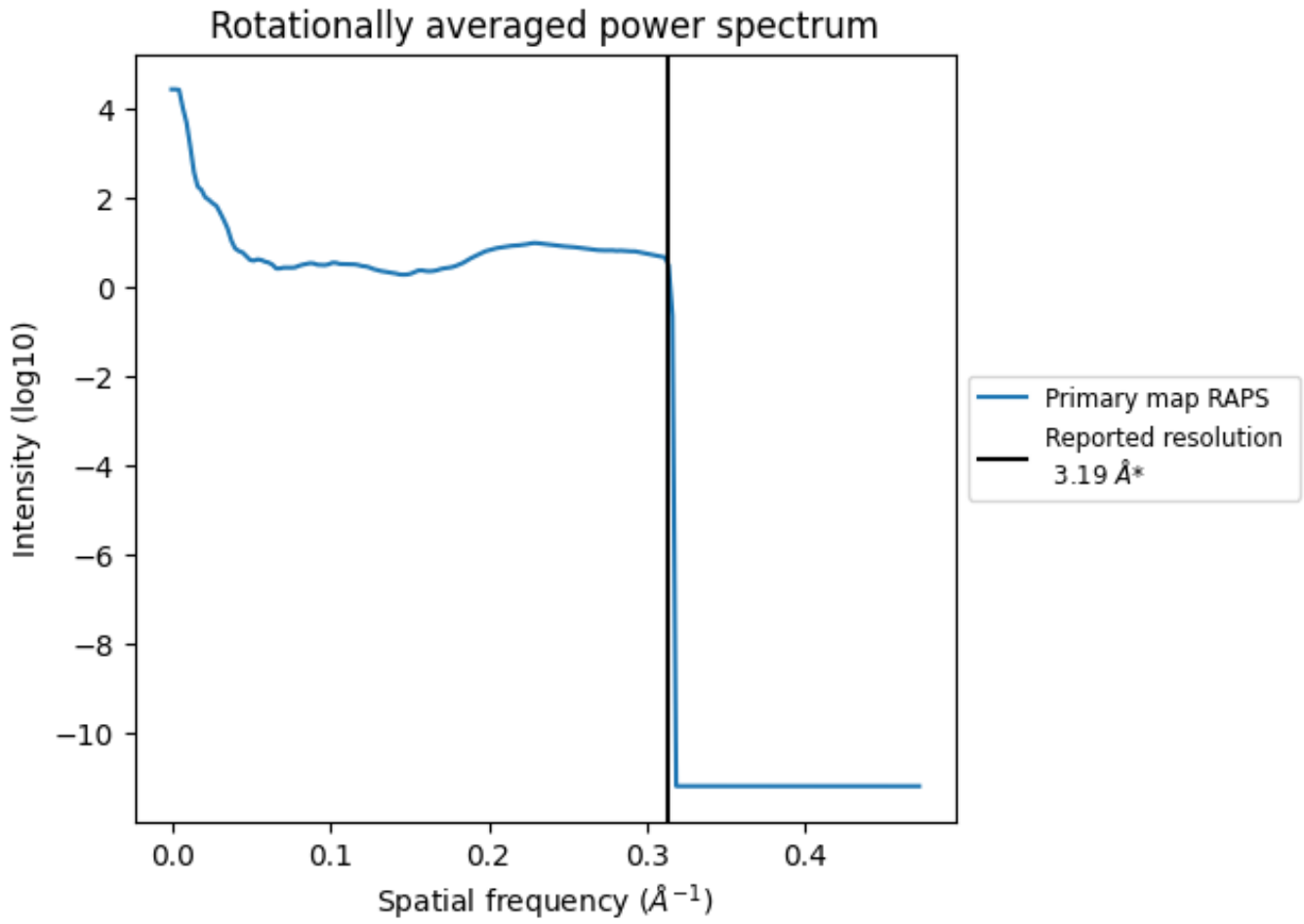
7.2 Volume estimate



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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)

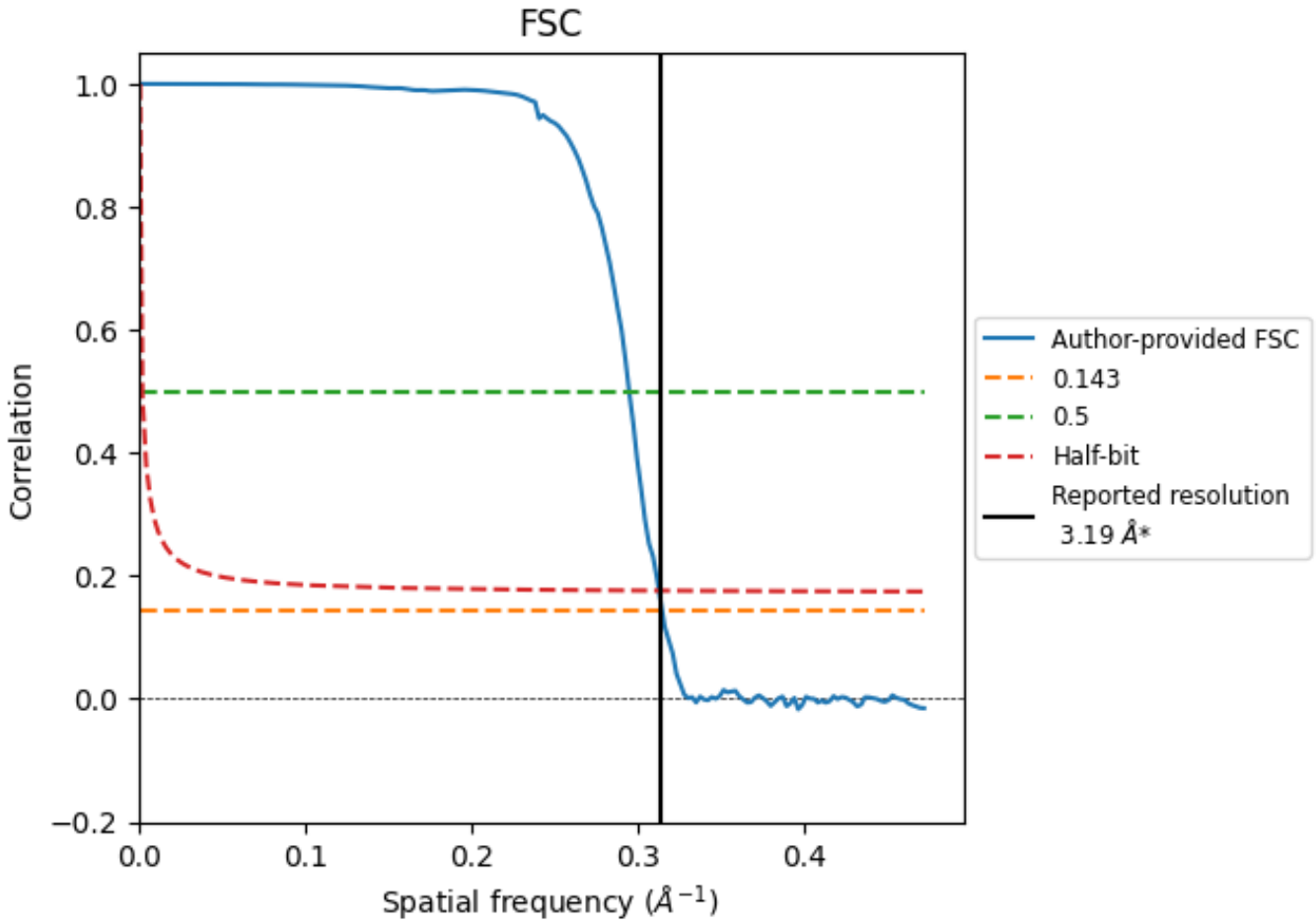


*Reported resolution corresponds to spatial frequency of 0.313 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.313 Å^{-1}

8.2 Resolution estimates (i)

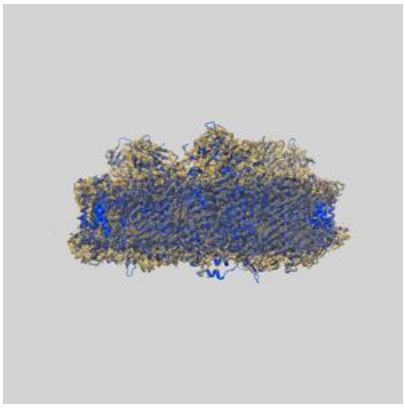
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.19	-	-
Author-provided FSC curve	3.18	3.39	3.20
Unmasked-calculated*	-	-	-

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

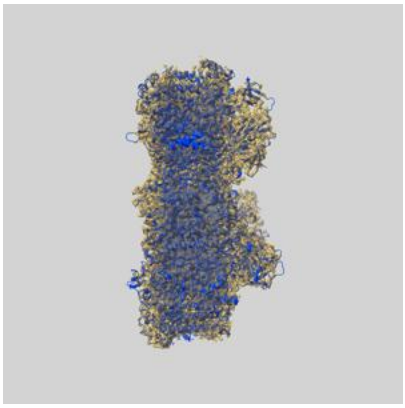
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20397 and PDB model 6PNJ. Per-residue inclusion information can be found in section 3 on page 37.

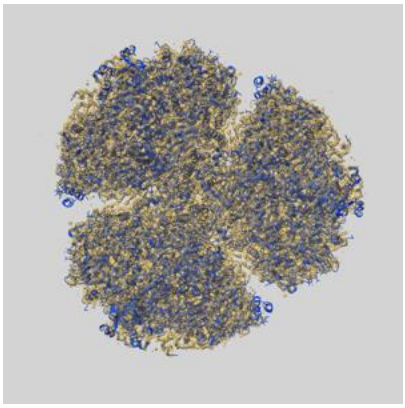
9.1 Map-model overlay



X



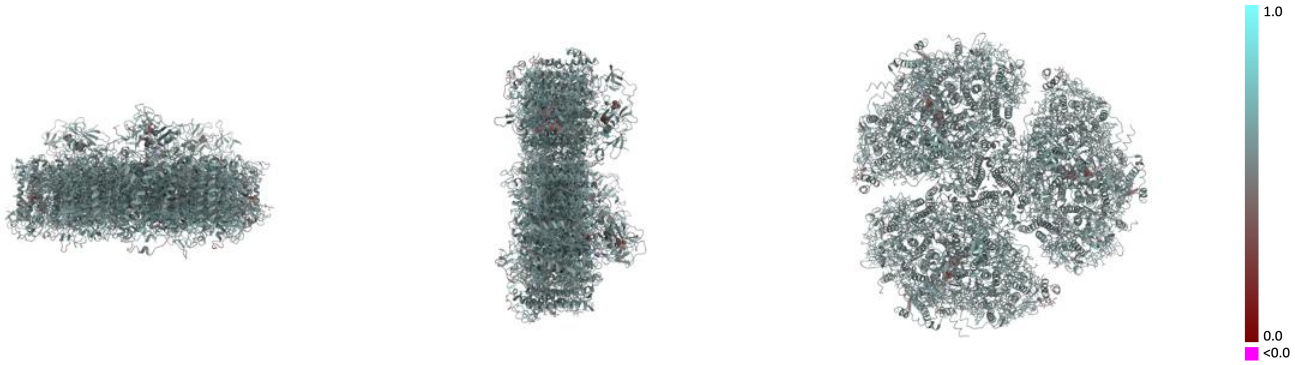
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0293 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.

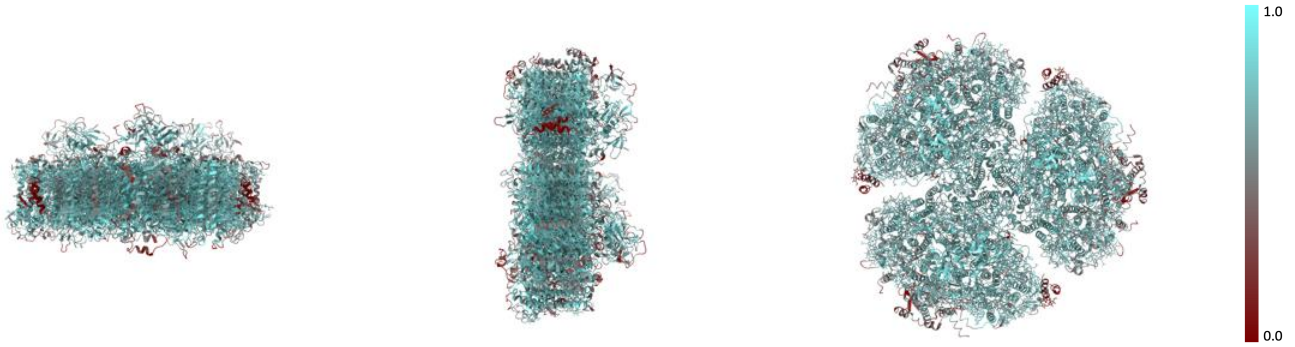
9.2 Q-score mapped to coordinate model



X Y Z

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

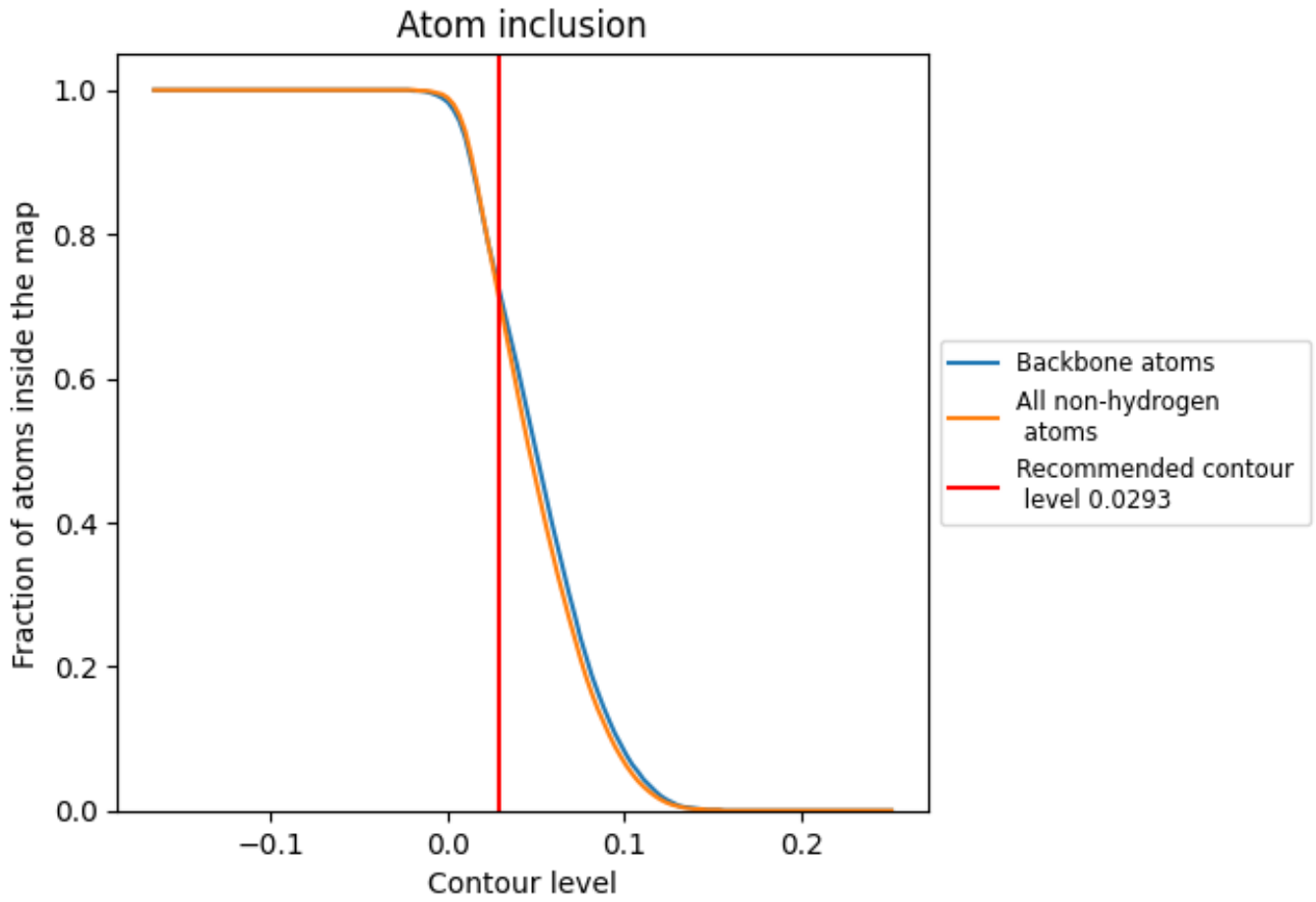
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.0293).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 71% 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 (0.0293) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7110	0.5660
A	0.7590	0.5750
B	0.7530	0.5760
C	0.7520	0.5500
D	0.6200	0.5530
E	0.5200	0.5330
F	0.3820	0.5160
G	0.7580	0.5750
H	0.7530	0.5760
I	0.7530	0.5820
J	0.4310	0.4890
K	0.0660	0.4440
L	0.7380	0.5700
M	0.6640	0.5450
N	0.7440	0.5490
O	0.6220	0.5540
P	0.5200	0.5320
Q	0.3800	0.5180
R	0.7580	0.5850
S	0.4230	0.4950
T	0.0660	0.4420
U	0.7340	0.5690
V	0.6790	0.5460
W	0.4870	0.5130
X	0.5090	0.5110
a	0.7600	0.5740
b	0.7550	0.5760
c	0.7390	0.5500
d	0.6170	0.5540
e	0.5110	0.5280
f	0.3870	0.5190
i	0.7550	0.5860
j	0.4310	0.4910
k	0.0660	0.4450
l	0.7320	0.5700

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Chain	Atom inclusion	Q-score
m	0.6820	0.5490
x	0.5050	0.5150