Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:54 AM UTC

PDB ID	:	7LX0 / pdb_00007lx0
EMDB ID	:	EMD-23563
Title	:	Quantitative assessment of chlorophyll types in cryo-EM maps of photosystem I acclimated to far-red light
Authors	:	Gisriel, C.J.; Wang, J.
Deposited on	:	2021-03-02
Resolution	:	2.96 Å(reported)

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

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

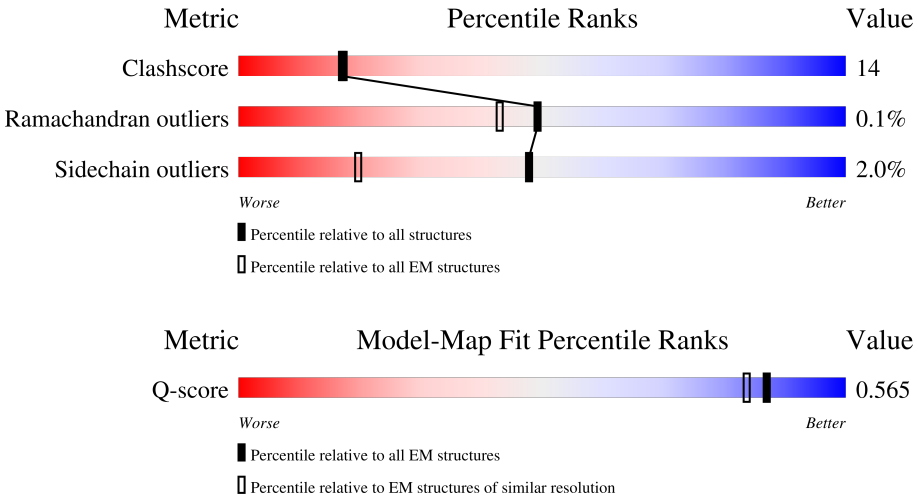
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.96 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	6% 69% 27% 5%
1	G	788	6% 69% 26% 5%
1	a	788	6% 69% 27% 5%
2	B	741	72% 28%

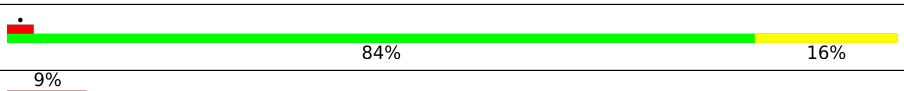
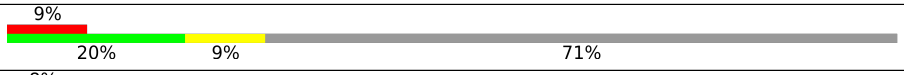
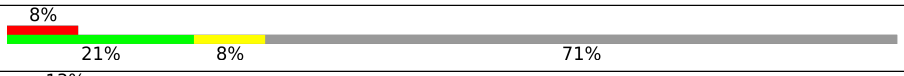
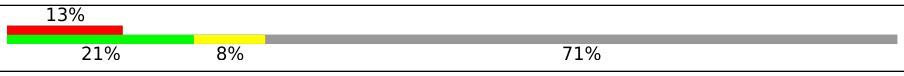
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Mol	Chain	Length	Quality of chain
2	H	741	72% 27%
2	b	741	72% 27%
3	C	81	75% 19% 5%
3	N	81	81% 12% 5%
3	c	81	77% 17% 5%
4	D	159	13% 66% 21% 13%
4	O	159	16% 66% 21% 13%
4	d	159	15% 65% 22% 13%
5	E	72	26% 68% 15% 14%
5	P	72	24% 74% 10% 14%
5	e	72	29% 72% 11% 14%
6	F	159	46% 55% 28% 15%
6	Q	159	44% 57% 26% 15%
6	f	159	44% 57% 25% 15%
7	I	67	6% 36% 27% 37%
7	R	67	6% 42% 21% 37%
7	i	67	7% 40% 22% 37%
8	J	48	40% 56% 27% 6% 10%
8	S	48	33% 56% 27% 6% 10%
8	j	48	38% 58% 25% 6% 10%
9	K	49	88% 78% 10% 10%
9	T	49	88% 78% 10% 10%
9	k	49	84% 78% 10% 10%
10	L	174	6% 71% 21% 6%
10	U	174	5% 72% 21% 6%

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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	1120	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	1122	X	-	-	-
14	CLA	A	1123	X	-	-	-
14	CLA	A	1124	X	-	-	-
14	CLA	A	1125	X	-	-	-
14	CLA	A	1126	X	-	-	-
14	CLA	A	1127	X	-	-	-
14	CLA	A	1128	X	-	-	-
14	CLA	A	1129	X	-	-	-
14	CLA	A	1130	X	-	-	-
14	CLA	A	1131	X	-	-	-
14	CLA	A	1132	X	-	-	-
14	CLA	A	1133	X	-	-	-
14	CLA	A	1134	X	-	-	-
14	CLA	A	1135	X	-	-	-
14	CLA	A	1136	X	-	-	-
14	CLA	A	1137	X	-	-	-
14	CLA	A	1138	X	-	-	-
14	CLA	A	1139	X	-	-	-
14	CLA	A	1140	X	-	-	-
14	CLA	B	1021	X	-	-	-
14	CLA	B	1022	X	-	-	-
14	CLA	B	1023	X	-	-	-
14	CLA	B	1201	X	-	-	-
14	CLA	B	1202	X	-	-	-
14	CLA	B	1203	X	-	-	-
14	CLA	B	1204	X	-	-	-
14	CLA	B	1205	X	-	-	-
14	CLA	B	1206	X	-	-	-
14	CLA	B	1208	X	-	-	-
14	CLA	B	1209	X	-	-	-
14	CLA	B	1210	X	-	-	-
14	CLA	B	1211	X	-	-	-
14	CLA	B	1212	X	-	-	-
14	CLA	B	1213	X	-	-	-
14	CLA	B	1214	X	-	-	-
14	CLA	B	1215	X	-	-	-
14	CLA	B	1216	X	-	-	-
14	CLA	B	1217	X	-	-	-
14	CLA	B	1218	X	-	-	-
14	CLA	B	1219	X	-	-	-
14	CLA	B	1220	X	-	-	-
14	CLA	B	1221	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	1222	X	-	-	-
14	CLA	B	1223	X	-	-	-
14	CLA	B	1224	X	-	-	-
14	CLA	B	1225	X	-	-	-
14	CLA	B	1226	X	-	-	-
14	CLA	B	1227	X	-	-	-
14	CLA	B	1228	X	-	-	-
14	CLA	B	1229	X	-	-	-
14	CLA	B	1231	X	-	-	-
14	CLA	B	1232	X	-	-	-
14	CLA	B	1233	X	-	-	-
14	CLA	B	1234	X	-	-	-
14	CLA	B	1235	X	-	-	-
14	CLA	B	1236	X	-	-	-
14	CLA	B	1239	X	-	-	-
14	CLA	G	1012	X	-	-	-
14	CLA	G	1013	X	-	-	-
14	CLA	G	1101	X	-	-	-
14	CLA	G	1102	X	-	-	-
14	CLA	G	1103	X	-	-	-
14	CLA	G	1104	X	-	-	-
14	CLA	G	1105	X	-	-	-
14	CLA	G	1106	X	-	-	-
14	CLA	G	1107	X	-	-	-
14	CLA	G	1108	X	-	-	-
14	CLA	G	1109	X	-	-	-
14	CLA	G	1110	X	-	-	-
14	CLA	G	1111	X	-	-	-
14	CLA	G	1112	X	-	-	-
14	CLA	G	1113	X	-	-	-
14	CLA	G	1114	X	-	-	-
14	CLA	G	1115	X	-	-	-
14	CLA	G	1116	X	-	-	-
14	CLA	G	1117	X	-	-	-
14	CLA	G	1118	X	-	-	-
14	CLA	G	1119	X	-	-	-
14	CLA	G	1120	X	-	-	-
14	CLA	G	1122	X	-	-	-
14	CLA	G	1123	X	-	-	-
14	CLA	G	1124	X	-	-	-
14	CLA	G	1125	X	-	-	-
14	CLA	G	1126	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	1127	X	-	-	-
14	CLA	G	1128	X	-	-	-
14	CLA	G	1129	X	-	-	-
14	CLA	G	1130	X	-	-	-
14	CLA	G	1131	X	-	-	-
14	CLA	G	1132	X	-	-	-
14	CLA	G	1133	X	-	-	-
14	CLA	G	1134	X	-	-	-
14	CLA	G	1135	X	-	-	-
14	CLA	G	1136	X	-	-	-
14	CLA	G	1137	X	-	-	-
14	CLA	G	1138	X	-	-	-
14	CLA	G	1139	X	-	-	-
14	CLA	G	1140	X	-	-	-
14	CLA	H	1021	X	-	-	-
14	CLA	H	1022	X	-	-	-
14	CLA	H	1023	X	-	-	-
14	CLA	H	1201	X	-	-	-
14	CLA	H	1202	X	-	-	-
14	CLA	H	1203	X	-	-	-
14	CLA	H	1204	X	-	-	-
14	CLA	H	1205	X	-	-	-
14	CLA	H	1206	X	-	-	-
14	CLA	H	1208	X	-	-	-
14	CLA	H	1209	X	-	-	-
14	CLA	H	1210	X	-	-	-
14	CLA	H	1211	X	-	-	-
14	CLA	H	1212	X	-	-	-
14	CLA	H	1213	X	-	-	-
14	CLA	H	1214	X	-	-	-
14	CLA	H	1215	X	-	-	-
14	CLA	H	1216	X	-	-	-
14	CLA	H	1217	X	-	-	-
14	CLA	H	1218	X	-	-	-
14	CLA	H	1219	X	-	-	-
14	CLA	H	1220	X	-	-	-
14	CLA	H	1221	X	-	-	-
14	CLA	H	1222	X	-	-	-
14	CLA	H	1223	X	-	-	-
14	CLA	H	1224	X	-	-	-
14	CLA	H	1225	X	-	-	-
14	CLA	H	1226	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	1227	X	-	-	-
14	CLA	H	1228	X	-	-	-
14	CLA	H	1229	X	-	-	-
14	CLA	H	1231	X	-	-	-
14	CLA	H	1232	X	-	-	-
14	CLA	H	1233	X	-	-	-
14	CLA	H	1234	X	-	-	-
14	CLA	H	1235	X	-	-	-
14	CLA	H	1236	X	-	-	-
14	CLA	H	1239	X	-	-	-
14	CLA	K	1401	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	1501	X	-	-	-
14	CLA	U	1502	X	-	-	-
14	CLA	U	1503	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	1012	X	-	-	-
14	CLA	a	1013	X	-	-	-
14	CLA	a	1101	X	-	-	-
14	CLA	a	1102	X	-	-	-
14	CLA	a	1103	X	-	-	-
14	CLA	a	1104	X	-	-	-
14	CLA	a	1105	X	-	-	-
14	CLA	a	1106	X	-	-	-
14	CLA	a	1107	X	-	-	-
14	CLA	a	1108	X	-	-	-
14	CLA	a	1109	X	-	-	-
14	CLA	a	1110	X	-	-	-
14	CLA	a	1111	X	-	-	-
14	CLA	a	1112	X	-	-	-
14	CLA	a	1113	X	-	-	-
14	CLA	a	1114	X	-	-	-
14	CLA	a	1115	X	-	-	-
14	CLA	a	1116	X	-	-	-
14	CLA	a	1117	X	-	-	-
14	CLA	a	1118	X	-	-	-
14	CLA	a	1119	X	-	-	-
14	CLA	a	1120	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	1122	X	-	-	-
14	CLA	a	1123	X	-	-	-
14	CLA	a	1124	X	-	-	-
14	CLA	a	1125	X	-	-	-
14	CLA	a	1126	X	-	-	-
14	CLA	a	1127	X	-	-	-
14	CLA	a	1128	X	-	-	-
14	CLA	a	1129	X	-	-	-
14	CLA	a	1130	X	-	-	-
14	CLA	a	1131	X	-	-	-
14	CLA	a	1132	X	-	-	-
14	CLA	a	1133	X	-	-	-
14	CLA	a	1134	X	-	-	-
14	CLA	a	1135	X	-	-	-
14	CLA	a	1136	X	-	-	-
14	CLA	a	1137	X	-	-	-
14	CLA	a	1138	X	-	-	-
14	CLA	a	1139	X	-	-	-
14	CLA	a	1140	X	-	-	-
14	CLA	b	1021	X	-	-	-
14	CLA	b	1022	X	-	-	-
14	CLA	b	1023	X	-	-	-
14	CLA	b	1201	X	-	-	-
14	CLA	b	1202	X	-	-	-
14	CLA	b	1203	X	-	-	-
14	CLA	b	1204	X	-	-	-
14	CLA	b	1205	X	-	-	-
14	CLA	b	1206	X	-	-	-
14	CLA	b	1208	X	-	-	-
14	CLA	b	1209	X	-	-	-
14	CLA	b	1210	X	-	-	-
14	CLA	b	1211	X	-	-	-
14	CLA	b	1212	X	-	-	-
14	CLA	b	1213	X	-	-	-
14	CLA	b	1214	X	-	-	-
14	CLA	b	1215	X	-	-	-
14	CLA	b	1216	X	-	-	-
14	CLA	b	1217	X	-	-	-
14	CLA	b	1218	X	-	-	-
14	CLA	b	1219	X	-	-	-
14	CLA	b	1220	X	-	-	-
14	CLA	b	1221	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	1222	X	-	-	-
14	CLA	b	1223	X	-	-	-
14	CLA	b	1224	X	-	-	-
14	CLA	b	1225	X	-	-	-
14	CLA	b	1226	X	-	-	-
14	CLA	b	1227	X	-	-	-
14	CLA	b	1228	X	-	-	-
14	CLA	b	1229	X	-	-	-
14	CLA	b	1231	X	-	-	-
14	CLA	b	1232	X	-	-	-
14	CLA	b	1233	X	-	-	-
14	CLA	b	1234	X	-	-	-
14	CLA	b	1235	X	-	-	-
14	CLA	b	1236	X	-	-	-
14	CLA	b	1239	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	1501	X	-	-	-
14	CLA	l	1502	X	-	-	-
14	CLA	l	1503	X	-	-	-
14	CLA	x	1701	X	-	-	-
15	F6C	A	1121	X	-	-	-
15	F6C	B	1207	X	-	-	-
15	F6C	B	1230	X	-	-	-
15	F6C	B	1237	X	-	-	-
15	F6C	B	1238	X	-	-	-
15	F6C	G	1121	X	-	-	-
15	F6C	H	1207	X	-	-	-
15	F6C	H	1230	X	-	-	-
15	F6C	H	1237	X	-	-	-
15	F6C	H	1238	X	-	-	-
15	F6C	a	1121	X	-	-	-
15	F6C	b	1207	X	-	-	-
15	F6C	b	1230	X	-	-	-
15	F6C	b	1237	X	-	-	-
15	F6C	b	1238	X	-	-	-

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 72462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	a	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		
1	A	751	Total	C	N	O	S	0	0
			5931	3892	1013	993	33		

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

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

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

- Molecule 10 is a protein called PSI subunit V.

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

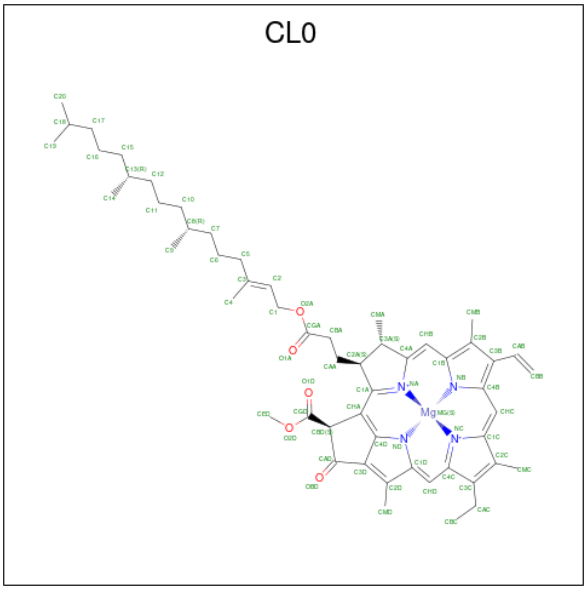
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 12 is a protein called Photosystem one PsaX.

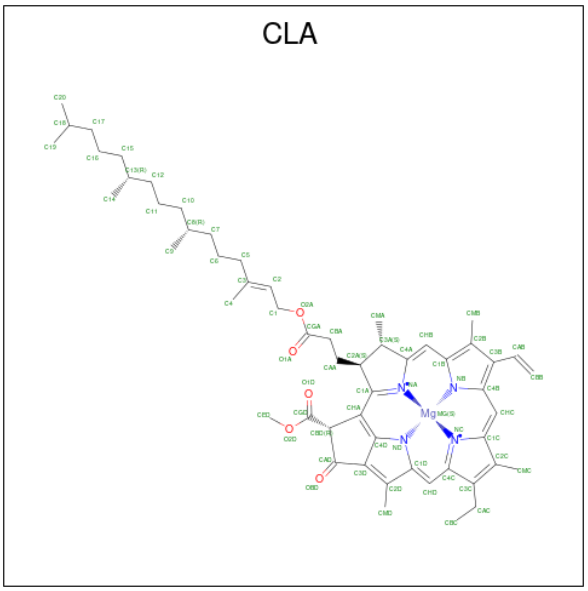
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	29	Total 246	C 172	N 36	O 38	0	0
12	x	29	Total 246	C 172	N 36	O 38	0	0
12	X	29	Total 246	C 172	N 36	O 38	0	0

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



Mol	Chain	Residues	Atoms					AltConf
13	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
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	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
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
			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
			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
			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
			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
			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
			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	

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

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

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

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

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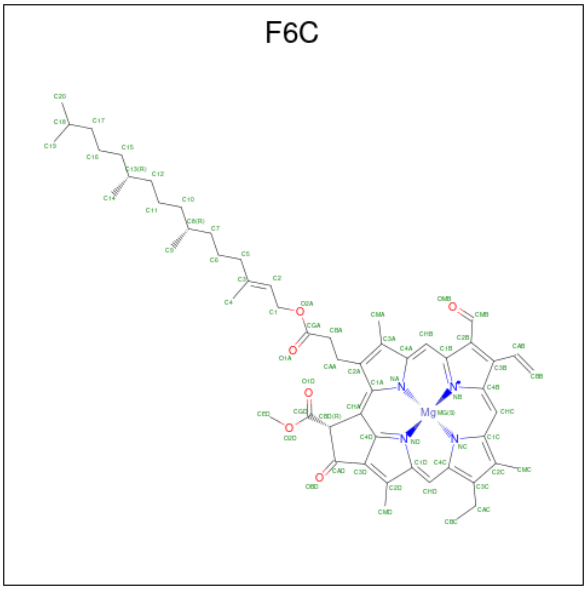
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0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

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



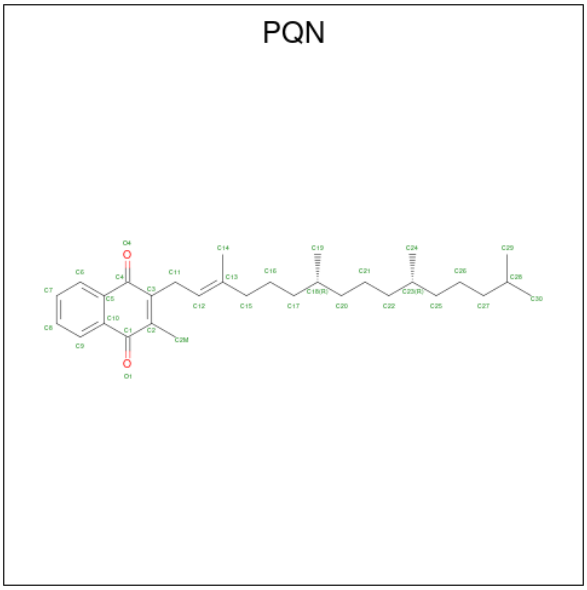
Mol	Chain	Residues	Atoms					AltConf
15	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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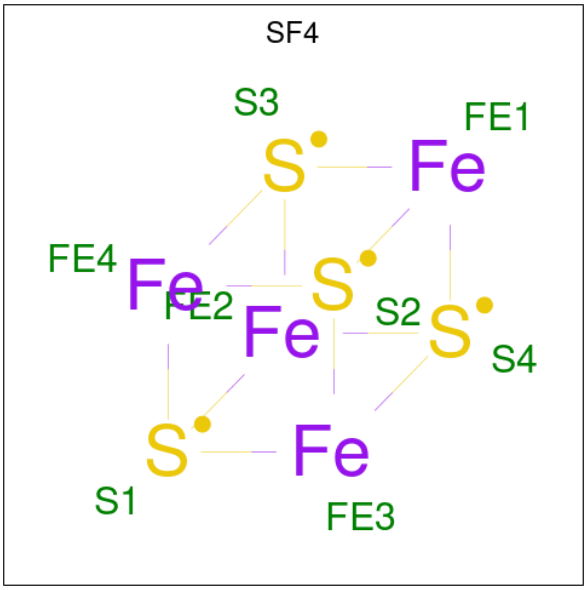
Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
15	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	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
			66	55	1	4	6	
15	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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



Mol	Chain	Residues	Atoms	AltConf
16	G	1	Total C O 33 31 2	0
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
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).



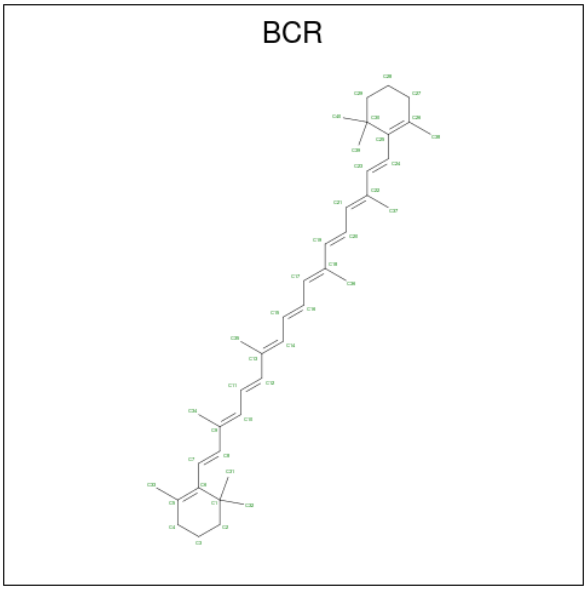
Mol	Chain	Residues	Atoms	AltConf
17	G	1	Total Fe S 8 4 4	0
17	N	1	Total Fe S 8 4 4	0
17	N	1	Total Fe S 8 4 4	0
17	a	1	Total Fe S 8 4 4	0
17	c	1	Total Fe S 8 4 4	0
17	c	1	Total Fe S 8 4 4	0

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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

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



Mol	Chain	Residues	Atoms	AltConf
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

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Mol	Chain	Residues	Atoms	AltConf
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	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

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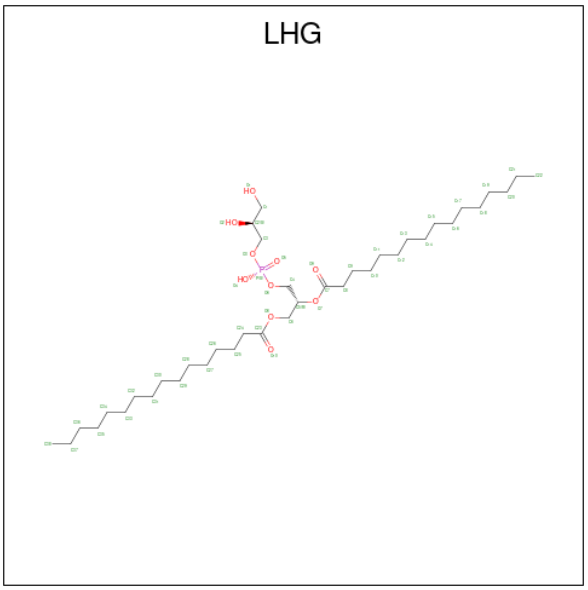
Mol	Chain	Residues	Atoms	AltConf
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	i	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	l	1	Total C 40 40	0
18	m	1	Total C 40 40	0
18	A	1	Total C 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	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: $C_{38}H_{75}O_{10}P$).



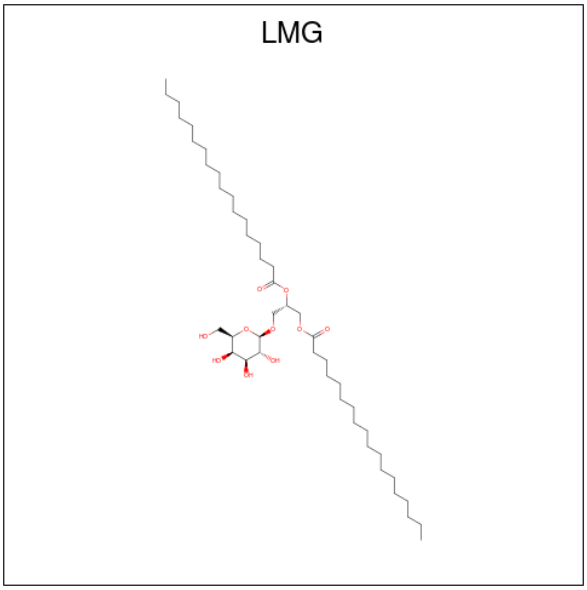
Mol	Chain	Residues	Atoms	AltConf
19	G	1	Total C O P 42 31 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
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	
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: $C_{45}H_{86}O_{10}$).



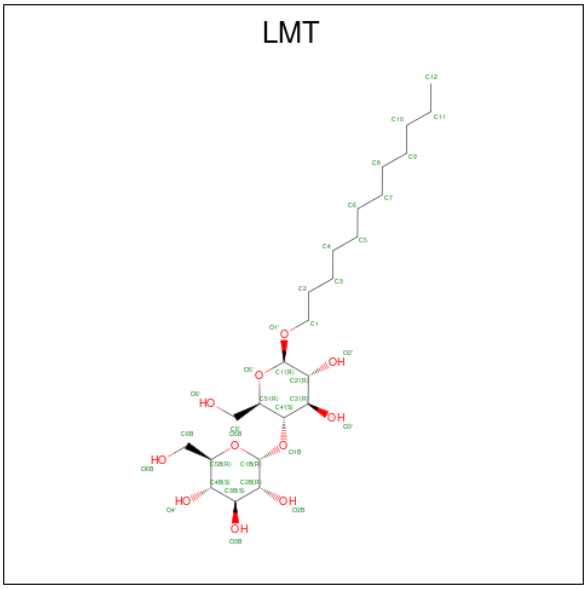
Mol	Chain	Residues	Atoms			AltConf
20	G	1	Total	C	O	0
			46	36	10	
20	H	1	Total	C	O	0
			46	36	10	
20	R	1	Total	C	O	0
			37	27	10	
20	U	1	Total	C	O	0
			50	40	10	
20	a	1	Total	C	O	0
			46	36	10	
20	b	1	Total	C	O	0
			46	36	10	

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Mol	Chain	Residues	Atoms	AltConf
20	i	1	Total C O 37 27 10	0
20	l	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	G	1	Total C O 31 20 11	0
21	G	1	Total C O 28 17 11	0
21	a	1	Total C O 31 20 11	0
21	a	1	Total C O 28 17 11	0
21	A	1	Total C O 31 20 11	0

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

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

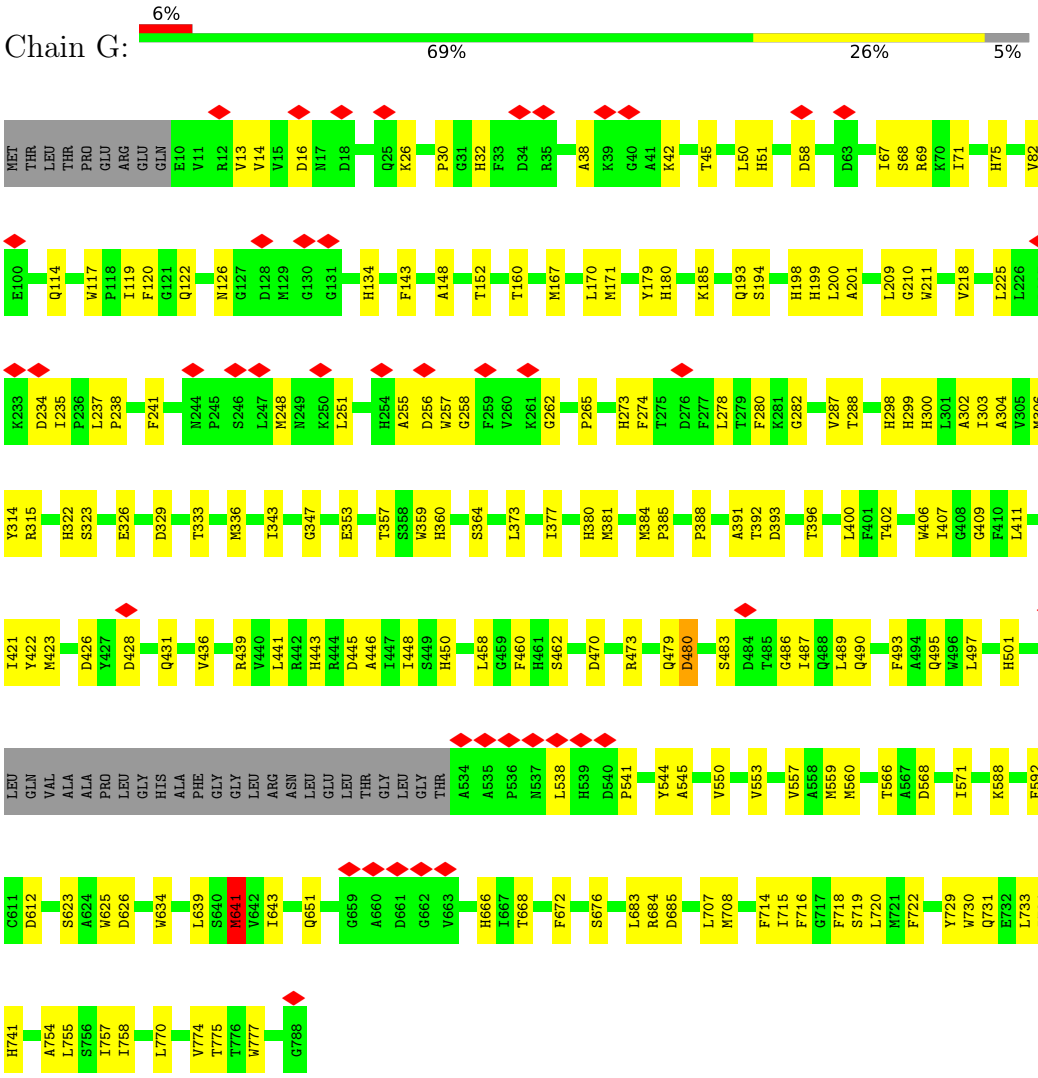
Mol	Chain	Residues	Atoms		AltConf
22	U	1	Total 1	Ca 1	0
22	l	1	Total 1	Ca 1	0
22	L	1	Total 1	Ca 1	0

3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

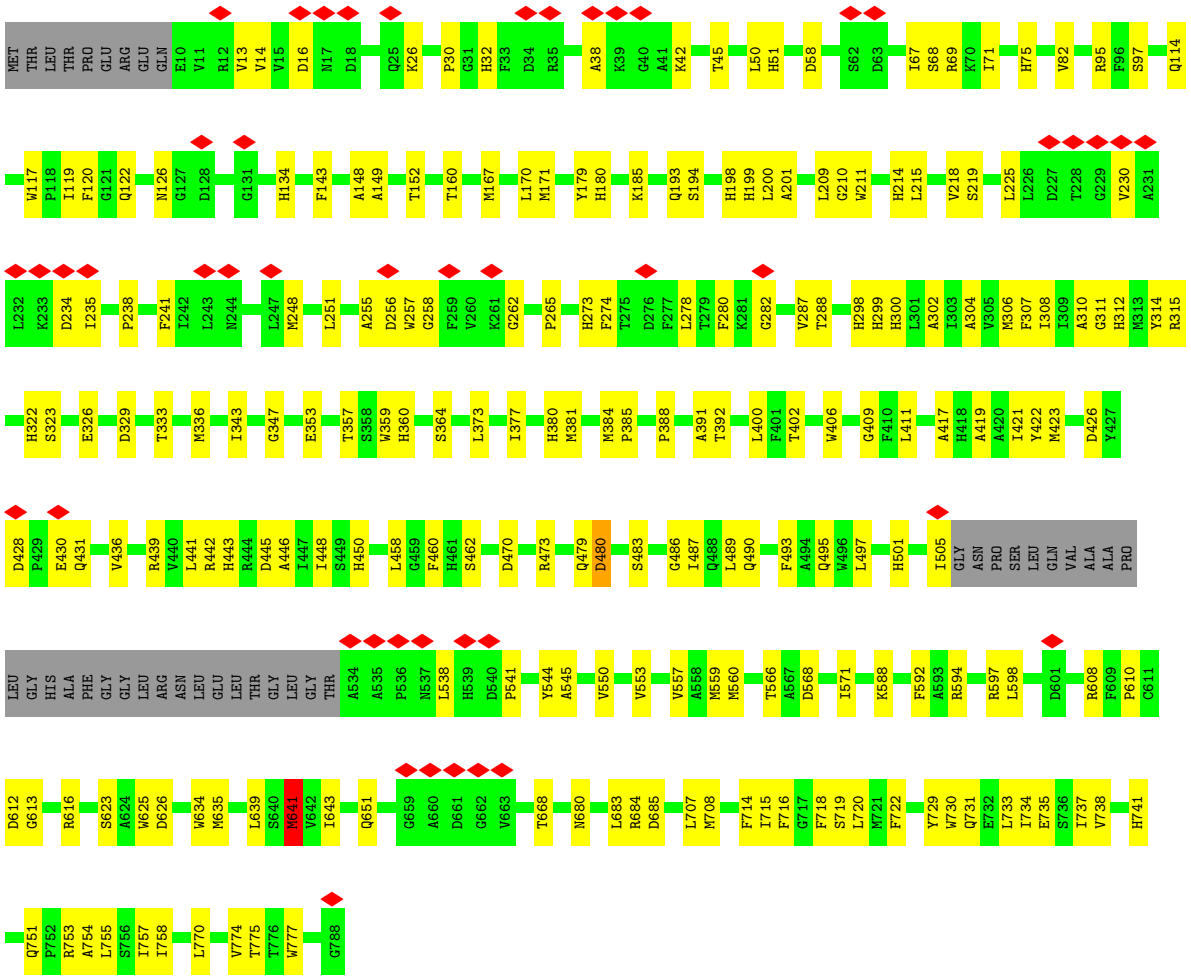
Chain G:



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:

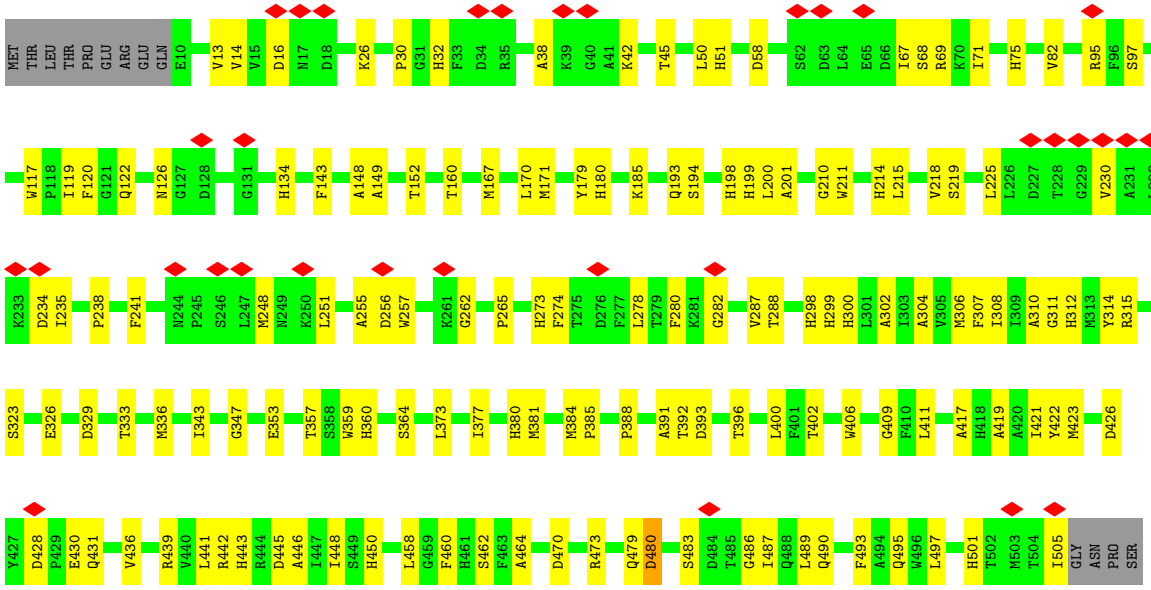


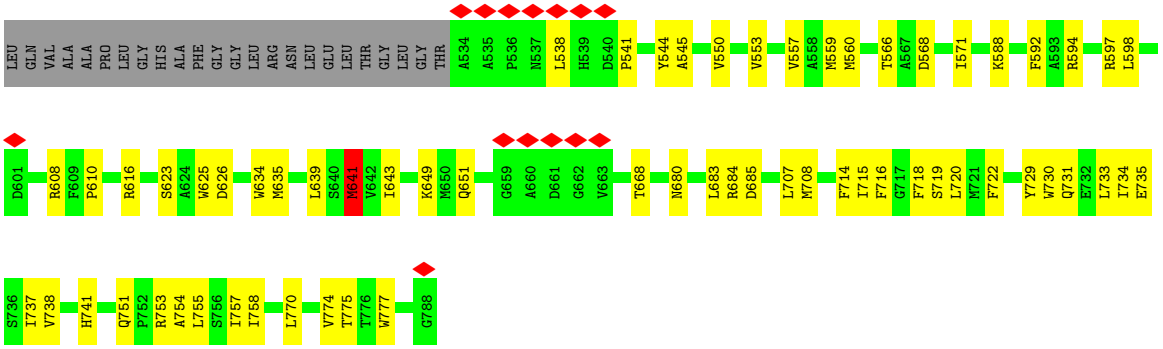


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



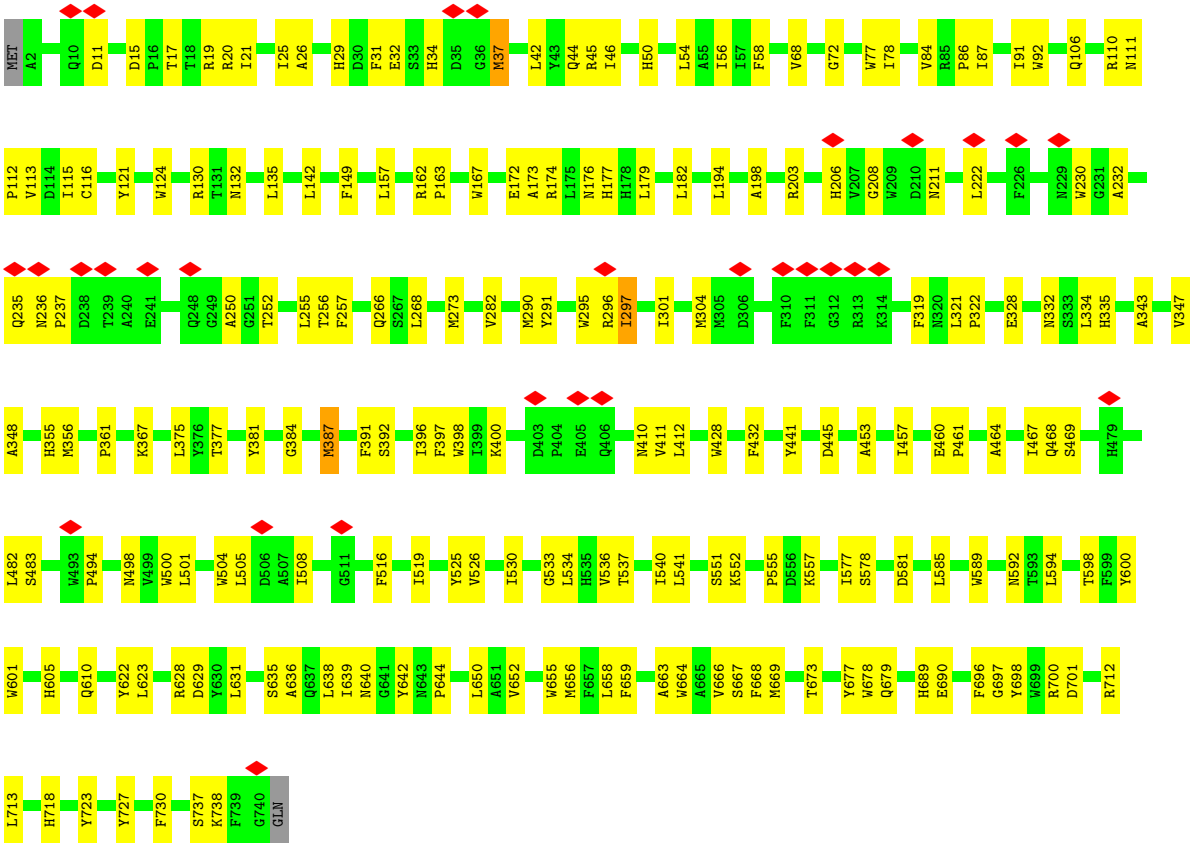




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H:

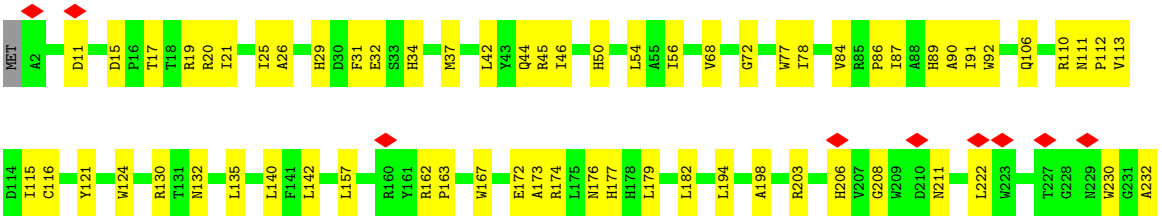


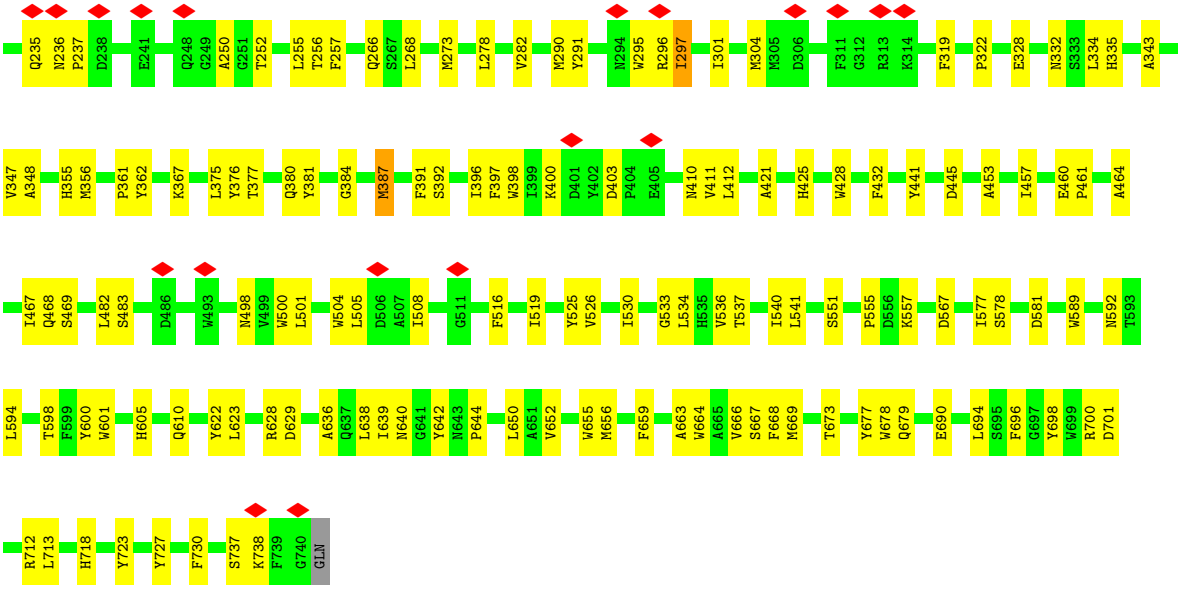


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



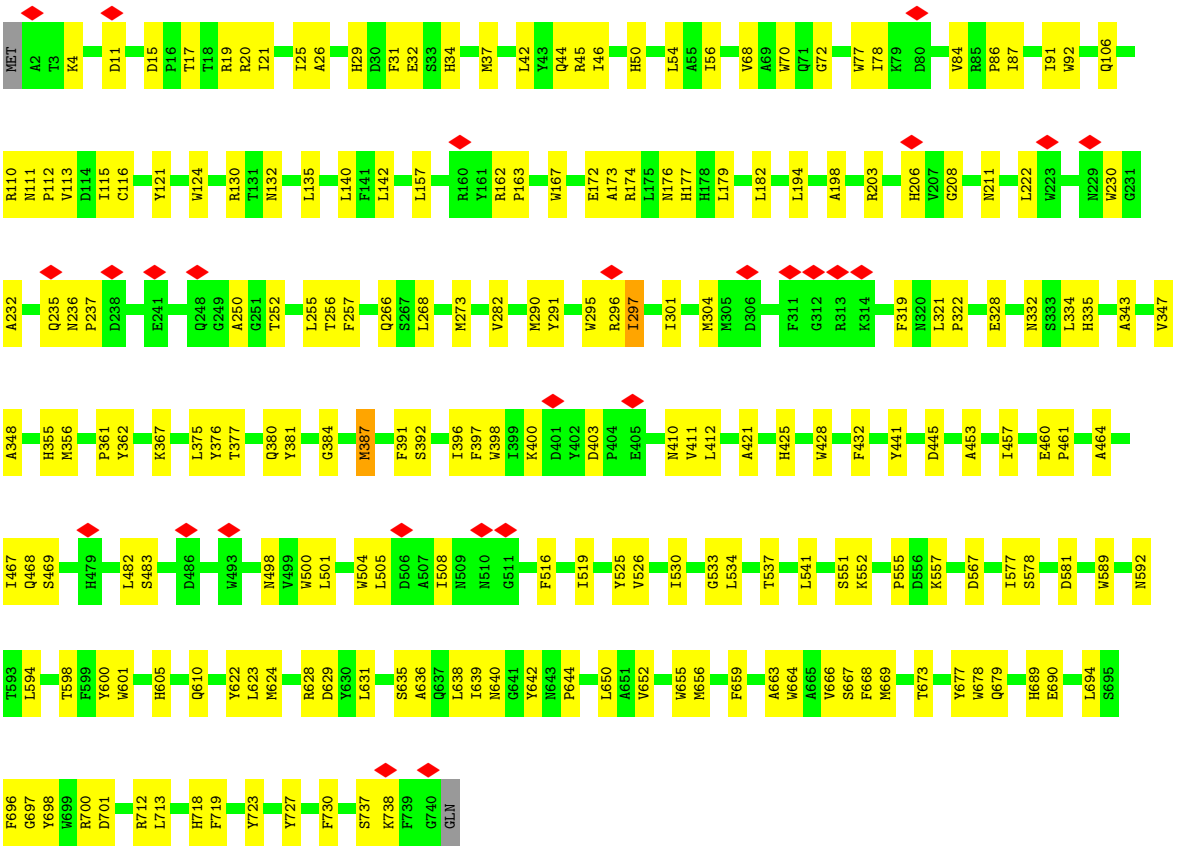




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

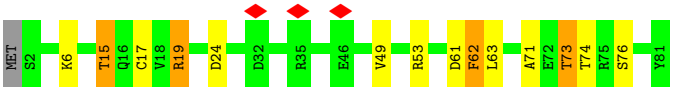




• Molecule 3: Photosystem I iron-sulfur center

Chain N:

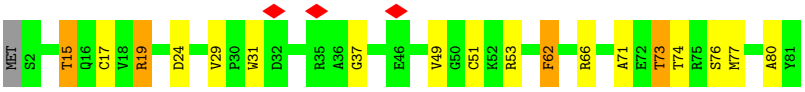




• Molecule 3: Photosystem I iron-sulfur center

Chain c:

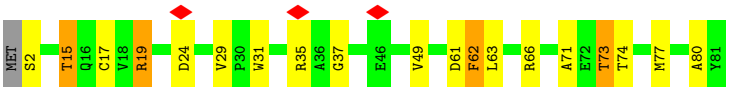




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

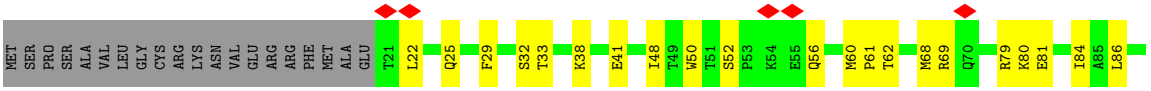


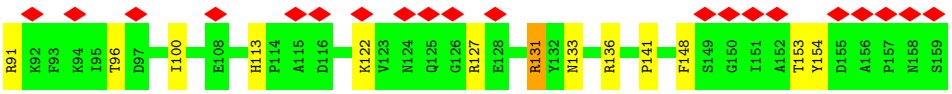


• Molecule 4: Photosystem I protein PsaD

Chain O:



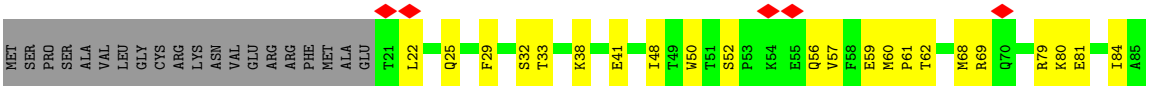


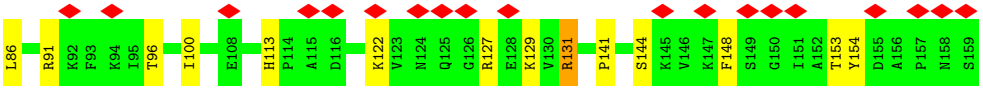


• Molecule 4: Photosystem I protein PsaD

Chain d:



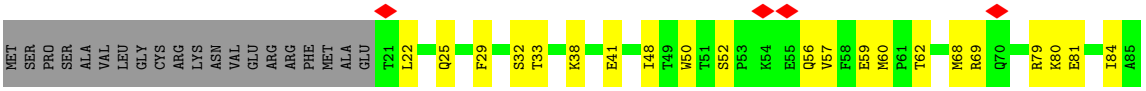


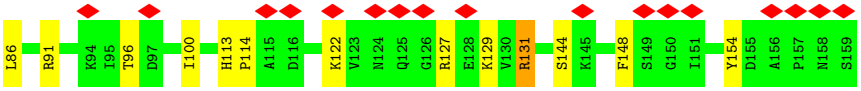


• Molecule 4: Photosystem I protein PsaD

Chain D:

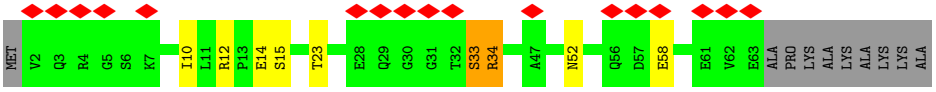






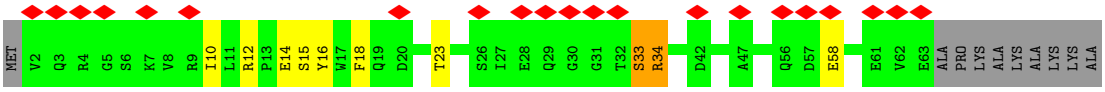
• Molecule 5: Photosystem I reaction center subunit IV





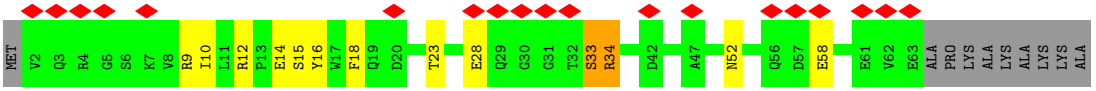
• Molecule 5: Photosystem I reaction center subunit IV





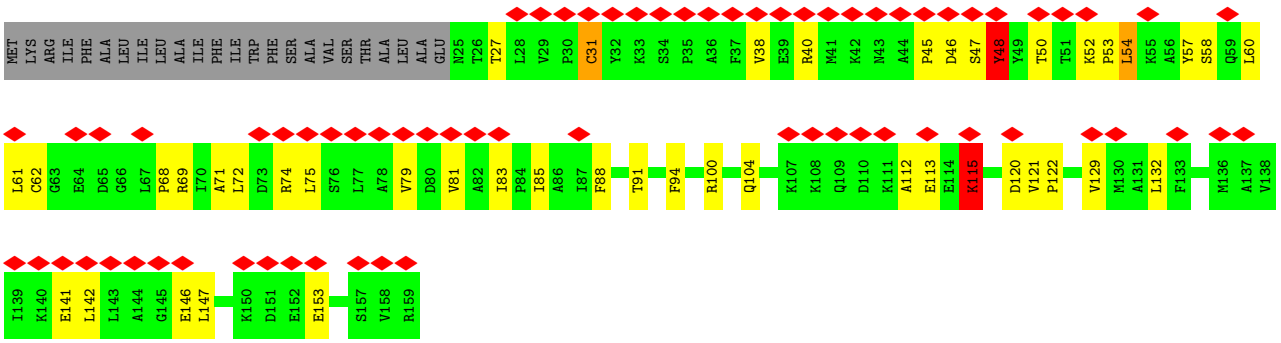
• Molecule 5: Photosystem I reaction center subunit IV



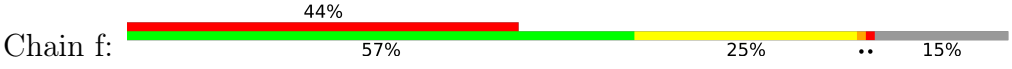


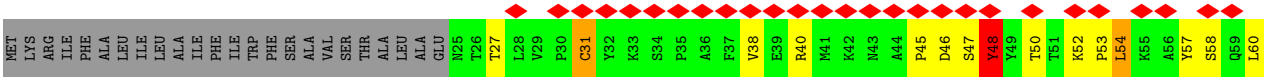
• Molecule 6: Photosystem I reaction center protein PsaF subunit III

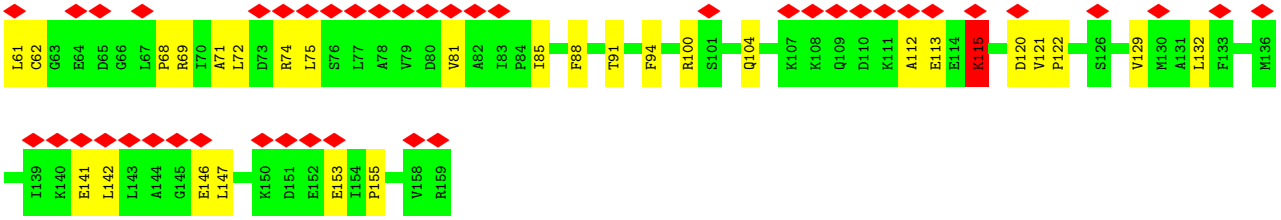




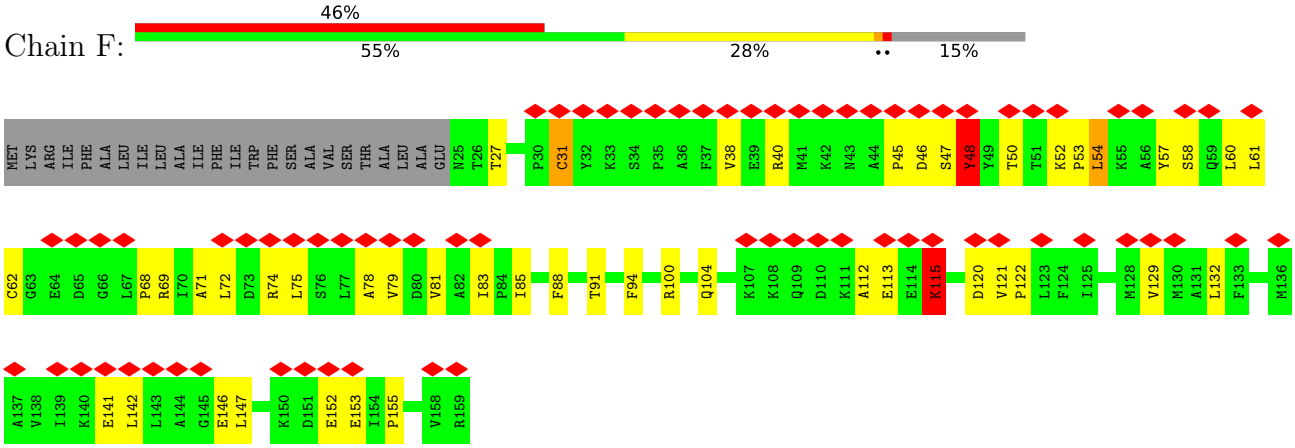
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



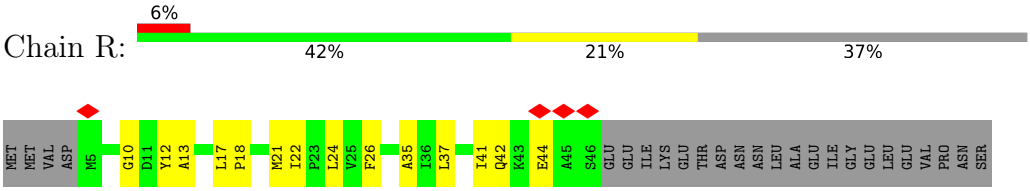




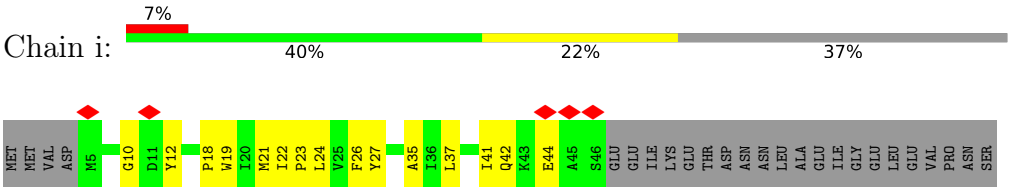
• Molecule 6: Photosystem I reaction center protein PsaF subunit III



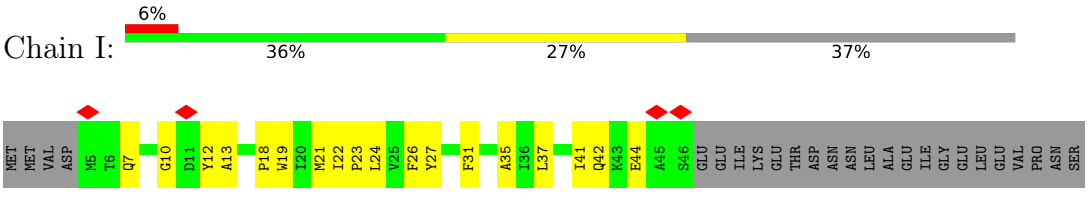
• Molecule 7: photosystem I subunit VIII



• Molecule 7: photosystem I subunit VIII



• Molecule 7: photosystem I subunit VIII



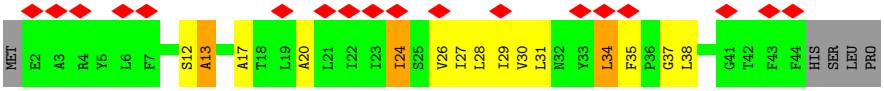
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ





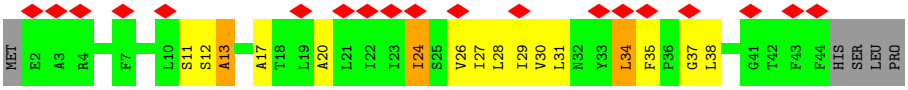
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



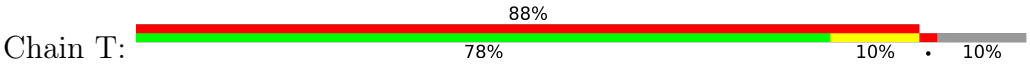


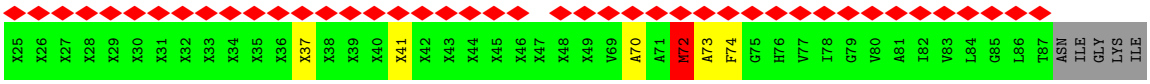
• Molecule 8: Photosystem I reaction centre subunit IX / PsaJ



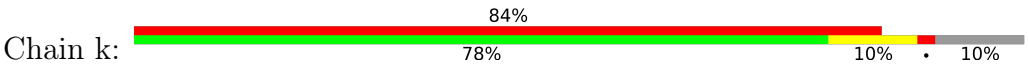


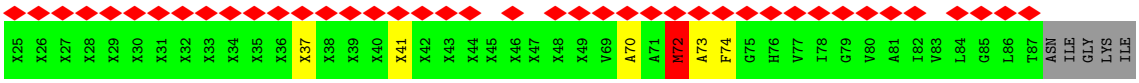
• Molecule 9: Photosystem I reaction center subunit PsaK



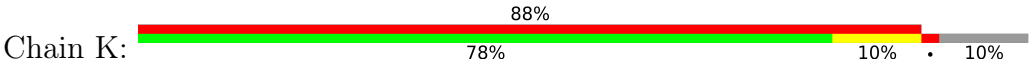


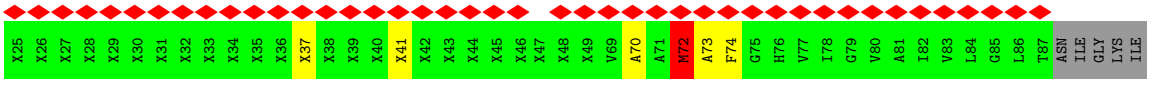
• Molecule 9: Photosystem I reaction center subunit PsaK





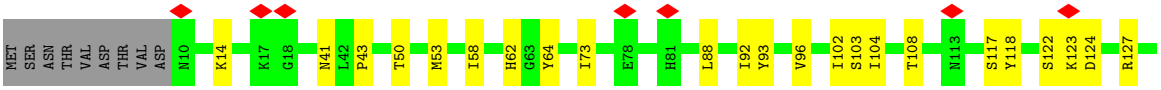
• Molecule 9: Photosystem I reaction center subunit PsaK





• Molecule 10: PSI subunit V

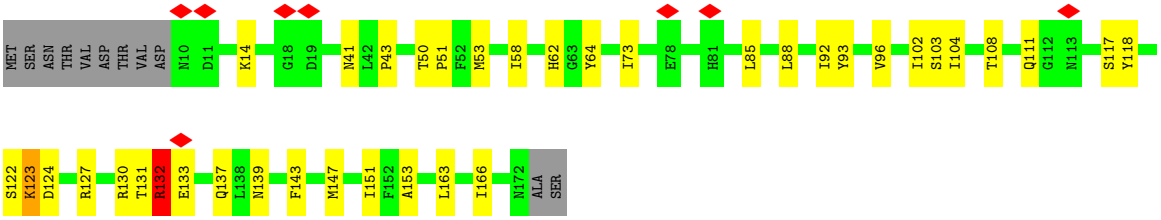






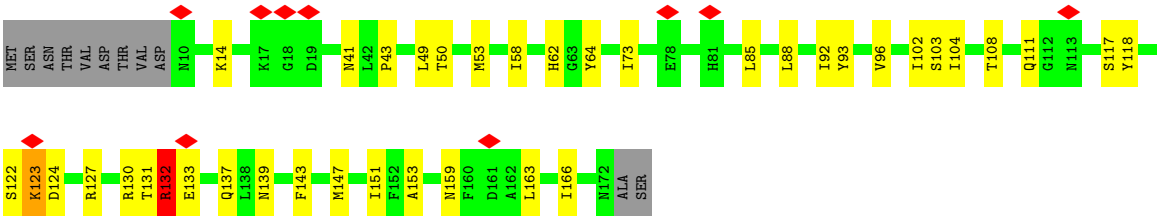
• Molecule 10: PSI subunit V



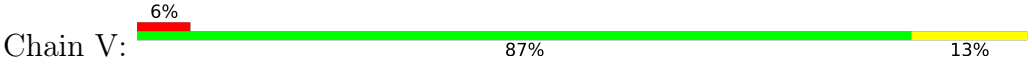


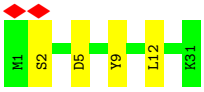
• Molecule 10: PSI subunit V



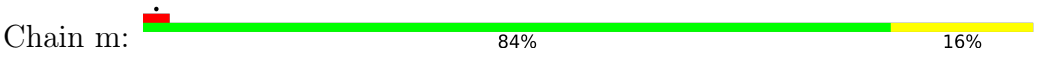


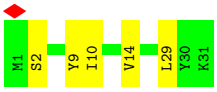
• Molecule 11: Photosystem I reaction center subunit XII



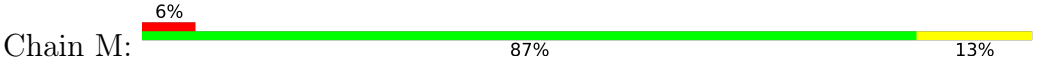


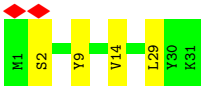
• Molecule 11: Photosystem I reaction center subunit XII





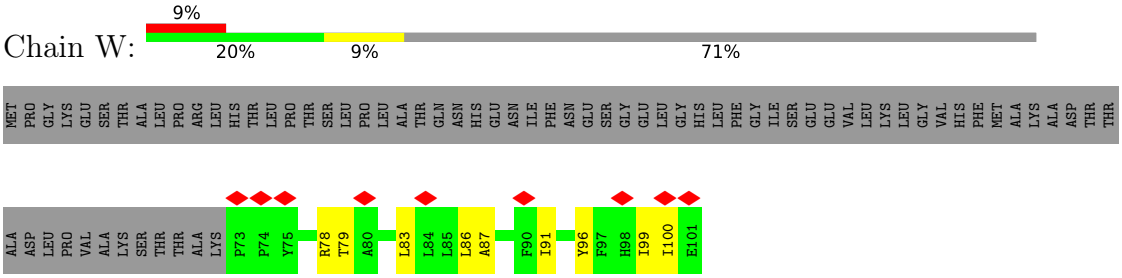
• Molecule 11: Photosystem I reaction center subunit XII





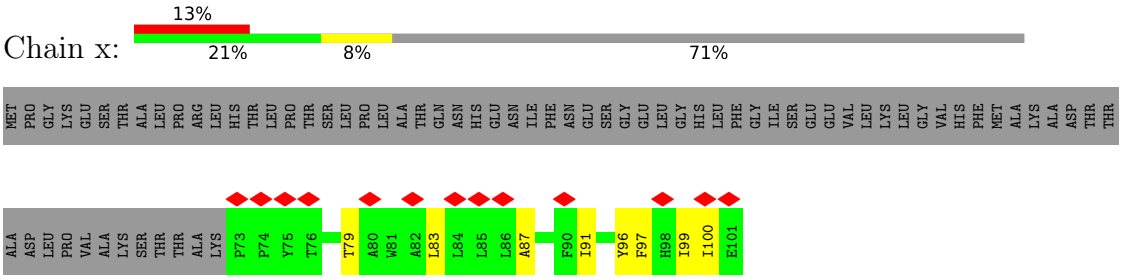
• Molecule 12: Photosystem one PsaX

Chain W:



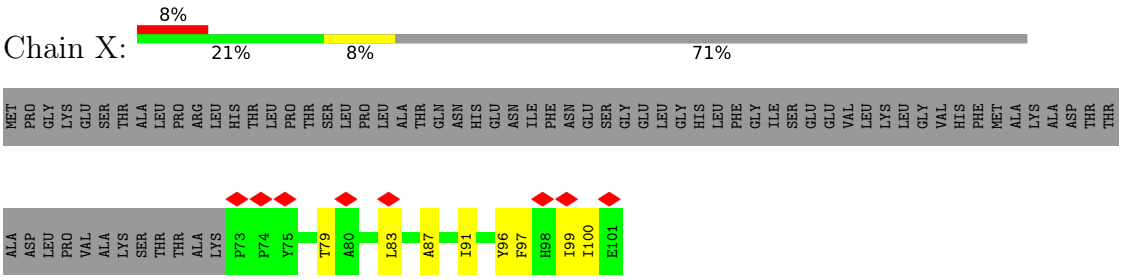
• Molecule 12: Photosystem one PsaX

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, Not provided	
Number of particles used	201104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	57.328	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	381.6013, 381.6013, 381.6013	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49063, 1.49063, 1.49063	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: F6C, SF4, BCR, CA, PQN, LMT, LHG, LMG, CL0, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.49	0/6138	0.50	1/8362 (0.0%)
1	G	0.49	0/6138	0.49	1/8362 (0.0%)
1	a	0.49	0/6138	0.49	1/8362 (0.0%)
2	B	0.50	0/6135	0.48	0/8385
2	H	0.50	0/6135	0.48	0/8385
2	b	0.50	0/6135	0.48	0/8385
3	C	0.52	0/611	0.76	2/828 (0.2%)
3	N	0.52	0/611	0.76	2/828 (0.2%)
3	c	0.52	0/611	0.76	2/828 (0.2%)
4	D	0.41	0/1116	0.58	0/1505
4	O	0.41	0/1116	0.58	0/1505
4	d	0.41	0/1116	0.58	0/1505
5	E	0.35	0/506	0.62	2/686 (0.3%)
5	P	0.35	0/506	0.62	2/686 (0.3%)
5	e	0.34	0/506	0.62	2/686 (0.3%)
6	F	0.35	0/1084	0.73	5/1470 (0.3%)
6	Q	0.35	0/1084	0.74	5/1470 (0.3%)
6	f	0.35	0/1084	0.74	5/1470 (0.3%)
7	I	0.51	0/365	0.66	0/502
7	R	0.50	0/365	0.67	0/502
7	i	0.50	0/365	0.66	0/502
8	J	0.31	0/353	0.85	2/482 (0.4%)
8	S	0.31	0/353	0.85	2/482 (0.4%)
8	j	0.31	0/353	0.85	0/482
9	K	0.22	0/129	1.03	2/175 (1.1%)
9	T	0.22	0/129	1.03	2/175 (1.1%)
9	k	0.22	0/129	1.03	2/175 (1.1%)
10	L	0.50	0/1255	0.76	4/1702 (0.2%)
10	U	0.50	0/1255	0.76	4/1702 (0.2%)
10	l	0.50	0/1255	0.76	4/1702 (0.2%)
11	M	0.37	0/250	0.57	0/340
11	V	0.38	0/250	0.57	0/340

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
11	m	0.37	0/250	0.57	0/340
12	W	0.26	0/256	0.41	0/350
12	X	0.26	0/256	0.41	0/350
12	x	0.26	0/256	0.41	0/350
All	All	0.47	0/54594	0.57	52/74361 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
1	a	0	1
6	F	0	2
6	Q	0	2
6	f	0	2
8	J	0	1
8	S	0	1
8	j	0	1
10	L	0	1
10	U	0	1
10	l	0	1
All	All	0	15

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	132	ARG	CG-CD-NE	12.10	138.61	112.00
10	L	132	ARG	CG-CD-NE	12.08	138.57	112.00
10	l	132	ARG	CG-CD-NE	12.07	138.55	112.00
10	l	132	ARG	CD-NE-CZ	9.51	137.72	124.40
10	L	132	ARG	CD-NE-CZ	9.50	137.70	124.40
10	U	132	ARG	CD-NE-CZ	9.49	137.68	124.40
9	K	72	MET	CB-CG-SD	9.37	140.81	112.70
9	T	72	MET	CB-CG-SD	9.37	140.80	112.70
9	k	72	MET	CB-CG-SD	9.37	140.80	112.70
10	l	132	ARG	CB-CG-CD	8.88	131.73	111.30
10	U	132	ARG	CB-CG-CD	8.87	131.71	111.30
10	L	132	ARG	CB-CG-CD	8.87	131.70	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	115	LYS	CB-CG-CD	7.79	129.21	111.30
6	F	115	LYS	CB-CG-CD	7.78	129.20	111.30
6	f	115	LYS	CB-CG-CD	7.78	129.20	111.30
9	K	72	MET	CA-CB-CG	6.57	127.24	114.10
9	k	72	MET	CA-CB-CG	6.56	127.23	114.10
9	T	72	MET	CA-CB-CG	6.55	127.21	114.10
1	a	641	MET	CB-CG-SD	6.15	131.15	112.70
1	G	641	MET	CB-CG-SD	6.15	131.15	112.70
1	A	641	MET	CB-CG-SD	6.14	131.11	112.70
6	f	31	CYS	CA-CB-SG	5.82	127.80	114.40
6	Q	31	CYS	CA-CB-SG	5.81	127.76	114.40
6	F	31	CYS	CA-CB-SG	5.80	127.75	114.40
5	P	33	SER	CA-C-N	5.73	132.49	121.54
5	P	33	SER	C-N-CA	5.73	132.49	121.54
5	e	33	SER	CA-C-N	5.73	132.48	121.54
5	e	33	SER	C-N-CA	5.73	132.48	121.54
5	E	33	SER	CA-C-N	5.72	132.47	121.54
5	E	33	SER	C-N-CA	5.72	132.47	121.54
6	Q	115	LYS	CG-CD-CE	5.60	124.18	111.30
6	f	115	LYS	CG-CD-CE	5.60	124.17	111.30
6	F	115	LYS	CG-CD-CE	5.59	124.16	111.30
10	l	132	ARG	NE-CZ-NH2	-5.58	114.18	119.20
10	L	132	ARG	NE-CZ-NH2	-5.54	114.21	119.20
10	U	132	ARG	NE-CZ-NH2	-5.49	114.26	119.20
3	N	62	PHE	CA-C-N	5.28	131.63	121.54
3	N	62	PHE	C-N-CA	5.28	131.63	121.54
3	c	62	PHE	CA-C-N	5.28	131.63	121.54
3	c	62	PHE	C-N-CA	5.28	131.63	121.54
3	C	62	PHE	CA-C-N	5.28	131.62	121.54
3	C	62	PHE	C-N-CA	5.28	131.62	121.54
6	F	46	ASP	CA-C-N	5.27	131.61	121.54
6	F	46	ASP	C-N-CA	5.27	131.61	121.54
6	Q	46	ASP	CA-C-N	5.26	131.58	121.54
6	Q	46	ASP	C-N-CA	5.26	131.58	121.54
6	f	46	ASP	CA-C-N	5.25	131.56	121.54
6	f	46	ASP	C-N-CA	5.25	131.56	121.54
8	J	11	SER	CA-C-N	-5.02	111.96	121.54
8	J	11	SER	C-N-CA	-5.02	111.96	121.54
8	S	11	SER	CA-C-N	-5.01	111.97	121.54
8	S	11	SER	C-N-CA	-5.01	111.97	121.54

There are no chirality outliers.

All (15) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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	5931	0	5774	169	0
1	G	5931	0	5774	162	0
1	a	5931	0	5774	169	0
2	B	5913	0	5669	174	0
2	H	5913	0	5669	170	0
2	b	5913	0	5669	170	0
3	C	601	0	577	15	0
3	N	601	0	577	11	0
3	c	601	0	577	15	0
4	D	1092	0	1098	29	0
4	O	1092	0	1098	27	0
4	d	1092	0	1098	30	0
5	E	497	0	482	10	0
5	P	497	0	482	7	0
5	e	497	0	482	7	0
6	F	1060	0	1091	32	0
6	Q	1060	0	1091	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	1060	0	1091	30	0
7	I	350	0	354	19	0
7	R	350	0	354	12	0
7	i	350	0	354	14	0
8	J	344	0	360	10	0
8	S	344	0	360	10	0
8	j	344	0	360	11	0
9	K	253	0	168	5	0
9	T	253	0	168	5	0
9	k	253	0	168	5	0
10	L	1227	0	1239	33	0
10	U	1227	0	1239	32	0
10	l	1227	0	1239	32	0
11	M	245	0	259	4	0
11	V	245	0	259	5	0
11	m	245	0	259	6	0
12	W	246	0	246	6	0
12	X	246	0	246	5	0
12	x	246	0	246	5	0
13	A	65	0	72	4	0
13	G	65	0	72	4	0
13	a	65	0	72	4	0
14	A	2315	0	2200	116	0
14	B	2220	0	2213	155	0
14	G	2315	0	2200	112	0
14	H	2220	0	2213	154	0
14	K	45	0	32	0	0
14	L	190	0	203	13	0
14	T	45	0	32	0	0
14	U	190	0	203	12	0
14	W	55	0	49	5	0
14	X	55	0	49	5	0
14	a	2315	0	2200	116	0
14	b	2220	0	2213	159	0
14	k	45	0	32	0	0
14	l	190	0	203	12	0
14	x	55	0	49	3	0
15	A	46	0	0	0	0
15	B	244	0	0	3	0
15	G	46	0	0	0	0
15	H	244	0	0	2	0
15	a	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b	244	0	0	2	0
16	A	33	0	46	11	0
16	B	33	0	46	6	0
16	G	33	0	46	8	0
16	H	33	0	46	6	0
16	a	33	0	46	10	0
16	b	33	0	46	5	0
17	A	8	0	0	0	0
17	C	16	0	0	1	0
17	G	8	0	0	0	0
17	N	16	0	0	1	0
17	a	8	0	0	0	0
17	c	16	0	0	1	0
18	A	240	0	293	18	0
18	B	360	0	438	32	0
18	G	240	0	293	21	0
18	H	360	0	438	33	0
18	I	80	0	96	11	0
18	L	80	0	97	9	0
18	M	40	0	48	4	0
18	R	80	0	96	10	0
18	U	80	0	97	7	0
18	V	40	0	48	4	0
18	a	240	0	293	21	0
18	b	360	0	438	33	0
18	i	80	0	96	8	0
18	l	80	0	97	8	0
18	m	40	0	48	5	0
19	A	42	0	54	3	0
19	B	44	0	61	1	0
19	G	42	0	54	2	0
19	H	44	0	61	3	0
19	a	42	0	54	3	0
19	b	44	0	61	0	0
20	A	46	0	65	5	0
20	B	46	0	62	4	0
20	G	46	0	65	5	0
20	H	46	0	62	4	0
20	I	37	0	44	1	0
20	L	50	0	70	5	0
20	R	37	0	44	4	0
20	U	50	0	70	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	a	46	0	65	2	0
20	b	46	0	62	4	0
20	i	37	0	44	1	0
20	l	50	0	70	4	0
21	A	59	0	58	1	0
21	G	59	0	57	1	0
21	a	59	0	58	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	72462	0	70691	1973	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 14.

All (1973) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:406:TRP:CD1	14:G:1126:CLA:HAB	2.09	0.87
1:A:406:TRP:CD1	14:A:1126:CLA:HAB	2.09	0.87
1:a:406:TRP:CD1	14:a:1126:CLA:HAB	2.09	0.87
14:B:1204:CLA:H43	7:I:21:MET:HE1	1.56	0.86
14:H:1205:CLA:H102	14:H:1205:CLA:H2	1.58	0.86
14:B:1205:CLA:H102	14:B:1205:CLA:H2	1.58	0.85
14:b:1205:CLA:H102	14:b:1205:CLA:H2	1.58	0.85
14:b:1204:CLA:H43	7:i:21:MET:HE1	1.60	0.83
14:H:1204:CLA:HHB	14:H:1205:CLA:HMB3	1.63	0.80
10:U:131:THR:HG22	10:U:133:GLU:H	1.47	0.80
14:b:1204:CLA:HHB	14:b:1205:CLA:HMB3	1.63	0.80
14:H:1023:CLA:H142	18:R:4018:BCR:H271	1.64	0.79
14:B:1204:CLA:HHB	14:B:1205:CLA:HMB3	1.63	0.79
10:L:131:THR:HG22	10:L:133:GLU:H	1.47	0.79
10:l:131:THR:HG22	10:l:133:GLU:H	1.47	0.79
1:A:409:GLY:HA3	1:A:639:LEU:HD11	1.67	0.76
1:a:409:GLY:HA3	1:a:639:LEU:HD11	1.67	0.76
10:U:124:ASP:H	10:U:130:ARG:HH22	1.34	0.76
1:G:409:GLY:HA3	1:G:639:LEU:HD11	1.67	0.75
10:l:124:ASP:H	10:l:130:ARG:HH22	1.34	0.75
10:L:124:ASP:H	10:L:130:ARG:HH22	1.34	0.75
1:G:588:LYS:NZ	2:H:677:TYR:O	2.20	0.74
14:H:1204:CLA:H43	7:R:21:MET:HE1	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:LYS:NZ	2:B:677:TYR:O	2.20	0.74
1:a:588:LYS:NZ	2:b:677:TYR:O	2.20	0.74
4:D:100:ILE:HB	4:D:113:HIS:HB3	1.70	0.74
6:Q:115:LYS:HZ1	6:Q:120:ASP:HB2	1.54	0.73
2:B:700:ARG:NH1	7:I:44:GLU:OE2	2.22	0.73
16:H:2002:PQN:H142	18:H:4017:BCR:H271	1.70	0.73
6:F:74:ARG:HG3	6:F:75:LEU:H	1.55	0.72
4:O:100:ILE:HB	4:O:113:HIS:HB3	1.70	0.72
6:Q:74:ARG:HG3	6:Q:75:LEU:H	1.55	0.72
16:b:2002:PQN:H142	18:b:4017:BCR:H271	1.70	0.72
6:f:74:ARG:HG3	6:f:75:LEU:H	1.55	0.72
16:B:2002:PQN:H142	18:B:4017:BCR:H271	1.70	0.72
4:d:100:ILE:HB	4:d:113:HIS:HB3	1.70	0.71
14:G:1103:CLA:H51	14:G:1111:CLA:H11	1.73	0.71
18:A:4001:BCR:H343	9:K:70:ALA:HB1	1.73	0.70
1:a:152:THR:HG21	1:a:235:ILE:HG21	1.73	0.70
1:A:152:THR:HG21	1:A:235:ILE:HG21	1.73	0.70
2:H:589:TRP:CH2	14:H:1022:CLA:HAB	2.26	0.70
14:a:1103:CLA:H51	14:a:1111:CLA:H11	1.73	0.70
2:B:589:TRP:CH2	14:B:1022:CLA:HAB	2.26	0.70
14:A:1103:CLA:H51	14:A:1111:CLA:H11	1.73	0.70
1:G:446:ALA:O	1:G:450:HIS:ND1	2.25	0.70
2:b:589:TRP:CH2	14:b:1022:CLA:HAB	2.26	0.70
18:G:4001:BCR:H343	9:T:70:ALA:HB1	1.73	0.70
1:A:241:PHE:HB3	1:A:248:MET:HE2	1.74	0.69
1:A:446:ALA:O	1:A:450:HIS:ND1	2.25	0.69
4:D:50:TRP:HE1	4:D:68:MET:HE3	1.57	0.69
1:G:193:GLN:NE2	1:G:322:HIS:O	2.26	0.69
2:B:578:SER:OG	2:B:581:ASP:OD2	2.11	0.69
1:G:152:THR:HG21	1:G:235:ILE:HG21	1.72	0.69
2:H:578:SER:OG	2:H:581:ASP:OD2	2.11	0.69
14:b:1228:CLA:HBC3	18:b:4016:BCR:H362	1.74	0.69
1:A:193:GLN:NE2	1:A:322:HIS:O	2.26	0.69
14:a:1119:CLA:HMB2	14:a:1123:CLA:HED2	1.75	0.69
14:b:1236:CLA:HBC2	14:x:1701:CLA:HBC3	1.73	0.69
4:d:50:TRP:HE1	4:d:68:MET:HE3	1.57	0.69
1:a:241:PHE:HB3	1:a:248:MET:HE2	1.74	0.69
2:b:578:SER:OG	2:b:581:ASP:OD2	2.11	0.69
14:b:1210:CLA:H101	14:b:1221:CLA:H43	1.75	0.69
1:a:193:GLN:NE2	1:a:322:HIS:O	2.26	0.68
14:B:1210:CLA:H101	14:B:1221:CLA:H43	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:4011:BCR:H362	14:b:1022:CLA:H42	1.75	0.68
6:f:45:PRO:O	6:f:50:THR:OG1	2.11	0.68
14:A:1119:CLA:HMB2	14:A:1123:CLA:HED2	1.75	0.68
2:B:111:ASN:HD22	7:I:10:GLY:HA2	1.59	0.68
1:G:241:PHE:HB3	1:G:248:MET:HE2	1.74	0.68
14:G:1119:CLA:HMB2	14:G:1123:CLA:HED2	1.75	0.68
14:H:1228:CLA:HBC3	18:H:4016:BCR:H362	1.74	0.68
6:F:115:LYS:HZ1	6:F:120:ASP:HB2	1.59	0.68
6:Q:45:PRO:O	6:Q:50:THR:OG1	2.11	0.68
14:B:1236:CLA:HBC2	14:X:1701:CLA:HBC3	1.74	0.68
14:H:1210:CLA:H101	14:H:1221:CLA:H43	1.75	0.67
4:O:50:TRP:HE1	4:O:68:MET:HE3	1.57	0.67
18:A:4011:BCR:H362	14:B:1022:CLA:H42	1.75	0.67
6:F:45:PRO:O	6:F:50:THR:OG1	2.11	0.67
3:N:24:ASP:OD2	4:O:113:HIS:ND1	2.26	0.67
2:B:70:TRP:NE1	7:I:13:ALA:O	2.18	0.67
14:B:1228:CLA:HBC3	18:B:4016:BCR:H362	1.74	0.67
6:F:129:VAL:HA	6:F:132:LEU:HD23	1.77	0.67
1:A:634:TRP:HH2	14:A:1012:CLA:HAB	1.60	0.67
1:G:385:PRO:HG2	1:G:391:ALA:HB2	1.76	0.66
1:a:446:ALA:O	1:a:450:HIS:ND1	2.25	0.66
1:a:385:PRO:HG2	1:a:391:ALA:HB2	1.76	0.66
1:A:385:PRO:HG2	1:A:391:ALA:HB2	1.76	0.66
2:H:589:TRP:HH2	14:H:1022:CLA:HAB	1.61	0.66
2:B:589:TRP:HH2	14:B:1022:CLA:HAB	1.61	0.66
18:G:4011:BCR:H362	14:H:1022:CLA:H42	1.75	0.66
2:b:589:TRP:HH2	14:b:1022:CLA:HAB	1.61	0.66
1:G:634:TRP:HH2	14:G:1012:CLA:HAB	1.60	0.66
1:a:634:TRP:HH2	14:a:1012:CLA:HAB	1.60	0.66
6:f:129:VAL:HA	6:f:132:LEU:HD23	1.77	0.66
1:A:114:GLN:NE2	14:A:1107:CLA:OBD	2.29	0.66
14:b:1214:CLA:HBA2	14:b:1223:CLA:HBB2	1.78	0.65
2:B:92:TRP:HB3	7:I:22:ILE:HG13	1.78	0.65
1:a:336:MET:HE3	1:a:343:ILE:HD11	1.78	0.65
2:b:457:ILE:O	2:b:525:TYR:OH	2.15	0.65
1:A:336:MET:HE3	1:A:343:ILE:HD11	1.78	0.65
14:A:1140:CLA:H71	16:A:2001:PQN:H202	1.78	0.65
14:B:1210:CLA:H141	14:B:1216:CLA:HBB2	1.79	0.65
2:H:173:ALA:O	2:H:177:HIS:ND1	2.28	0.65
10:U:163:LEU:HD12	10:U:166:ILE:HD11	1.78	0.65
14:a:1138:CLA:HED2	2:b:428:TRP:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:129:VAL:HA	6:Q:132:LEU:HD23	1.77	0.65
7:R:13:ALA:HB1	11:V:5:ASP:HA	1.76	0.65
10:L:163:LEU:HD12	10:L:166:ILE:HD11	1.78	0.65
1:G:336:MET:HE3	1:G:343:ILE:HD11	1.78	0.65
4:d:25:GLN:HG3	4:d:69:ARG:HG3	1.79	0.65
14:a:1140:CLA:H71	16:a:2001:PQN:H202	1.78	0.65
2:H:86:PRO:HB2	2:H:116:CYS:HB3	1.80	0.64
2:B:44:GLN:NE2	2:B:163:PRO:O	2.30	0.64
4:D:25:GLN:HG3	4:D:69:ARG:HG3	1.79	0.64
1:G:114:GLN:NE2	14:G:1107:CLA:OBD	2.29	0.64
1:G:380:HIS:ND1	14:G:1116:CLA:OBD	2.30	0.64
14:G:1138:CLA:HED2	2:H:428:TRP:HB2	1.78	0.64
2:b:319:PHE:HA	14:b:1219:CLA:HAB	1.80	0.64
14:G:1140:CLA:H71	16:G:2001:PQN:H202	1.78	0.64
10:l:163:LEU:HD12	10:l:166:ILE:HD11	1.78	0.64
14:A:1138:CLA:HED2	2:B:428:TRP:HB2	1.78	0.64
2:B:282:VAL:HG11	14:B:1213:CLA:H143	1.80	0.64
2:H:664:TRP:O	2:H:667:SER:OG	2.15	0.64
3:N:73:THR:OG1	3:N:74:THR:N	2.28	0.64
4:O:25:GLN:HG3	4:O:69:ARG:HG3	1.79	0.64
1:A:380:HIS:ND1	14:A:1116:CLA:OBD	2.30	0.64
2:H:319:PHE:HA	14:H:1219:CLA:HAB	1.80	0.64
14:H:1210:CLA:H141	14:H:1216:CLA:HBB2	1.78	0.64
1:a:114:GLN:NE2	14:a:1107:CLA:OBD	2.29	0.64
2:b:222:LEU:HD11	14:b:1212:CLA:HBA2	1.80	0.64
2:b:700:ARG:NH1	7:i:44:GLU:OE2	2.31	0.64
2:H:222:LEU:HD11	14:H:1212:CLA:HBA2	1.80	0.64
6:Q:72:LEU:HB3	14:W:1701:CLA:H12	1.79	0.64
2:b:173:ALA:O	2:b:177:HIS:ND1	2.28	0.64
2:B:222:LEU:HD11	14:B:1212:CLA:HBA2	1.80	0.64
2:B:457:ILE:O	2:B:525:TYR:OH	2.15	0.64
14:b:1210:CLA:H141	14:b:1216:CLA:HBB2	1.78	0.64
3:c:73:THR:OG1	3:c:74:THR:N	2.28	0.64
2:B:86:PRO:HB2	2:B:116:CYS:HB3	1.80	0.64
2:b:86:PRO:HB2	2:b:116:CYS:HB3	1.80	0.64
2:B:664:TRP:O	2:B:667:SER:OG	2.15	0.64
1:A:479:GLN:HG2	1:A:480:ASP:OD1	1.98	0.63
2:H:457:ILE:O	2:H:525:TYR:OH	2.15	0.63
20:R:5006:LMG:HC61	20:l:5007:LMG:H322	1.80	0.63
14:H:1214:CLA:HBA2	14:H:1223:CLA:HBB2	1.78	0.63
2:B:173:ALA:O	2:B:177:HIS:ND1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:380:HIS:ND1	14:a:1116:CLA:OBD	2.30	0.63
1:A:445:ASP:H	4:D:33:THR:HG21	1.64	0.63
7:I:37:LEU:HD21	18:L:4019:BCR:H312	1.80	0.63
1:a:634:TRP:CH2	14:a:1012:CLA:HAB	2.34	0.63
1:A:634:TRP:CH2	14:A:1012:CLA:HAB	2.34	0.63
2:H:257:PHE:HE2	2:H:500:TRP:CE3	2.17	0.63
18:H:4009:BCR:H383	18:H:4010:BCR:H272	1.81	0.63
6:Q:54:LEU:HA	6:Q:57:TYR:HD1	1.64	0.63
18:B:4009:BCR:H383	18:B:4010:BCR:H272	1.81	0.63
2:H:44:GLN:NE2	2:H:163:PRO:O	2.30	0.63
14:H:1023:CLA:H122	18:R:4018:BCR:H281	1.81	0.63
2:b:92:TRP:HB3	7:i:22:ILE:HG13	1.81	0.63
14:B:1214:CLA:HBA2	14:B:1223:CLA:HBB2	1.79	0.63
14:b:1229:CLA:HAC2	6:f:85:ILE:HG13	1.81	0.63
4:O:38:LYS:NZ	10:U:122:SER:O	2.32	0.62
1:a:445:ASP:H	4:d:33:THR:HG21	1.64	0.62
2:B:319:PHE:HA	14:B:1219:CLA:HAB	1.80	0.62
1:G:479:GLN:HG2	1:G:480:ASP:OD1	1.98	0.62
2:H:54:LEU:HD12	14:H:1210:CLA:HED1	1.81	0.62
18:H:4016:BCR:H272	14:W:1701:CLA:H71	1.81	0.62
2:b:44:GLN:NE2	2:b:163:PRO:O	2.30	0.62
2:B:257:PHE:HE2	2:B:500:TRP:CE3	2.17	0.62
6:F:54:LEU:HA	6:F:57:TYR:HD1	1.64	0.62
14:H:1229:CLA:HAC2	6:Q:85:ILE:HG13	1.81	0.62
2:b:282:VAL:HG11	14:b:1213:CLA:H143	1.80	0.62
6:f:54:LEU:HA	6:f:57:TYR:HD1	1.64	0.62
2:B:54:LEU:HD12	14:B:1210:CLA:HED1	1.81	0.62
2:B:696:PHE:O	10:L:118:TYR:OH	2.17	0.62
2:H:282:VAL:HG11	14:H:1213:CLA:H143	1.80	0.62
14:U:1501:CLA:H192	20:U:5007:LMG:H222	1.80	0.62
1:a:307:PHE:HE1	14:a:1119:CLA:HAB	1.65	0.62
14:l:1501:CLA:H192	20:l:5007:LMG:H222	1.80	0.62
14:L:1501:CLA:H192	20:L:5007:LMG:H222	1.80	0.62
1:a:623:SER:OG	1:a:626:ASP:OD1	2.17	0.62
1:a:479:GLN:HG2	1:a:480:ASP:OD1	1.98	0.62
2:b:257:PHE:HE2	2:b:500:TRP:CE3	2.17	0.62
3:C:24:ASP:OD2	4:D:113:HIS:ND1	2.32	0.62
2:b:664:TRP:O	2:b:667:SER:OG	2.15	0.62
14:b:1228:CLA:H2	18:b:4016:BCR:H353	1.82	0.62
18:b:4009:BCR:H383	18:b:4010:BCR:H272	1.81	0.62
1:G:307:PHE:HE1	14:G:1119:CLA:HAB	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:54:LEU:HD12	14:b:1210:CLA:HED1	1.81	0.61
1:a:406:TRP:HD1	14:a:1126:CLA:HAB	1.65	0.61
1:a:30:PRO:HB2	1:a:50:LEU:HD11	1.83	0.61
2:b:537:THR:HG21	14:b:1222:CLA:HBC3	1.82	0.61
1:G:623:SER:OG	1:G:626:ASP:OD1	2.17	0.61
2:H:132:ASN:HD22	11:V:2:SER:HA	1.65	0.61
1:A:30:PRO:HB2	1:A:50:LEU:HD11	1.83	0.61
1:G:171:MET:HE1	14:G:1111:CLA:H92	1.83	0.61
1:a:171:MET:HE1	14:a:1111:CLA:H92	1.83	0.61
1:a:612:ASP:OD2	3:c:53:ARG:NH2	2.33	0.61
1:A:623:SER:OG	1:A:626:ASP:OD1	2.17	0.61
1:G:634:TRP:CH2	14:G:1012:CLA:HAB	2.34	0.61
2:H:668:PHE:HB2	14:H:1023:CLA:HMC2	1.83	0.61
2:b:668:PHE:HB2	14:b:1023:CLA:HMC2	1.83	0.61
14:B:1229:CLA:HAC2	6:F:85:ILE:HG13	1.81	0.61
4:O:79:ARG:NH2	4:O:81:GLU:OE1	2.34	0.61
1:A:307:PHE:HE1	14:A:1119:CLA:HAB	1.65	0.61
2:H:537:THR:HG21	14:H:1222:CLA:HBC3	1.82	0.61
1:a:167:MET:HE3	1:a:171:MET:HE3	1.82	0.61
1:A:167:MET:HE3	1:A:171:MET:HE3	1.83	0.61
1:G:406:TRP:HD1	14:G:1126:CLA:HAB	1.66	0.61
4:D:79:ARG:NH2	4:D:81:GLU:OE1	2.34	0.61
1:A:171:MET:HE1	14:A:1111:CLA:H92	1.83	0.60
2:H:355:HIS:ND1	14:H:1214:CLA:OBD	2.34	0.60
2:b:650:LEU:HD11	2:b:737:SER:HB3	1.84	0.60
4:d:79:ARG:NH2	4:d:81:GLU:OE1	2.34	0.60
2:b:268:LEU:HB2	2:b:273:MET:HE3	1.84	0.60
1:G:30:PRO:HB2	1:G:50:LEU:HD11	1.83	0.60
2:B:537:THR:HG21	14:B:1222:CLA:HBC3	1.82	0.60
2:H:68:VAL:HG21	2:H:124:TRP:HZ3	1.67	0.60
18:a:4001:BCR:H343	9:k:70:ALA:HB1	1.83	0.60
1:G:167:MET:HE3	1:G:171:MET:HE3	1.83	0.60
2:H:650:LEU:HD11	2:H:737:SER:HB3	1.84	0.60
2:B:668:PHE:HB2	14:B:1023:CLA:HMC2	1.83	0.60
2:H:696:PHE:O	10:U:118:TYR:OH	2.17	0.60
14:H:1228:CLA:H2	18:H:4016:BCR:H353	1.82	0.60
14:a:1125:CLA:HMB3	14:a:1133:CLA:H12	1.84	0.60
1:A:282:GLY:HA3	1:A:538:LEU:HD11	1.84	0.60
2:H:15:ASP:HB3	2:H:20:ARG:HB3	1.84	0.59
14:A:1125:CLA:HMB3	14:A:1133:CLA:H12	1.84	0.59
2:B:355:HIS:ND1	14:B:1214:CLA:OBD	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:334:LEU:HD13	14:b:1202:CLA:HAC1	1.85	0.59
14:B:1228:CLA:H2	18:B:4016:BCR:H353	1.82	0.59
1:G:684:ARG:NH1	1:G:685:ASP:OD2	2.36	0.59
3:c:24:ASP:OD2	4:d:113:HIS:ND1	2.34	0.59
2:B:68:VAL:HG21	2:B:124:TRP:HZ3	1.66	0.59
2:B:650:LEU:HD11	2:B:737:SER:HB3	1.84	0.59
2:b:15:ASP:HB3	2:b:20:ARG:HB3	1.84	0.59
2:B:268:LEU:HB2	2:B:273:MET:HE3	1.84	0.59
1:G:282:GLY:HA3	1:G:538:LEU:HD11	1.84	0.59
1:G:641:MET:HE2	1:G:641:MET:HA	1.85	0.59
14:G:1125:CLA:HMB3	14:G:1133:CLA:H12	1.84	0.59
1:a:282:GLY:HA3	1:a:538:LEU:HD11	1.84	0.59
2:B:334:LEU:HD13	14:B:1202:CLA:HAC1	1.84	0.59
2:b:381:TYR:CD1	14:b:1224:CLA:HAB	2.38	0.59
2:b:355:HIS:ND1	14:b:1214:CLA:OBD	2.34	0.59
2:B:381:TYR:CD1	14:B:1224:CLA:HAB	2.38	0.59
10:L:58:ILE:O	10:L:62:HIS:ND1	2.36	0.59
14:A:1131:CLA:HBB2	10:L:73:ILE:HD11	1.85	0.59
2:B:15:ASP:HB3	2:B:20:ARG:HB3	1.84	0.59
1:G:684:ARG:HH22	2:H:644:PRO:HD3	1.68	0.59
1:A:684:ARG:NH1	1:A:685:ASP:OD2	2.36	0.59
10:U:58:ILE:O	10:U:62:HIS:ND1	2.36	0.58
14:a:1131:CLA:HBB2	10:l:73:ILE:HD11	1.85	0.58
3:C:73:THR:OG1	3:C:74:THR:N	2.28	0.58
2:b:111:ASN:HD22	7:i:10:GLY:HA2	1.66	0.58
2:b:319:PHE:HA	14:b:1219:CLA:CAB	2.34	0.58
2:H:255:LEU:HD11	14:H:1212:CLA:HBC1	1.86	0.58
2:H:381:TYR:CD1	14:H:1224:CLA:HAB	2.38	0.58
1:A:545:ALA:HB2	1:A:559:MET:HE2	1.85	0.58
1:A:557:VAL:HG11	1:A:560:MET:HG3	1.86	0.58
2:b:68:VAL:HG21	2:b:124:TRP:HZ3	1.67	0.58
4:d:122:LYS:O	4:d:127:ARG:NH2	2.37	0.58
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.85	0.58
2:H:268:LEU:HB2	2:H:273:MET:HE3	1.84	0.58
2:H:319:PHE:HA	14:H:1219:CLA:CAB	2.33	0.58
1:a:545:ALA:HB2	1:a:559:MET:HE2	1.85	0.58
1:A:641:MET:HE2	1:A:641:MET:HA	1.85	0.58
2:B:319:PHE:HA	14:B:1219:CLA:CAB	2.33	0.58
1:G:460:PHE:HB3	14:G:1132:CLA:HBB2	1.86	0.58
2:H:91:ILE:HB	2:H:112:PRO:HB2	1.86	0.58
1:A:306:MET:HG3	14:A:1115:CLA:H192	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:MET:HG3	14:G:1115:CLA:H192	1.86	0.58
1:G:489:LEU:HB2	1:G:566:THR:HG23	1.85	0.58
1:a:489:LEU:HB2	1:a:566:THR:HG23	1.85	0.58
1:a:684:ARG:HH22	2:b:644:PRO:HD3	1.68	0.58
1:a:58:ASP:OD2	1:a:360:HIS:NE2	2.37	0.58
1:a:641:MET:HA	1:a:641:MET:HE2	1.85	0.58
1:a:684:ARG:NH1	1:a:685:ASP:OD2	2.36	0.58
2:B:255:LEU:HD11	14:B:1212:CLA:HBC1	1.86	0.58
2:H:445:ASP:OD1	2:H:623:LEU:N	2.37	0.58
10:l:58:ILE:O	10:l:62:HIS:ND1	2.36	0.58
4:D:122:LYS:O	4:D:127:ARG:NH2	2.37	0.58
2:H:334:LEU:HD13	14:H:1202:CLA:HAC1	1.84	0.57
14:H:1211:CLA:HMA3	18:H:4006:BCR:H292	1.86	0.57
1:A:489:LEU:HB2	1:A:566:THR:HG23	1.85	0.57
1:G:210:GLY:C	14:G:1112:CLA:HAB	2.29	0.57
1:A:460:PHE:HB3	14:A:1132:CLA:HBB2	1.86	0.57
1:G:470:ASP:OD2	2:H:642:TYR:OH	2.18	0.57
1:a:651:GLN:HB3	1:a:668:THR:HG23	1.87	0.57
2:b:696:PHE:O	10:l:118:TYR:OH	2.17	0.57
1:A:58:ASP:OD2	1:A:360:HIS:NE2	2.37	0.57
1:a:179:TYR:HB3	1:a:180:HIS:HD2	1.69	0.57
1:A:651:GLN:HB3	1:A:668:THR:HG23	1.87	0.57
1:G:557:VAL:HG11	1:G:560:MET:HG3	1.86	0.57
20:R:5006:LMG:H361	18:V:4021:BCR:H392	1.85	0.57
2:b:255:LEU:HD11	14:b:1212:CLA:HBC1	1.86	0.57
14:b:1211:CLA:HMA3	18:b:4006:BCR:H292	1.86	0.57
2:B:328:GLU:O	2:B:332:ASN:ND2	2.38	0.57
1:G:179:TYR:HB3	1:G:180:HIS:HD2	1.69	0.57
1:G:193:GLN:HE21	1:G:315:ARG:H	1.52	0.57
1:G:545:ALA:HB2	1:G:559:MET:HE2	1.85	0.57
14:G:1131:CLA:HBB2	10:U:73:ILE:HD11	1.85	0.57
2:b:468:GLN:NE2	14:b:1234:CLA:OBD	2.38	0.57
2:H:453:ALA:HB3	6:Q:40:ARG:HH22	1.70	0.57
14:H:1204:CLA:H2	18:R:4018:BCR:HC41	1.87	0.57
1:a:210:GLY:C	14:a:1112:CLA:HAB	2.29	0.57
14:B:1211:CLA:HMA3	18:B:4006:BCR:H292	1.86	0.57
4:O:122:LYS:O	4:O:127:ARG:NH2	2.37	0.57
2:b:91:ILE:HB	2:b:112:PRO:HB2	1.85	0.57
1:A:210:GLY:C	14:A:1112:CLA:HAB	2.29	0.57
1:A:684:ARG:HH22	2:B:644:PRO:HD3	1.68	0.57
2:H:328:GLU:O	2:H:332:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:17:LEU:HD21	11:V:12:LEU:HD11	1.87	0.57
1:a:392:THR:HG21	1:a:553:VAL:HB	1.86	0.57
2:b:467:ILE:HD11	14:b:1234:CLA:H12	1.87	0.57
2:b:592:ASN:HB2	14:b:1022:CLA:HBC2	1.87	0.57
1:A:392:THR:HG21	1:A:553:VAL:HB	1.86	0.56
2:B:445:ASP:OD1	2:B:623:LEU:N	2.37	0.56
2:B:453:ALA:HB3	6:F:40:ARG:HH22	1.70	0.56
3:C:61:ASP:HB3	5:E:52:ASN:ND2	2.20	0.56
1:a:460:PHE:HB3	14:a:1132:CLA:HBB2	1.86	0.56
1:a:557:VAL:HG11	1:a:560:MET:HG3	1.86	0.56
2:B:467:ILE:HD11	14:B:1234:CLA:H12	1.87	0.56
1:G:651:GLN:HB3	1:G:668:THR:HG23	1.87	0.56
2:H:468:GLN:NE2	14:H:1234:CLA:OBD	2.38	0.56
4:O:136:ARG:HD2	5:P:14:GLU:OE2	2.05	0.56
2:b:453:ALA:HB3	6:f:40:ARG:HH22	1.70	0.56
1:A:193:GLN:HE21	1:A:315:ARG:H	1.52	0.56
2:H:592:ASN:HB2	14:H:1022:CLA:HBC2	1.88	0.56
2:H:713:LEU:HD23	20:H:5002:LMG:H141	1.88	0.56
1:a:193:GLN:HE21	1:a:315:ARG:H	1.52	0.56
2:b:328:GLU:O	2:b:332:ASN:ND2	2.38	0.56
1:G:735:GLU:OE1	2:H:551:SER:OG	2.23	0.56
2:H:78:ILE:HD11	2:H:130:ARG:HD3	1.88	0.56
2:b:384:GLY:HA3	2:b:594:LEU:HD11	1.88	0.56
14:b:1023:CLA:H142	18:i:4018:BCR:H271	1.87	0.56
4:d:52:SER:OG	4:d:69:ARG:O	2.24	0.56
6:f:115:LYS:HZ1	6:f:120:ASP:HB2	1.70	0.56
3:C:17:CYS:HB3	17:C:3003:SF4:S4	2.45	0.56
1:G:392:THR:HG21	1:G:553:VAL:HB	1.86	0.56
12:W:79:THR:HG23	12:W:83:LEU:HD23	1.88	0.56
3:c:17:CYS:HB3	17:c:3003:SF4:S4	2.45	0.56
1:A:735:GLU:OE1	2:B:551:SER:OG	2.23	0.56
14:G:1113:CLA:HBB1	18:G:4001:BCR:H382	1.88	0.56
4:O:52:SER:OG	4:O:69:ARG:O	2.24	0.56
1:a:735:GLU:OE1	2:b:551:SER:OG	2.23	0.56
1:A:179:TYR:HB3	1:A:180:HIS:HD2	1.69	0.56
1:A:406:TRP:HD1	14:A:1126:CLA:HAB	1.66	0.56
2:B:384:GLY:HA3	2:B:594:LEU:HD11	1.88	0.56
2:H:467:ILE:HD11	14:H:1234:CLA:H12	1.87	0.56
1:a:306:MET:HG3	14:a:1115:CLA:H192	1.86	0.56
2:b:505:LEU:HA	2:b:508:ILE:HG22	1.88	0.56
4:d:131:ARG:HG3	4:d:131:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:384:GLY:HA3	2:H:594:LEU:HD11	1.88	0.55
2:b:713:LEU:HD23	20:b:5002:LMG:H141	1.88	0.55
2:B:68:VAL:HG21	2:B:124:TRP:CZ3	2.42	0.55
1:a:470:ASP:OD2	2:b:642:TYR:OH	2.18	0.55
14:a:1113:CLA:HBB1	18:a:4001:BCR:H382	1.88	0.55
14:H:1225:CLA:H202	18:H:4005:BCR:H352	1.89	0.55
3:N:17:CYS:HB3	17:N:3003:SF4:S4	2.45	0.55
2:B:257:PHE:HE2	2:B:500:TRP:HE3	1.54	0.55
1:G:58:ASP:OD2	1:G:360:HIS:NE2	2.37	0.55
4:O:131:ARG:HH11	4:O:131:ARG:HG3	1.71	0.55
1:a:568:ASP:HA	1:a:571:ILE:HG22	1.89	0.55
1:a:683:LEU:HD12	14:a:1012:CLA:HED1	1.88	0.55
2:b:78:ILE:HD11	2:b:130:ARG:HD3	1.87	0.55
2:b:257:PHE:HE2	2:b:500:TRP:HE3	1.54	0.55
2:B:468:GLN:NE2	14:B:1234:CLA:OBD	2.38	0.55
4:D:52:SER:OG	4:D:69:ARG:O	2.24	0.55
1:G:683:LEU:HD12	14:G:1012:CLA:HED1	1.88	0.55
1:G:274:PHE:HB3	1:G:278:LEU:HD12	1.89	0.55
14:A:1140:CLA:HAC1	16:A:2001:PQN:H161	1.89	0.55
2:B:78:ILE:HD11	2:B:130:ARG:HD3	1.88	0.55
4:D:131:ARG:HH11	4:D:131:ARG:HG3	1.71	0.55
14:G:1124:CLA:H12	14:G:1136:CLA:HBA1	1.89	0.55
2:H:257:PHE:HE2	2:H:500:TRP:HE3	1.54	0.55
4:d:48:ILE:HG21	4:d:86:LEU:HD23	1.89	0.55
2:b:445:ASP:OD1	2:b:623:LEU:N	2.37	0.55
14:A:1113:CLA:HBB1	18:A:4001:BCR:H382	1.88	0.55
2:B:592:ASN:HB2	14:B:1022:CLA:HBC2	1.87	0.55
2:B:713:LEU:HD23	20:B:5002:LMG:H141	1.88	0.55
14:B:1225:CLA:H202	18:B:4005:BCR:H352	1.89	0.55
2:H:50:HIS:HE1	14:H:1202:CLA:H121	1.72	0.55
2:H:68:VAL:HG21	2:H:124:TRP:CZ3	2.42	0.55
2:H:505:LEU:HA	2:H:508:ILE:HG22	1.88	0.55
2:b:68:VAL:HG21	2:b:124:TRP:CZ3	2.42	0.55
8:j:20:ALA:O	8:j:24:ILE:N	2.39	0.55
14:A:1124:CLA:H12	14:A:1136:CLA:HBA1	1.89	0.55
1:G:568:ASP:HA	1:G:571:ILE:HG22	1.89	0.54
2:H:700:ARG:NH1	7:R:44:GLU:OE2	2.40	0.54
1:A:470:ASP:OD2	2:B:642:TYR:OH	2.18	0.54
14:U:1501:CLA:H101	14:U:1503:CLA:H201	1.90	0.54
1:a:353:GLU:O	1:a:357:THR:OG1	2.23	0.54
2:b:50:HIS:HE1	14:b:1202:CLA:H121	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:LEU:HA	2:B:508:ILE:HG22	1.88	0.54
8:J:26:VAL:HA	8:J:29:ILE:HG12	1.90	0.54
12:X:79:THR:HG23	12:X:83:LEU:HD23	1.88	0.54
14:a:1132:CLA:HAC1	14:b:1206:CLA:HBB2	1.89	0.54
14:a:1140:CLA:H102	16:a:2001:PQN:H202	1.90	0.54
12:x:79:THR:HG23	12:x:83:LEU:HD23	1.88	0.54
1:G:218:VAL:HG13	1:G:238:PRO:HB3	1.90	0.54
1:G:265:PRO:HB3	1:G:273:HIS:HD2	1.73	0.54
2:b:555:PRO:HD2	3:c:62:PHE:CE1	2.43	0.54
8:j:26:VAL:HA	8:j:29:ILE:HG12	1.89	0.54
2:H:468:GLN:HG2	2:H:516:PHE:HD1	1.73	0.54
14:a:1124:CLA:H12	14:a:1136:CLA:HBA1	1.89	0.54
1:G:68:SER:OG	1:G:359:TRP:NE1	2.38	0.54
1:a:265:PRO:HB3	1:a:273:HIS:HD2	1.73	0.54
1:A:218:VAL:HG13	1:A:238:PRO:HB3	1.90	0.54
1:A:265:PRO:HB3	1:A:273:HIS:HD2	1.73	0.54
14:A:1140:CLA:H102	16:A:2001:PQN:H202	1.90	0.54
14:L:1501:CLA:H101	14:L:1503:CLA:H201	1.90	0.54
14:G:1140:CLA:H102	16:G:2001:PQN:H202	1.90	0.54
2:H:581:ASP:OD1	2:H:712:ARG:NH1	2.40	0.54
2:b:581:ASP:OD1	2:b:712:ARG:NH1	2.40	0.54
14:b:1225:CLA:H202	18:b:4005:BCR:H352	1.89	0.54
2:B:581:ASP:OD1	2:B:712:ARG:NH1	2.40	0.54
14:B:1205:CLA:HAB	14:B:1206:CLA:O1A	2.08	0.54
10:U:131:THR:HG22	10:U:133:GLU:N	2.21	0.54
2:b:396:ILE:HG23	2:b:400:LYS:HD2	1.89	0.54
4:D:48:ILE:HG21	4:D:86:LEU:HD23	1.89	0.54
2:b:230:TRP:HZ3	14:b:1213:CLA:H102	1.73	0.54
14:b:1205:CLA:HAB	14:b:1206:CLA:O1A	2.08	0.54
13:A:1011:CL0:H15	13:A:1011:CL0:H2	1.90	0.54
20:A:5005:LMG:H362	20:A:5005:LMG:H291	1.90	0.54
2:B:50:HIS:HE1	14:B:1202:CLA:H121	1.72	0.54
1:a:218:VAL:HG13	1:a:238:PRO:HB3	1.90	0.54
1:G:230:VAL:HB	1:G:234:ASP:HB2	1.90	0.53
13:G:1011:CL0:H15	13:G:1011:CL0:H2	1.90	0.53
14:G:1132:CLA:HAC1	14:H:1206:CLA:HBB2	1.89	0.53
2:b:468:GLN:HG2	2:b:516:PHE:HD1	1.73	0.53
1:A:230:VAL:HB	1:A:234:ASP:HB2	1.90	0.53
1:A:597:ARG:HD3	3:C:80:ALA:HB3	1.90	0.53
1:A:683:LEU:HD12	14:A:1012:CLA:HED1	1.88	0.53
2:B:256:THR:HA	14:B:1213:CLA:HED1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:256:THR:HA	14:H:1213:CLA:HED1	1.89	0.53
15:B:1207:F6C:CAB	7:I:26:PHE:HB3	2.38	0.53
1:A:568:ASP:HA	1:A:571:ILE:HG22	1.89	0.53
14:A:1136:CLA:H193	18:I:4020:BCR:H371	1.91	0.53
2:B:230:TRP:HZ3	14:B:1213:CLA:H102	1.73	0.53
2:B:468:GLN:HG2	2:B:516:PHE:HD1	1.73	0.53
1:G:733:LEU:HD21	14:G:1013:CLA:HED2	1.91	0.53
14:a:1140:CLA:HAC1	16:a:2001:PQN:H161	1.89	0.53
20:a:5005:LMG:H362	20:a:5005:LMG:H291	1.90	0.53
2:b:256:THR:HA	14:b:1213:CLA:HED1	1.89	0.53
7:i:37:LEU:HD21	18:l:4019:BCR:H312	1.90	0.53
14:A:1132:CLA:HAC1	14:B:1206:CLA:HBB2	1.89	0.53
2:B:622:TYR:OH	2:B:628:ARG:NH2	2.40	0.53
14:G:1140:CLA:HAC1	16:G:2001:PQN:H161	1.89	0.53
2:H:396:ILE:HG23	2:H:400:LYS:HD2	1.89	0.53
1:a:733:LEU:HD21	14:a:1013:CLA:HED2	1.91	0.53
2:H:230:TRP:HZ3	14:H:1213:CLA:H102	1.73	0.53
2:H:622:TYR:OH	2:H:628:ARG:NH2	2.40	0.53
8:S:26:VAL:HA	8:S:29:ILE:HG12	1.89	0.53
10:U:96:VAL:HG22	10:U:143:PHE:HE1	1.74	0.53
2:B:396:ILE:HG23	2:B:400:LYS:HD2	1.89	0.53
20:G:5005:LMG:H291	20:G:5005:LMG:H362	1.90	0.53
2:H:31:PHE:HA	2:H:34:HIS:CD2	2.44	0.53
4:O:48:ILE:HG21	4:O:86:LEU:HD23	1.89	0.53
1:a:287:VAL:HG13	1:a:288:THR:HG23	1.91	0.53
13:a:1011:CL0:H15	13:a:1011:CL0:H2	1.90	0.53
2:b:387:MET:HE1	18:b:4010:BCR:H361	1.91	0.53
2:b:469:SER:O	2:b:483:SER:OG	2.23	0.53
10:l:96:VAL:HG22	10:l:143:PHE:HE1	1.74	0.53
20:R:5006:LMG:H141	20:l:5007:LMG:H411	1.90	0.53
1:a:230:VAL:HB	1:a:234:ASP:HB2	1.90	0.53
2:b:31:PHE:HA	2:b:34:HIS:CD2	2.44	0.53
10:l:131:THR:HG22	10:l:133:GLU:N	2.21	0.53
1:G:287:VAL:HG13	1:G:288:THR:HG23	1.91	0.53
1:G:608:ARG:NH2	19:G:5001:LHG:O2	2.42	0.53
1:A:274:PHE:HB3	1:A:278:LEU:HD12	1.89	0.53
2:B:504:TRP:HD1	2:B:505:LEU:HD12	1.74	0.53
2:H:361:PRO:HG3	14:H:1215:CLA:HBA1	1.90	0.53
2:H:387:MET:HE1	18:H:4010:BCR:H361	1.91	0.53
2:H:504:TRP:HD1	2:H:505:LEU:HD12	1.75	0.53
10:L:96:VAL:HG22	10:L:143:PHE:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:274:PHE:HB3	1:a:278:LEU:HD12	1.89	0.52
14:l:1501:CLA:H101	14:l:1503:CLA:H201	1.90	0.52
1:A:733:LEU:HD21	14:A:1013:CLA:HED2	1.91	0.52
1:A:751:GLN:NE2	5:E:16:TYR:OH	2.41	0.52
14:A:1140:CLA:H112	16:A:2001:PQN:H222	1.91	0.52
1:A:287:VAL:HG13	1:A:288:THR:HG23	1.91	0.52
1:A:458:LEU:O	1:A:462:SER:OG	2.20	0.52
2:H:636:ALA:O	2:H:640:ASN:ND2	2.40	0.52
2:B:31:PHE:HA	2:B:34:HIS:CD2	2.44	0.52
2:B:208:GLY:H	2:B:211:ASN:HB3	1.75	0.52
2:B:361:PRO:HG3	14:B:1215:CLA:HBA1	1.90	0.52
14:H:1205:CLA:HAB	14:H:1206:CLA:O1A	2.08	0.52
8:S:20:ALA:O	8:S:24:ILE:N	2.40	0.52
2:b:636:ALA:O	2:b:640:ASN:ND2	2.40	0.52
10:L:131:THR:HG22	10:L:133:GLU:N	2.21	0.52
1:G:458:LEU:O	1:G:462:SER:OG	2.20	0.52
14:G:1140:CLA:H112	16:G:2001:PQN:H222	1.91	0.52
2:H:42:LEU:HD22	4:O:148:PHE:HZ	1.75	0.52
18:m:4021:BCR:H282	20:A:5005:LMG:H431	1.91	0.52
1:A:16:ASP:OD2	1:A:69:ARG:NH2	2.41	0.52
2:B:526:VAL:HG11	2:B:600:TYR:HB2	1.92	0.52
1:a:75:HIS:ND1	14:a:1111:CLA:OBD	2.43	0.52
2:b:361:PRO:HG3	14:b:1215:CLA:HBA1	1.90	0.52
2:b:526:VAL:HG11	2:b:600:TYR:HB2	1.92	0.52
2:b:622:TYR:OH	2:b:628:ARG:NH2	2.40	0.52
6:f:60:LEU:HD12	6:f:68:PRO:HB3	1.92	0.52
1:G:729:TYR:OH	14:G:1013:CLA:OBD	2.27	0.52
2:H:526:VAL:HG11	2:H:600:TYR:HB2	1.92	0.52
1:a:201:ALA:HB2	1:a:311:GLY:HA3	1.92	0.52
2:b:504:TRP:HD1	2:b:505:LEU:HD12	1.74	0.52
1:A:608:ARG:NH2	19:A:5001:LHG:O2	2.42	0.52
1:A:730:TRP:O	1:A:734:ILE:HG12	2.10	0.52
2:H:206:HIS:O	2:H:211:ASN:ND2	2.43	0.52
2:H:700:ARG:NH2	10:U:108:THR:O	2.43	0.52
1:A:199:HIS:ND1	14:A:1123:CLA:OBD	2.43	0.52
2:b:206:HIS:O	2:b:211:ASN:ND2	2.43	0.52
2:b:208:GLY:H	2:b:211:ASN:HB3	1.75	0.52
1:A:75:HIS:ND1	14:A:1111:CLA:OBD	2.43	0.52
2:B:206:HIS:O	2:B:211:ASN:ND2	2.43	0.52
2:B:700:ARG:NH2	10:L:108:THR:O	2.43	0.52
2:B:319:PHE:HB2	14:B:1220:CLA:HMA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:20:ALA:O	8:J:24:ILE:N	2.40	0.52
1:G:16:ASP:OD2	1:G:69:ARG:NH2	2.41	0.51
1:a:608:ARG:NH2	19:a:5001:LHG:O2	2.43	0.51
10:l:147:MET:SD	18:l:4022:BCR:H24C	2.51	0.51
1:A:737:ILE:HD13	14:A:1138:CLA:HMD2	1.92	0.51
2:B:387:MET:HE1	18:B:4010:BCR:H361	1.91	0.51
3:C:15:THR:HB	3:C:19:ARG:NH1	2.25	0.51
1:G:737:ILE:HD13	14:G:1138:CLA:HMD2	1.92	0.51
2:H:319:PHE:HB2	14:H:1220:CLA:HMA2	1.91	0.51
3:N:15:THR:HB	3:N:19:ARG:NH1	2.25	0.51
10:U:50:THR:HG23	10:U:53:MET:H	1.75	0.51
1:A:225:LEU:HD21	1:A:251:LEU:HD11	1.92	0.51
6:F:60:LEU:HD12	6:F:68:PRO:HB3	1.92	0.51
10:L:50:THR:HG23	10:L:53:MET:H	1.75	0.51
1:G:550:VAL:HG22	1:G:560:MET:HG2	1.92	0.51
1:G:730:TRP:O	1:G:734:ILE:HG12	2.10	0.51
1:a:716:PHE:O	1:a:719:SER:OG	2.27	0.51
1:a:737:ILE:HD13	14:a:1138:CLA:HMD2	1.92	0.51
10:l:50:THR:HG23	10:l:53:MET:H	1.75	0.51
1:G:423:MET:HE1	1:G:441:LEU:HD11	1.92	0.51
6:Q:60:LEU:HD12	6:Q:68:PRO:HB3	1.92	0.51
1:a:423:MET:HE1	1:a:441:LEU:HD11	1.92	0.51
1:A:423:MET:HE1	1:A:441:LEU:HD11	1.92	0.51
1:a:550:VAL:HG22	1:a:560:MET:HG2	1.92	0.51
1:a:730:TRP:O	1:a:734:ILE:HG12	2.10	0.51
14:a:1140:CLA:H112	16:a:2001:PQN:H222	1.91	0.51
20:U:5007:LMG:H322	20:I:5006:LMG:HC61	1.91	0.51
2:b:700:ARG:NH2	10:l:108:THR:O	2.43	0.51
2:B:673:THR:HG23	2:B:678:TRP:HE1	1.76	0.51
1:G:225:LEU:HD21	1:G:251:LEU:HD11	1.92	0.51
1:a:448:ILE:HG13	1:a:592:PHE:HE2	1.75	0.51
2:b:673:THR:HG23	2:b:678:TRP:HE1	1.76	0.51
14:H:1201:CLA:HBC1	20:H:5002:LMG:H201	1.93	0.51
1:a:225:LEU:HD21	1:a:251:LEU:HD11	1.92	0.51
14:a:1124:CLA:H8	18:a:4008:BCR:H392	1.93	0.51
2:b:236:ASN:OD1	2:b:252:THR:OG1	2.26	0.51
14:A:1124:CLA:H8	18:A:4008:BCR:H392	1.93	0.51
1:G:448:ILE:HG13	1:G:592:PHE:HE2	1.75	0.51
20:G:5005:LMG:H431	18:M:4021:BCR:H282	1.93	0.51
2:H:673:THR:HG23	2:H:678:TRP:HE1	1.76	0.51
2:B:236:ASN:OD1	2:B:252:THR:OG1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:636:ALA:O	2:B:640:ASN:ND2	2.40	0.51
2:H:208:GLY:H	2:H:211:ASN:HB3	1.75	0.51
1:a:751:GLN:NE2	5:e:16:TYR:OH	2.43	0.51
2:b:319:PHE:HB2	14:b:1220:CLA:HMA2	1.91	0.51
7:i:41:ILE:HG13	7:i:42:GLN:HG3	1.93	0.51
1:A:448:ILE:HG13	1:A:592:PHE:HE2	1.75	0.51
10:L:147:MET:SD	18:L:4022:BCR:H24C	2.51	0.51
1:G:505:ILE:HG21	1:G:541:PRO:HA	1.94	0.50
3:c:15:THR:HB	3:c:19:ARG:NH1	2.25	0.50
1:A:201:ALA:HB2	1:A:311:GLY:HA3	1.92	0.50
1:A:716:PHE:O	1:A:719:SER:OG	2.27	0.50
10:U:147:MET:SD	18:U:4022:BCR:H24C	2.50	0.50
2:B:398:TRP:HE1	18:B:4010:BCR:H271	1.76	0.50
7:I:41:ILE:HG13	7:I:42:GLN:HG3	1.93	0.50
18:I:4020:BCR:C20	14:L:1502:CLA:HAB	2.41	0.50
18:G:4001:BCR:HC8	9:T:74:PHE:HB2	1.93	0.50
2:B:403:ASP:HB3	4:D:144:SER:OG	2.12	0.50
1:G:411:LEU:HD11	14:G:1104:CLA:H142	1.94	0.50
14:H:1216:CLA:HBA1	14:H:1221:CLA:C3B	2.42	0.50
1:a:737:ILE:O	1:a:741:HIS:ND1	2.39	0.50
1:G:199:HIS:ND1	14:G:1123:CLA:OBD	2.43	0.50
7:R:41:ILE:HG13	7:R:42:GLN:HG3	1.93	0.50
10:U:151:ILE:HG13	18:U:4022:BCR:H291	1.93	0.50
1:a:16:ASP:OD2	1:a:69:ARG:NH2	2.41	0.50
2:b:652:VAL:HG21	14:b:1205:CLA:HAC1	1.94	0.50
14:L:1501:CLA:H202	14:L:1503:CLA:H142	1.94	0.50
2:H:398:TRP:HE1	18:H:4010:BCR:H271	1.76	0.50
10:U:103:SER:HB3	10:U:139:ASN:ND2	2.27	0.50
1:a:505:ILE:HG21	1:a:541:PRO:HA	1.94	0.50
2:B:498:ASN:HB3	2:B:501:LEU:HB2	1.94	0.50
1:G:14:VAL:HG13	1:G:185:LYS:HB2	1.94	0.50
1:G:201:ALA:HB2	1:G:311:GLY:HA3	1.92	0.50
2:H:469:SER:O	2:H:483:SER:OG	2.23	0.50
2:H:498:ASN:HB3	2:H:501:LEU:HB2	1.94	0.50
12:W:87:ALA:O	12:W:91:ILE:HG13	2.12	0.50
2:b:498:ASN:HB3	2:b:501:LEU:HB2	1.94	0.50
2:b:567:ASP:OD1	3:c:66:ARG:NH2	2.42	0.50
1:A:505:ILE:HG21	1:A:541:PRO:HA	1.94	0.50
1:A:729:TYR:OH	14:A:1013:CLA:OBD	2.27	0.50
14:B:1216:CLA:HBA1	14:B:1221:CLA:C3B	2.42	0.50
2:b:132:ASN:HD22	11:m:2:SER:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:1216:CLA:HBA1	14:b:1221:CLA:C3B	2.42	0.50
3:c:19:ARG:HH11	3:c:19:ARG:HG3	1.77	0.50
4:d:80:LYS:HE2	4:d:84:ILE:HD11	1.94	0.50
1:A:411:LEU:HD11	14:A:1104:CLA:H142	1.94	0.50
1:A:417:ALA:O	1:A:421:ILE:HG13	2.12	0.50
1:A:550:VAL:HG22	1:A:560:MET:HG2	1.92	0.50
14:B:1201:CLA:HBC1	20:B:5002:LMG:H201	1.93	0.50
4:D:80:LYS:HE2	4:D:84:ILE:HD11	1.93	0.50
1:G:417:ALA:O	1:G:421:ILE:HG13	2.12	0.50
19:H:5004:LHG:H362	14:W:1701:CLA:HBC1	1.92	0.50
4:O:91:ARG:HG2	4:O:96:THR:HG22	1.94	0.50
10:l:103:SER:HB3	10:l:139:ASN:ND2	2.27	0.50
1:A:14:VAL:HG13	1:A:185:LYS:HB2	1.94	0.50
14:L:1501:CLA:HBA2	14:L:1503:CLA:H172	1.93	0.50
3:N:19:ARG:HH11	3:N:19:ARG:HG3	1.77	0.49
4:O:80:LYS:HE2	4:O:84:ILE:HD11	1.93	0.49
2:b:403:ASP:HB3	4:d:144:SER:OG	2.12	0.49
8:J:27:ILE:HG13	8:J:28:LEU:HD12	1.94	0.49
2:H:652:VAL:HG21	14:H:1205:CLA:HAC1	1.94	0.49
3:C:19:ARG:HH11	3:C:19:ARG:HG3	1.77	0.49
12:X:87:ALA:O	12:X:91:ILE:HG13	2.12	0.49
1:G:353:GLU:O	1:G:357:THR:OG1	2.23	0.49
4:d:91:ARG:HG2	4:d:96:THR:HG22	1.94	0.49
2:b:461:PRO:HG2	2:b:519:ILE:HG22	1.95	0.49
14:b:1021:CLA:H18	14:b:1022:CLA:HMB3	1.95	0.49
6:f:72:LEU:HB3	14:x:1701:CLA:H12	1.94	0.49
12:x:87:ALA:O	12:x:91:ILE:HG13	2.12	0.49
2:B:461:PRO:HG2	2:B:519:ILE:HG22	1.95	0.49
2:H:157:LEU:O	2:H:162:ARG:NH2	2.45	0.49
1:a:14:VAL:HG13	1:a:185:LYS:HB2	1.94	0.49
1:a:417:ALA:O	1:a:421:ILE:HG13	2.12	0.49
14:l:1501:CLA:HBA2	14:l:1503:CLA:H172	1.93	0.49
1:A:616:ARG:HA	3:C:77:MET:HA	1.95	0.49
18:A:4001:BCR:HC8	9:K:74:PHE:HB2	1.93	0.49
2:B:652:VAL:HG21	14:B:1205:CLA:HAC1	1.94	0.49
10:L:103:SER:HB3	10:L:139:ASN:ND2	2.27	0.49
4:O:60:MET:HG3	4:O:62:THR:H	1.77	0.49
1:a:199:HIS:ND1	14:a:1123:CLA:OBD	2.43	0.49
1:a:411:LEU:HD11	14:a:1104:CLA:H142	1.94	0.49
2:b:157:LEU:O	2:b:162:ARG:NH2	2.45	0.49
2:b:398:TRP:HE1	18:b:4010:BCR:H271	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:1205:CLA:HBB1	14:b:1205:CLA:HMB1	1.95	0.49
8:j:30:VAL:HG13	8:j:34:LEU:HD23	1.94	0.49
14:B:1205:CLA:HMB1	14:B:1205:CLA:HBB1	1.95	0.49
10:L:102:ILE:HD11	10:L:139:ASN:HA	1.94	0.49
2:H:387:MET:HA	2:H:387:MET:HE3	1.95	0.49
14:H:1223:CLA:H2	18:H:4010:BCR:H14C	1.95	0.49
10:U:147:MET:HB3	18:U:4022:BCR:H393	1.94	0.49
14:U:1501:CLA:H202	14:U:1503:CLA:H142	1.94	0.49
14:U:1501:CLA:HBA2	14:U:1503:CLA:H172	1.93	0.49
4:d:60:MET:HG3	4:d:62:THR:H	1.77	0.49
9:k:37:UNK:O	9:k:41:UNK:N	2.46	0.49
10:l:43:PRO:HG3	14:l:1502:CLA:HED2	1.95	0.49
10:l:102:ILE:HD11	10:l:139:ASN:HA	1.94	0.49
2:B:222:LEU:HG	14:B:1212:CLA:HBD	1.95	0.49
2:B:257:PHE:CE2	2:B:500:TRP:HB3	2.48	0.49
14:B:1227:CLA:HAB	14:B:1236:CLA:HBB2	1.95	0.49
4:D:91:ARG:HG2	4:D:96:THR:HG22	1.94	0.49
9:K:37:UNK:O	9:K:41:UNK:N	2.46	0.49
20:G:5005:LMG:H412	18:M:4021:BCR:H281	1.95	0.49
2:H:690:GLU:HG2	2:H:698:TYR:HE1	1.78	0.49
1:a:256:ASP:HB3	1:a:262:GLY:HA2	1.95	0.49
1:a:400:LEU:HD11	14:a:1127:CLA:HED3	1.95	0.49
2:b:257:PHE:CE2	2:b:500:TRP:HB3	2.48	0.49
14:b:1205:CLA:H91	14:b:1224:CLA:H202	1.94	0.49
14:b:1217:CLA:HBB1	14:b:1217:CLA:H8	1.95	0.49
2:B:530:ILE:HG21	14:B:1234:CLA:HAB	1.95	0.49
14:G:1124:CLA:H8	18:G:4008:BCR:H392	1.93	0.49
10:U:43:PRO:HG3	14:U:1502:CLA:HED2	1.95	0.49
2:b:387:MET:HE3	2:b:387:MET:HA	1.95	0.49
14:b:1223:CLA:H2	18:b:4010:BCR:H14C	1.95	0.49
10:l:147:MET:HB3	18:l:4022:BCR:H393	1.94	0.49
14:B:1021:CLA:H18	14:B:1022:CLA:HMB3	1.95	0.49
18:B:4009:BCR:H402	18:B:4010:BCR:H383	1.95	0.49
4:D:60:MET:HG3	4:D:62:THR:H	1.77	0.49
7:I:35:ALA:HB1	10:L:104:ILE:HG21	1.94	0.49
13:G:1011:CL0:H10	13:G:1011:CL0:H72	1.62	0.48
2:H:111:ASN:HD22	7:R:10:GLY:HA2	1.78	0.48
14:H:1217:CLA:H8	14:H:1217:CLA:HBB1	1.95	0.48
14:a:1140:CLA:H41	14:a:1140:CLA:H62	1.57	0.48
14:l:1501:CLA:H202	14:l:1503:CLA:H142	1.94	0.48
1:A:737:ILE:O	1:A:741:HIS:ND1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:PHE:HZ	2:B:412:LEU:HD21	1.78	0.48
1:G:75:HIS:ND1	14:G:1111:CLA:OBD	2.43	0.48
14:G:1131:CLA:H91	16:H:2002:PQN:H221	1.95	0.48
2:H:236:ASN:OD1	2:H:252:THR:OG1	2.26	0.48
14:H:1205:CLA:H91	14:H:1224:CLA:H202	1.95	0.48
1:a:729:TYR:OH	14:a:1013:CLA:OBD	2.27	0.48
2:b:397:PHE:HZ	2:b:412:LEU:HD21	1.78	0.48
10:l:151:ILE:HG13	18:l:4022:BCR:H291	1.93	0.48
6:F:72:LEU:HB3	14:X:1701:CLA:H12	1.95	0.48
10:L:43:PRO:HG3	14:L:1502:CLA:HED2	1.95	0.48
1:G:400:LEU:HD11	14:G:1127:CLA:HED3	1.95	0.48
1:G:716:PHE:O	1:G:719:SER:OG	2.27	0.48
2:H:461:PRO:HG2	2:H:519:ILE:HG22	1.95	0.48
2:H:530:ILE:HG21	14:H:1234:CLA:HAB	1.95	0.48
5:P:10:ILE:HG22	5:P:12:ARG:H	1.79	0.48
10:U:159:ASN:HB3	10:L:85:LEU:HD22	1.95	0.48
10:U:170:ALA:HB2	7:I:7:GLN:HG2	1.95	0.48
2:b:530:ILE:HG21	14:b:1234:CLA:HAB	1.95	0.48
14:b:1204:CLA:H111	14:b:1204:CLA:H72	1.65	0.48
18:H:4009:BCR:H402	18:H:4010:BCR:H383	1.95	0.48
14:b:1201:CLA:HBC1	20:b:5002:LMG:H201	1.93	0.48
14:A:1115:CLA:H92	14:A:1115:CLA:H61	1.71	0.48
14:A:1116:CLA:H62	14:A:1116:CLA:H41	1.57	0.48
8:J:30:VAL:HG13	8:J:34:LEU:HD23	1.94	0.48
14:G:1109:CLA:H91	14:G:1109:CLA:H111	1.62	0.48
2:H:397:PHE:HZ	2:H:412:LEU:HD21	1.78	0.48
14:H:1215:CLA:HBA2	14:H:1215:CLA:H3A	1.59	0.48
8:S:30:VAL:HG13	8:S:34:LEU:HD23	1.94	0.48
9:T:37:UNK:O	9:T:41:UNK:N	2.46	0.48
8:j:27:ILE:HG13	8:j:28:LEU:HD12	1.94	0.48
1:A:400:LEU:HD11	14:A:1127:CLA:HED3	1.95	0.48
14:B:1203:CLA:H43	20:B:5002:LMG:H302	1.96	0.48
10:L:151:ILE:HG13	18:L:4022:BCR:H291	1.93	0.48
2:H:72:GLY:HA2	2:H:87:ILE:HB	1.96	0.48
14:H:1204:CLA:H72	14:H:1204:CLA:H111	1.65	0.48
14:H:1225:CLA:H3A	14:H:1225:CLA:HBA2	1.51	0.48
4:d:56:GLN:O	4:d:68:MET:HG2	2.14	0.48
14:B:1205:CLA:H43	14:B:1224:CLA:H11	1.96	0.48
14:B:1217:CLA:HBB1	14:B:1217:CLA:H8	1.95	0.48
14:G:1125:CLA:H162	14:G:1125:CLA:H141	1.72	0.48
2:H:222:LEU:HG	14:H:1212:CLA:HBD	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:257:PHE:CE2	2:H:500:TRP:HB3	2.48	0.48
8:S:27:ILE:HG13	8:S:28:LEU:HD12	1.94	0.48
2:b:222:LEU:HG	14:b:1212:CLA:HBD	1.95	0.48
14:b:1227:CLA:HAB	14:b:1236:CLA:HBB2	1.95	0.48
18:l:4022:BCR:H351	18:l:4022:BCR:H15C	1.61	0.48
1:A:68:SER:OG	1:A:359:TRP:NE1	2.38	0.48
2:B:690:GLU:HG2	2:B:698:TYR:HE1	1.78	0.48
18:B:4010:BCR:H24C	18:B:4010:BCR:H371	1.65	0.48
10:L:147:MET:HB3	18:L:4022:BCR:H393	1.94	0.48
14:b:1208:CLA:H201	14:b:1211:CLA:H191	1.96	0.48
6:f:115:LYS:NZ	6:f:120:ASP:HB2	2.28	0.48
14:A:1131:CLA:HMA2	18:I:4018:BCR:H272	1.96	0.48
2:B:72:GLY:HA2	2:B:87:ILE:HB	1.96	0.48
14:B:1021:CLA:H112	14:B:1021:CLA:H151	1.44	0.48
4:D:56:GLN:O	4:D:68:MET:HG2	2.14	0.48
2:H:182:LEU:HG	14:H:1210:CLA:H43	1.96	0.48
2:H:322:PRO:HB2	2:H:410:ASN:HA	1.96	0.48
14:H:1205:CLA:HMB1	14:H:1205:CLA:HBB1	1.95	0.48
4:O:56:GLN:O	4:O:68:MET:HG2	2.14	0.48
1:A:483:SER:HB2	1:A:486:GLY:H	1.79	0.48
14:A:1104:CLA:H193	14:A:1104:CLA:H161	1.72	0.48
18:A:4007:BCR:H351	18:A:4007:BCR:H15C	1.64	0.48
2:B:387:MET:HA	2:B:387:MET:HE3	1.95	0.48
14:B:1223:CLA:H2	18:B:4010:BCR:H14C	1.95	0.48
14:G:1115:CLA:H193	14:G:1115:CLA:H162	1.75	0.48
14:H:1227:CLA:HAB	14:H:1236:CLA:HBB2	1.95	0.48
6:Q:112:ALA:HA	6:Q:115:LYS:HB2	1.96	0.48
18:b:4017:BCR:H351	18:b:4017:BCR:H15C	1.59	0.48
14:A:1138:CLA:HBA2	2:B:428:TRP:CD1	2.49	0.48
2:B:132:ASN:HD22	11:M:2:SER:HA	1.78	0.48
2:B:157:LEU:O	2:B:162:ARG:NH2	2.45	0.48
2:B:469:SER:O	2:B:483:SER:OG	2.23	0.48
5:E:10:ILE:HG22	5:E:12:ARG:H	1.79	0.48
6:F:115:LYS:NZ	6:F:120:ASP:HB2	2.28	0.48
12:X:99:ILE:HG22	12:X:100:ILE:HG23	1.96	0.48
1:G:445:ASP:H	4:O:33:THR:HG21	1.78	0.47
14:G:1119:CLA:H72	14:G:1119:CLA:H112	1.65	0.47
2:b:322:PRO:HB2	2:b:410:ASN:HA	1.96	0.47
14:b:1205:CLA:H112	14:b:1224:CLA:H161	1.95	0.47
20:i:5006:LMG:HC61	20:L:5007:LMG:H322	1.96	0.47
12:x:99:ILE:HG22	12:x:100:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1117:CLA:HBA2	14:A:1117:CLA:H3A	1.60	0.47
14:A:1120:CLA:HBA2	14:A:1120:CLA:H3A	1.51	0.47
14:B:1205:CLA:H91	14:B:1224:CLA:H202	1.95	0.47
14:B:1215:CLA:HBA2	14:B:1215:CLA:H3A	1.59	0.47
14:B:1231:CLA:H42	14:B:1232:CLA:HBA1	1.95	0.47
14:H:1021:CLA:H18	14:H:1022:CLA:HMB3	1.95	0.47
14:H:1231:CLA:H42	14:H:1232:CLA:HBA1	1.95	0.47
14:a:1131:CLA:H91	16:b:2002:PQN:H221	1.95	0.47
2:b:72:GLY:HA2	2:b:87:ILE:HB	1.96	0.47
1:A:256:ASP:HB3	1:A:262:GLY:HA2	1.95	0.47
1:A:610:PRO:HB3	1:A:757:ILE:HB	1.97	0.47
14:G:1138:CLA:HBA2	2:H:428:TRP:CD1	2.49	0.47
10:U:102:ILE:HD11	10:U:139:ASN:HA	1.94	0.47
2:b:237:PRO:HB3	2:b:256:THR:HG21	1.96	0.47
14:b:1205:CLA:H43	14:b:1224:CLA:H11	1.95	0.47
14:b:1231:CLA:H42	14:b:1232:CLA:HBA1	1.95	0.47
1:A:353:GLU:O	1:A:357:THR:OG1	2.23	0.47
14:B:1205:CLA:H112	14:B:1224:CLA:H161	1.95	0.47
14:B:1208:CLA:H201	14:B:1211:CLA:H191	1.96	0.47
14:G:1116:CLA:H3A	14:G:1116:CLA:HBA2	1.48	0.47
14:G:1131:CLA:H143	16:H:2002:PQN:H191	1.97	0.47
2:H:56:ILE:HD11	18:V:4021:BCR:HC7	1.97	0.47
2:H:441:TYR:CE2	2:H:525:TYR:HB3	2.50	0.47
18:R:4020:BCR:HC41	10:U:93:TYR:CD1	2.49	0.47
14:b:1217:CLA:H3A	14:b:1217:CLA:HBA2	1.49	0.47
18:b:4009:BCR:H402	18:b:4010:BCR:H383	1.95	0.47
14:l:1502:CLA:HAC2	18:l:4019:BCR:H393	1.97	0.47
1:A:493:PHE:HZ	20:A:5005:LMG:H401	1.80	0.47
14:A:1109:CLA:H61	14:A:1109:CLA:H41	1.56	0.47
14:A:1131:CLA:H91	16:B:2002:PQN:H221	1.95	0.47
1:G:612:ASP:OD2	3:N:53:ARG:NH2	2.40	0.47
2:H:347:VAL:HG13	14:H:1222:CLA:HED1	1.97	0.47
14:H:1021:CLA:H203	14:H:1021:CLA:H161	1.77	0.47
14:a:1138:CLA:HBA2	2:b:428:TRP:CD1	2.49	0.47
2:b:347:VAL:HG13	14:b:1222:CLA:HED1	1.97	0.47
2:b:441:TYR:CE2	2:b:525:TYR:HB3	2.50	0.47
6:f:115:LYS:HZ3	6:f:115:LYS:HA	1.79	0.47
1:A:439:ARG:O	1:A:443:HIS:ND1	2.44	0.47
2:B:20:ARG:NH1	7:I:41:ILE:O	2.46	0.47
2:B:347:VAL:HG13	14:B:1222:CLA:HED1	1.96	0.47
14:L:1502:CLA:HAC2	18:L:4019:BCR:H393	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:ASP:HB3	1:G:262:GLY:HA2	1.95	0.47
1:a:402:THR:HG23	1:a:643:ILE:HG21	1.97	0.47
1:a:483:SER:HB2	1:a:486:GLY:H	1.79	0.47
14:B:1227:CLA:HMC2	18:B:4009:BCR:H281	1.97	0.47
1:G:483:SER:HB2	1:G:486:GLY:H	1.79	0.47
14:H:1021:CLA:H112	14:H:1021:CLA:H151	1.45	0.47
14:H:1203:CLA:H43	20:H:5002:LMG:H302	1.96	0.47
14:H:1205:CLA:H112	14:H:1224:CLA:H161	1.95	0.47
5:P:33:SER:O	5:P:34:ARG:HG2	2.15	0.47
7:R:35:ALA:HB1	10:U:104:ILE:HG21	1.97	0.47
1:a:68:SER:OG	1:a:359:TRP:NE1	2.38	0.47
1:a:194:SER:O	1:a:198:HIS:ND1	2.39	0.47
1:a:302:ALA:HB2	14:a:1116:CLA:HAB	1.97	0.47
14:b:1021:CLA:H203	14:b:1021:CLA:H161	1.77	0.47
5:e:33:SER:O	5:e:34:ARG:HG2	2.14	0.47
6:f:112:ALA:HA	6:f:115:LYS:HB2	1.96	0.47
2:B:56:ILE:HD11	18:M:4021:BCR:HC7	1.96	0.47
14:B:1216:CLA:H3A	14:B:1216:CLA:HBA2	1.55	0.47
14:B:1228:CLA:H93	14:B:1228:CLA:H62	1.79	0.47
7:I:44:GLU:HG2	10:L:111:GLN:OE1	2.15	0.47
14:L:1503:CLA:H141	14:L:1503:CLA:H162	1.65	0.47
1:G:381:MET:HE1	14:G:1127:CLA:O1D	2.15	0.47
20:G:5005:LMG:H351	20:G:5005:LMG:H321	1.61	0.47
1:a:598:LEU:HD21	2:b:679:GLN:HG2	1.97	0.47
2:b:295:TRP:O	2:b:297:ILE:HG22	2.14	0.47
2:b:690:GLU:HG2	2:b:698:TYR:HE1	1.78	0.47
6:f:31:CYS:HB2	6:f:58:SER:HA	1.97	0.47
18:i:4018:BCR:H371	18:i:4018:BCR:H24C	1.71	0.47
2:B:441:TYR:CE2	2:B:525:TYR:HB3	2.50	0.47
6:F:112:ALA:HA	6:F:115:LYS:HB2	1.95	0.47
1:G:493:PHE:HZ	20:G:5005:LMG:H401	1.79	0.47
1:G:610:PRO:HB3	1:G:757:ILE:HB	1.96	0.47
14:G:1136:CLA:H111	14:G:1137:CLA:HBC1	1.97	0.47
18:U:4022:BCR:H24C	18:U:4022:BCR:H371	1.69	0.47
18:a:4001:BCR:HC8	9:k:74:PHE:HB2	1.95	0.47
18:b:4009:BCR:H351	18:b:4009:BCR:H15C	1.53	0.47
5:e:10:ILE:HG22	5:e:12:ARG:H	1.79	0.47
13:A:1011:CL0:H10	13:A:1011:CL0:H72	1.62	0.47
2:B:237:PRO:HB3	2:B:256:THR:HG21	1.96	0.47
2:B:664:TRP:CD2	14:B:1021:CLA:HMA2	2.50	0.47
14:B:1210:CLA:H142	14:B:1210:CLA:H112	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:ALA:HB2	14:G:1116:CLA:HAB	1.97	0.47
1:G:402:THR:HG23	1:G:643:ILE:HG21	1.97	0.47
1:G:598:LEU:HD21	2:H:679:GLN:HG2	1.96	0.47
2:H:92:TRP:HB3	7:R:22:ILE:HG13	1.97	0.47
14:H:1235:CLA:H41	14:H:1235:CLA:H62	1.72	0.47
1:a:308:ILE:O	1:a:312:HIS:ND1	2.48	0.47
1:a:493:PHE:HZ	20:a:5005:LMG:H401	1.80	0.47
1:a:597:ARG:HD3	3:c:80:ALA:HB3	1.97	0.47
2:b:77:TRP:HA	2:b:84:VAL:HG11	1.97	0.47
4:d:131:ARG:HG3	4:d:131:ARG:NH1	2.30	0.47
7:i:19:TRP:CE3	20:L:5007:LMG:H361	2.50	0.47
1:A:568:ASP:OD2	1:A:649:LYS:NZ	2.34	0.47
1:A:598:LEU:HD21	2:B:679:GLN:HG2	1.96	0.47
14:A:1131:CLA:H143	16:B:2002:PQN:H191	1.97	0.47
14:B:1204:CLA:HED2	7:I:18:PRO:HB3	1.97	0.47
2:H:664:TRP:CD2	14:H:1021:CLA:HMA2	2.50	0.46
14:H:1225:CLA:H112	18:H:4005:BCR:H19C	1.98	0.46
1:a:126:ASN:HB3	1:a:134:HIS:HB3	1.97	0.46
1:a:722:PHE:HA	16:a:2001:PQN:H9	1.96	0.46
14:a:1106:CLA:HBA2	14:a:1106:CLA:H3A	1.32	0.46
14:a:1109:CLA:H41	14:a:1109:CLA:H61	1.56	0.46
14:b:1203:CLA:H43	20:b:5002:LMG:H302	1.96	0.46
1:A:302:ALA:HB2	14:A:1116:CLA:HAB	1.97	0.46
2:B:322:PRO:HB2	2:B:410:ASN:HA	1.96	0.46
6:F:31:CYS:HB2	6:F:58:SER:HA	1.97	0.46
1:G:720:LEU:HB2	14:G:1013:CLA:HMC2	1.98	0.46
14:G:1140:CLA:H62	14:G:1140:CLA:H41	1.57	0.46
14:H:1204:CLA:HBC2	11:V:12:LEU:HD23	1.96	0.46
15:H:1238:F6C:CAB	16:H:2002:PQN:H141	2.45	0.46
18:H:4009:BCR:H351	18:H:4009:BCR:H15C	1.53	0.46
2:b:182:LEU:HG	14:b:1210:CLA:H43	1.96	0.46
14:A:1125:CLA:H141	14:A:1125:CLA:H162	1.72	0.46
14:A:1126:CLA:H62	14:A:1126:CLA:H41	1.73	0.46
16:A:2001:PQN:H243	16:A:2001:PQN:H261	1.73	0.46
2:B:182:LEU:HG	14:B:1210:CLA:H43	1.96	0.46
18:B:4006:BCR:H351	18:B:4006:BCR:H15C	1.68	0.46
18:B:4014:BCR:H371	18:B:4014:BCR:H24C	1.68	0.46
1:G:608:ARG:HG2	1:G:758:ILE:HG21	1.97	0.46
18:G:4003:BCR:H351	18:G:4003:BCR:H15C	1.68	0.46
2:H:295:TRP:O	2:H:297:ILE:HG22	2.15	0.46
14:H:1205:CLA:H43	14:H:1224:CLA:H11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:610:PRO:HB3	1:a:757:ILE:HB	1.97	0.46
2:b:176:ASN:ND2	2:b:291:TYR:O	2.44	0.46
14:b:1203:CLA:H112	14:b:1203:CLA:H152	1.47	0.46
14:b:1211:CLA:H12	14:b:1211:CLA:H51	1.70	0.46
15:b:1238:F6C:CAB	16:b:2002:PQN:H141	2.45	0.46
1:A:308:ILE:O	1:A:312:HIS:ND1	2.48	0.46
1:A:381:MET:HE1	14:A:1127:CLA:O1D	2.15	0.46
18:B:4017:BCR:H15C	18:B:4017:BCR:H351	1.59	0.46
4:D:131:ARG:HG3	4:D:131:ARG:NH1	2.30	0.46
14:G:1111:CLA:H71	14:G:1111:CLA:H112	1.74	0.46
14:H:1211:CLA:H51	14:H:1211:CLA:H12	1.70	0.46
4:O:131:ARG:HG3	4:O:131:ARG:NH1	2.30	0.46
14:U:1502:CLA:HAC2	18:U:4019:BCR:H393	1.97	0.46
1:a:720:LEU:HB2	14:a:1013:CLA:HMC2	1.98	0.46
14:a:1120:CLA:H3A	14:a:1120:CLA:HBA2	1.51	0.46
18:b:4014:BCR:H343	6:f:88:PHE:HD1	1.81	0.46
14:l:1503:CLA:H141	14:l:1503:CLA:H162	1.66	0.46
1:A:402:THR:HG23	1:A:643:ILE:HG21	1.97	0.46
2:B:77:TRP:HA	2:B:84:VAL:HG11	1.97	0.46
2:B:106:GLN:HG3	2:B:115:ILE:HD11	1.97	0.46
14:B:1219:CLA:HBC3	18:B:4009:BCR:H323	1.98	0.46
14:B:1225:CLA:HBA2	14:B:1225:CLA:H3A	1.51	0.46
1:G:117:TRP:CE2	18:H:4013:BCR:HC41	2.51	0.46
1:G:731:GLN:NE2	1:G:754:ALA:H	2.14	0.46
1:G:774:VAL:HG22	18:G:4011:BCR:HC21	1.98	0.46
14:G:1115:CLA:H71	14:G:1115:CLA:H112	1.76	0.46
14:G:1135:CLA:H3A	14:G:1135:CLA:HBA1	1.46	0.46
14:H:1227:CLA:HMC2	18:H:4009:BCR:H281	1.97	0.46
14:a:1106:CLA:H93	14:a:1106:CLA:H61	1.75	0.46
14:b:1228:CLA:H42	6:f:142:LEU:HD22	1.98	0.46
2:B:172:GLU:HG3	2:B:301:ILE:HD12	1.98	0.46
2:B:638:LEU:HD22	2:B:730:PHE:HA	1.98	0.46
15:B:1238:F6C:CAB	16:B:2002:PQN:H141	2.45	0.46
2:H:194:LEU:HA	2:H:198:ALA:HB3	1.98	0.46
2:H:237:PRO:HB3	2:H:256:THR:HG21	1.96	0.46
14:H:1219:CLA:HBC3	18:H:4009:BCR:H323	1.98	0.46
14:H:1228:CLA:H42	6:Q:142:LEU:HD22	1.98	0.46
12:W:99:ILE:HG22	12:W:100:ILE:HG23	1.96	0.46
14:a:1122:CLA:H62	14:a:1122:CLA:H41	1.69	0.46
2:b:29:HIS:HB2	14:b:1226:CLA:HBA1	1.97	0.46
1:A:126:ASN:HB3	1:A:134:HIS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLN:NE2	1:A:495:GLN:HE22	2.14	0.46
1:A:722:PHE:HA	16:A:2001:PQN:H9	1.96	0.46
18:A:4008:BCR:H24C	18:A:4008:BCR:H371	1.75	0.46
2:B:295:TRP:O	2:B:297:ILE:HG22	2.15	0.46
14:B:1214:CLA:H112	14:B:1214:CLA:H71	1.68	0.46
2:H:391:PHE:HB3	2:H:541:LEU:HB3	1.98	0.46
3:N:61:ASP:HB3	5:P:52:ASN:ND2	2.31	0.46
6:Q:100:ARG:CZ	6:Q:104:GLN:HE22	2.29	0.46
1:a:117:TRP:CE2	18:b:4013:BCR:HC41	2.51	0.46
1:a:439:ARG:O	1:a:443:HIS:ND1	2.44	0.46
1:a:608:ARG:HG2	1:a:758:ILE:HG21	1.97	0.46
14:a:1124:CLA:HBA2	14:a:1124:CLA:H3A	1.58	0.46
14:a:1136:CLA:H102	14:a:1136:CLA:H61	1.82	0.46
2:b:172:GLU:HG3	2:b:301:ILE:HD12	1.98	0.46
2:b:391:PHE:HB3	2:b:541:LEU:HB3	1.98	0.46
2:b:664:TRP:CD2	14:b:1021:CLA:HMA2	2.50	0.46
4:d:32:SER:OG	4:d:33:THR:N	2.49	0.46
6:f:91:THR:HA	6:f:94:PHE:HB3	1.98	0.46
1:A:120:PHE:CE2	8:J:31:LEU:HD22	2.51	0.46
1:A:193:GLN:NE2	1:A:323:SER:HA	2.31	0.46
14:B:1229:CLA:HBB1	14:B:1229:CLA:HMB3	1.98	0.46
14:B:1235:CLA:H91	14:B:1235:CLA:H111	1.77	0.46
5:E:33:SER:O	5:E:34:ARG:HG2	2.14	0.46
14:L:1503:CLA:H41	14:L:1503:CLA:H61	1.68	0.46
1:G:126:ASN:HB3	1:G:134:HIS:HB3	1.97	0.46
1:G:722:PHE:HA	16:G:2001:PQN:H9	1.97	0.46
2:H:37:MET:HE2	2:H:37:MET:HB2	1.81	0.46
1:a:193:GLN:NE2	1:a:323:SER:HA	2.31	0.46
14:a:1131:CLA:H143	16:b:2002:PQN:H191	1.97	0.46
14:a:1136:CLA:H111	14:a:1137:CLA:HBC1	1.97	0.46
8:j:26:VAL:O	8:j:30:VAL:N	2.43	0.46
14:A:1136:CLA:H111	14:A:1137:CLA:HBC1	1.97	0.46
2:B:176:ASN:ND2	2:B:291:TYR:O	2.44	0.46
14:B:1222:CLA:HED2	14:B:1223:CLA:HBD	1.98	0.46
1:G:117:TRP:CZ3	18:H:4013:BCR:HC8	2.51	0.46
1:G:439:ARG:O	1:G:443:HIS:ND1	2.44	0.46
14:G:1112:CLA:H61	14:G:1112:CLA:H2	1.64	0.46
14:H:1208:CLA:H201	14:H:1211:CLA:H191	1.96	0.46
14:H:1236:CLA:HBC2	14:W:1701:CLA:HBC3	1.98	0.46
1:a:381:MET:HE1	14:a:1127:CLA:O1D	2.15	0.46
14:a:1135:CLA:H112	14:a:1135:CLA:H142	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:194:LEU:HA	2:b:198:ALA:HB3	1.98	0.46
14:b:1208:CLA:H202	14:b:1208:CLA:H161	1.79	0.46
1:A:608:ARG:HG2	1:A:758:ILE:HG21	1.97	0.46
1:A:714:PHE:CD2	18:A:4011:BCR:H363	2.51	0.46
14:A:1128:CLA:H61	14:A:1128:CLA:H41	1.79	0.46
18:A:4008:BCR:H15C	18:A:4008:BCR:H351	1.65	0.46
2:B:179:LEU:HD21	14:B:1216:CLA:C3B	2.46	0.46
18:I:4020:BCR:C19	14:L:1502:CLA:HAB	2.45	0.46
14:G:1013:CLA:CGA	14:G:1013:CLA:H3A	2.46	0.46
2:H:179:LEU:HD21	14:H:1216:CLA:C3B	2.46	0.46
1:a:117:TRP:CZ3	18:b:4013:BCR:HC8	2.51	0.46
1:a:200:LEU:HD23	1:a:200:LEU:HA	1.75	0.46
2:b:56:ILE:HD11	18:m:4021:BCR:HC7	1.97	0.46
2:b:638:LEU:HD22	2:b:730:PHE:HA	1.98	0.46
14:b:1225:CLA:H112	18:b:4005:BCR:H19C	1.98	0.46
6:f:100:ARG:CZ	6:f:104:GLN:HE22	2.29	0.46
8:j:31:LEU:O	8:j:31:LEU:HD23	2.16	0.46
1:A:117:TRP:CZ3	18:B:4013:BCR:HC8	2.51	0.46
14:A:1111:CLA:H112	14:A:1111:CLA:H71	1.74	0.46
18:G:4008:BCR:H351	18:G:4008:BCR:H15C	1.65	0.45
14:H:1206:CLA:HMB1	14:H:1206:CLA:HBB1	1.98	0.45
14:H:1222:CLA:HED2	14:H:1223:CLA:HBD	1.98	0.45
6:Q:91:THR:HA	6:Q:94:PHE:HB3	1.98	0.45
1:a:97:SER:HB2	1:a:143:PHE:HZ	1.80	0.45
1:a:442:ARG:HG2	4:d:32:SER:HA	1.98	0.45
18:a:4007:BCR:H15C	18:a:4007:BCR:H351	1.64	0.45
2:b:106:GLN:HG3	2:b:115:ILE:HD11	1.97	0.45
2:b:179:LEU:HD21	14:b:1216:CLA:C3B	2.46	0.45
18:m:4021:BCR:H281	20:A:5005:LMG:H412	1.98	0.45
14:B:1217:CLA:H3A	14:B:1217:CLA:HBA2	1.49	0.45
2:H:77:TRP:HA	2:H:84:VAL:HG11	1.97	0.45
2:H:172:GLU:HG3	2:H:301:ILE:HD12	1.98	0.45
14:a:1116:CLA:H62	14:a:1116:CLA:H41	1.57	0.45
14:a:1138:CLA:H91	14:a:1138:CLA:H111	1.77	0.45
14:b:1227:CLA:HMC2	18:b:4009:BCR:H281	1.97	0.45
14:l:1503:CLA:H41	14:l:1503:CLA:H61	1.68	0.45
1:A:720:LEU:HB2	14:A:1013:CLA:HMC2	1.98	0.45
2:B:29:HIS:HB2	14:B:1226:CLA:HBA1	1.98	0.45
2:B:391:PHE:HB3	2:B:541:LEU:HB3	1.98	0.45
2:B:727:TYR:HB2	14:B:1021:CLA:HED3	1.98	0.45
14:B:1225:CLA:H112	18:B:4005:BCR:H19C	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:4014:BCR:H343	6:F:88:PHE:HD1	1.81	0.45
6:F:91:THR:HA	6:F:94:PHE:HB3	1.98	0.45
1:G:714:PHE:CD2	18:G:4011:BCR:H363	2.51	0.45
1:G:718:PHE:HZ	14:G:1140:CLA:HBC2	1.82	0.45
18:G:4002:BCR:H351	18:G:4002:BCR:H15C	1.67	0.45
18:G:4007:BCR:H351	18:G:4007:BCR:H15C	1.64	0.45
2:H:29:HIS:HB2	14:H:1226:CLA:HBA1	1.97	0.45
2:H:727:TYR:HB2	14:H:1021:CLA:HED3	1.98	0.45
14:H:1224:CLA:H11	14:H:1224:CLA:H51	1.64	0.45
6:Q:31:CYS:HB2	6:Q:58:SER:HA	1.97	0.45
8:S:31:LEU:HD23	8:S:31:LEU:O	2.16	0.45
14:U:1503:CLA:H141	14:U:1503:CLA:H162	1.66	0.45
11:V:9:TYR:HB3	18:V:4021:BCR:H401	1.99	0.45
1:A:97:SER:HB2	1:A:143:PHE:HZ	1.80	0.45
14:B:1216:CLA:H162	14:B:1216:CLA:H122	1.34	0.45
18:B:4009:BCR:H24C	18:B:4009:BCR:H371	1.73	0.45
1:G:308:ILE:O	1:G:312:HIS:ND1	2.48	0.45
14:G:1124:CLA:HAB	18:G:4008:BCR:C8	2.47	0.45
14:G:1131:CLA:HAA1	18:R:4020:BCR:C17	2.46	0.45
2:H:638:LEU:HD22	2:H:730:PHE:HA	1.98	0.45
18:H:4014:BCR:H343	6:Q:88:PHE:HD1	1.81	0.45
6:Q:81:VAL:O	6:Q:85:ILE:HD13	2.17	0.45
1:a:377:ILE:HD13	14:a:1127:CLA:HHD	1.98	0.45
1:a:406:TRP:HB3	14:a:1126:CLA:HMC2	1.98	0.45
1:a:480:ASP:HB3	14:a:1132:CLA:CED	2.47	0.45
1:a:594:ARG:HH21	4:d:59:GLU:CD	2.24	0.45
14:a:1112:CLA:H2	14:a:1112:CLA:H61	1.64	0.45
14:a:1115:CLA:HBD	14:a:1115:CLA:HBA1	1.99	0.45
2:b:667:SER:HB3	2:b:718:HIS:HB2	1.99	0.45
14:b:1219:CLA:HBC3	18:b:4009:BCR:H323	1.98	0.45
18:b:4006:BCR:H351	18:b:4006:BCR:H15C	1.68	0.45
1:A:594:ARG:HH21	4:D:59:GLU:CD	2.24	0.45
14:A:1102:CLA:HBB1	14:A:1102:CLA:HMB1	1.99	0.45
14:A:1135:CLA:H3A	14:A:1135:CLA:HBA1	1.46	0.45
14:A:1140:CLA:HBA2	14:A:1140:CLA:H3A	1.64	0.45
14:B:1222:CLA:H11	14:B:1222:CLA:H52	1.85	0.45
4:D:38:LYS:NZ	10:L:122:SER:O	2.50	0.45
1:G:120:PHE:CE2	8:S:31:LEU:HD22	2.51	0.45
2:H:68:VAL:HG23	2:H:135:LEU:HD13	1.99	0.45
2:H:106:GLN:HG3	2:H:115:ILE:HD11	1.97	0.45
14:b:1213:CLA:H41	14:b:1213:CLA:H61	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:1222:CLA:HED2	14:b:1223:CLA:HBD	1.98	0.45
1:A:422:TYR:CD1	1:A:426:ASP:HB2	2.52	0.45
1:A:731:GLN:NE2	1:A:754:ALA:H	2.14	0.45
20:A:5005:LMG:H321	20:A:5005:LMG:H351	1.61	0.45
2:B:42:LEU:O	2:B:46:ILE:HG12	2.17	0.45
1:G:193:GLN:NE2	1:G:323:SER:HA	2.31	0.45
1:G:393:ASP:OD2	1:G:396:THR:OG1	2.28	0.45
1:G:541:PRO:HG2	1:G:544:TYR:HE1	1.82	0.45
14:G:1122:CLA:H41	14:G:1122:CLA:H62	1.69	0.45
18:H:4017:BCR:H351	18:H:4017:BCR:H15C	1.59	0.45
4:O:38:LYS:NZ	10:U:124:ASP:HB2	2.31	0.45
7:R:21:MET:HA	7:R:24:LEU:HB2	1.98	0.45
1:a:120:PHE:CE2	8:j:31:LEU:HD22	2.51	0.45
1:a:541:PRO:HG2	1:a:544:TYR:CE1	2.52	0.45
2:b:167:TRP:CE2	14:b:1210:CLA:HAC2	2.52	0.45
2:b:375:LEU:HD11	14:b:1225:CLA:HED3	1.99	0.45
14:b:1222:CLA:H93	14:b:1222:CLA:H61	1.79	0.45
1:A:82:VAL:HG11	14:A:1103:CLA:H41	1.99	0.45
1:A:280:PHE:HE2	14:A:1134:CLA:HED1	1.82	0.45
14:B:1219:CLA:H3A	14:B:1219:CLA:HBA2	1.71	0.45
14:B:1228:CLA:H42	6:F:142:LEU:HD22	1.98	0.45
8:J:31:LEU:HD23	8:J:31:LEU:O	2.16	0.45
1:G:541:PRO:HG2	1:G:544:TYR:CE1	2.52	0.45
14:G:1117:CLA:HBA2	14:G:1117:CLA:H3A	1.60	0.45
14:G:1126:CLA:H41	14:G:1126:CLA:H62	1.73	0.45
2:H:42:LEU:O	2:H:46:ILE:HG12	2.17	0.45
14:a:1102:CLA:HBB1	14:a:1102:CLA:HMB1	1.99	0.45
2:b:500:TRP:CD1	14:b:1231:CLA:HED1	2.52	0.45
14:b:1227:CLA:H3A	14:b:1227:CLA:HBA2	1.48	0.45
14:b:1228:CLA:H93	14:b:1228:CLA:H62	1.79	0.45
4:d:38:LYS:NZ	10:l:122:SER:O	2.50	0.45
6:f:81:VAL:O	6:f:85:ILE:HD13	2.17	0.45
1:A:117:TRP:CE2	18:B:4013:BCR:HC41	2.51	0.45
1:A:377:ILE:HD13	14:A:1127:CLA:HHD	1.98	0.45
1:A:707:LEU:HD12	14:A:1107:CLA:HAC1	1.99	0.45
1:A:708:MET:HG3	1:A:777:TRP:HZ3	1.82	0.45
2:B:694:LEU:HB2	18:I:4020:BCR:H282	1.99	0.45
14:B:1210:CLA:H202	14:B:1210:CLA:H162	1.77	0.45
14:B:1224:CLA:H11	14:B:1224:CLA:H51	1.64	0.45
6:F:100:ARG:CZ	6:F:104:GLN:HE22	2.29	0.45
7:I:21:MET:HA	7:I:24:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:TYR:CD1	1:G:426:ASP:HB2	2.52	0.45
1:G:480:ASP:HB3	14:G:1132:CLA:CED	2.47	0.45
1:G:490:GLN:NE2	1:G:495:GLN:HE22	2.14	0.45
1:G:505:ILE:HD13	1:G:541:PRO:HB3	1.99	0.45
14:H:1221:CLA:H71	14:H:1223:CLA:H42	1.99	0.45
14:H:1229:CLA:HMB3	14:H:1229:CLA:HBB1	1.98	0.45
18:R:4020:BCR:H312	18:R:4020:BCR:HC32	1.77	0.45
1:a:422:TYR:CD1	1:a:426:ASP:HB2	2.52	0.45
2:b:11:ASP:HB2	3:c:71:ALA:HB2	1.98	0.45
2:b:42:LEU:O	2:b:46:ILE:HG12	2.17	0.45
14:b:1216:CLA:H62	14:b:1216:CLA:H41	1.74	0.45
18:b:4004:BCR:H15C	18:b:4004:BCR:H351	1.69	0.45
11:m:9:TYR:HB3	18:m:4021:BCR:H401	1.99	0.45
1:A:480:ASP:OD1	1:A:480:ASP:N	2.50	0.45
14:A:1118:CLA:H41	14:A:1118:CLA:H62	1.84	0.45
14:A:1119:CLA:H112	14:A:1119:CLA:H72	1.65	0.45
14:A:1124:CLA:HAB	18:A:4008:BCR:C8	2.47	0.45
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.98	0.45
2:B:500:TRP:CD1	14:B:1231:CLA:HED1	2.52	0.45
14:B:1021:CLA:H141	14:B:1021:CLA:H162	1.74	0.45
14:B:1211:CLA:H93	18:B:4006:BCR:H362	1.99	0.45
14:B:1222:CLA:HBA2	14:B:1222:CLA:H3A	1.63	0.45
18:I:4020:BCR:H351	18:I:4020:BCR:H15C	1.63	0.45
1:G:82:VAL:HG11	14:G:1103:CLA:H41	1.99	0.45
1:G:97:SER:HB2	1:G:143:PHE:HZ	1.80	0.45
1:G:419:ALA:O	1:G:423:MET:HG2	2.17	0.45
14:G:1115:CLA:HBD	14:G:1115:CLA:HBA1	1.99	0.45
14:G:1124:CLA:HBA2	14:G:1124:CLA:H3A	1.58	0.45
16:G:2001:PQN:H292	8:S:17:ALA:HB1	1.99	0.45
2:H:176:ASN:ND2	2:H:291:TYR:O	2.44	0.45
2:H:375:LEU:HD11	14:H:1225:CLA:HED3	1.99	0.45
14:H:1210:CLA:H171	14:H:1215:CLA:HBB2	1.99	0.45
14:a:1124:CLA:HAB	18:a:4008:BCR:C8	2.47	0.45
14:b:1221:CLA:H61	14:b:1221:CLA:H2	1.65	0.45
14:b:1222:CLA:H72	14:b:1234:CLA:H92	1.99	0.45
14:b:1229:CLA:HBB1	14:b:1229:CLA:HMB3	1.98	0.45
1:A:442:ARG:HG2	4:D:32:SER:HA	1.98	0.45
1:A:487:ILE:HD11	14:A:1132:CLA:HED1	1.99	0.45
1:A:541:PRO:HG2	1:A:544:TYR:CE1	2.52	0.45
1:A:716:PHE:CG	13:A:1011:CL0:H5	2.52	0.45
14:A:1109:CLA:H91	14:A:1109:CLA:H111	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:1116:CLA:HBA2	14:A:1116:CLA:H3A	1.48	0.45
14:A:1135:CLA:H12	14:A:1135:CLA:H51	1.82	0.45
2:B:669:MET:HE1	14:B:1239:CLA:HBC3	1.99	0.45
14:B:1206:CLA:HBB1	14:B:1206:CLA:HMB1	1.99	0.45
1:G:13:VAL:HG11	14:G:1108:CLA:HAA2	1.99	0.45
1:G:323:SER:OG	1:G:326:GLU:HG3	2.18	0.45
1:a:505:ILE:HD13	1:a:541:PRO:HB3	1.99	0.45
1:a:541:PRO:HG2	1:a:544:TYR:HE1	1.82	0.45
1:a:714:PHE:CD2	18:a:4011:BCR:H363	2.51	0.45
1:a:718:PHE:HZ	14:a:1140:CLA:HBC2	1.82	0.45
14:a:1013:CLA:CGA	14:a:1013:CLA:H3A	2.46	0.45
1:G:67:ILE:O	1:G:71:ILE:HG12	2.17	0.44
1:G:716:PHE:CG	13:G:1011:CL0:H5	2.52	0.44
14:G:1102:CLA:HMB1	14:G:1102:CLA:HBB1	1.99	0.44
14:G:1109:CLA:H61	14:G:1109:CLA:H41	1.55	0.44
14:G:1138:CLA:H91	14:G:1138:CLA:H111	1.77	0.44
14:H:1216:CLA:HBA2	14:H:1216:CLA:H3A	1.55	0.44
15:H:1230:F6C:O1D	8:S:37:GLY:HA2	2.17	0.44
4:O:100:ILE:HD12	4:O:113:HIS:CD2	2.52	0.44
10:U:122:SER:HB3	10:U:130:ARG:NH1	2.32	0.44
1:a:13:VAL:HG11	14:a:1108:CLA:HAA2	1.99	0.44
1:a:160:THR:HG23	18:a:4002:BCR:H312	1.99	0.44
1:a:487:ILE:HD11	14:a:1132:CLA:HED1	1.99	0.44
14:b:1210:CLA:H171	14:b:1215:CLA:HBB2	1.99	0.44
14:b:1235:CLA:H91	14:b:1235:CLA:H111	1.77	0.44
10:l:122:SER:HB3	10:l:130:ARG:NH1	2.32	0.44
2:B:4:LYS:HE3	2:B:4:LYS:HB3	1.83	0.44
2:B:167:TRP:CE2	14:B:1210:CLA:HAC2	2.52	0.44
14:B:1227:CLA:H3A	14:B:1227:CLA:HBA2	1.48	0.44
4:D:100:ILE:HD12	4:D:113:HIS:CD2	2.53	0.44
14:H:1234:CLA:H202	12:W:86:LEU:HG	1.98	0.44
10:U:147:MET:HG3	18:U:4022:BCR:H382	2.00	0.44
1:a:323:SER:OG	1:a:326:GLU:HG3	2.17	0.44
14:a:1140:CLA:H141	14:a:1140:CLA:H161	1.71	0.44
2:b:68:VAL:HG23	2:b:135:LEU:HD13	1.99	0.44
2:b:322:PRO:O	2:b:411:VAL:N	2.50	0.44
2:b:601:TRP:CD1	14:b:1234:CLA:HBC2	2.53	0.44
14:b:1206:CLA:HBA2	14:b:1206:CLA:H3A	1.60	0.44
14:b:1229:CLA:H93	14:b:1229:CLA:H112	1.80	0.44
4:d:29:PHE:HZ	4:d:32:SER:HB2	1.83	0.44
6:f:141:GLU:HB3	6:f:147:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASP:HB3	14:A:1132:CLA:CED	2.47	0.44
1:A:718:PHE:HZ	14:A:1140:CLA:HBC2	1.81	0.44
1:A:774:VAL:HG22	18:A:4011:BCR:HC21	1.98	0.44
14:A:1115:CLA:HBD	14:A:1115:CLA:HBA1	1.99	0.44
2:B:631:LEU:O	2:B:635:SER:OG	2.22	0.44
14:B:1221:CLA:H61	14:B:1221:CLA:H2	1.65	0.44
4:D:29:PHE:HZ	4:D:32:SER:HB2	1.83	0.44
14:G:1120:CLA:HBA2	14:G:1120:CLA:H3A	1.51	0.44
2:H:557:LYS:HE2	2:H:577:ILE:HG12	1.99	0.44
14:H:1221:CLA:H141	14:H:1221:CLA:H162	1.75	0.44
6:Q:53:PRO:HB3	8:S:37:GLY:HA3	2.00	0.44
6:Q:141:GLU:HB3	6:Q:147:LEU:HB2	2.00	0.44
14:b:1206:CLA:HBB1	14:b:1206:CLA:HMB1	1.99	0.44
5:e:12:ARG:HG2	5:e:14:GLU:HG2	2.00	0.44
6:f:53:PRO:HB3	8:j:37:GLY:HA3	2.00	0.44
1:A:541:PRO:HG2	1:A:544:TYR:HE1	1.82	0.44
2:B:432:PHE:CE2	14:B:1235:CLA:HAB	2.53	0.44
15:B:1230:F6C:O1D	8:J:37:GLY:HA2	2.17	0.44
6:F:81:VAL:O	6:F:85:ILE:HD13	2.17	0.44
1:G:360:HIS:CD2	14:G:1103:CLA:HBC1	2.53	0.44
1:G:708:MET:HG3	1:G:777:TRP:HZ3	1.82	0.44
14:G:1013:CLA:H92	14:G:1013:CLA:H61	1.74	0.44
2:H:167:TRP:CE2	14:H:1210:CLA:HAC2	2.52	0.44
14:H:1222:CLA:H72	14:H:1234:CLA:H92	1.99	0.44
4:O:32:SER:OG	4:O:33:THR:N	2.49	0.44
1:a:67:ILE:O	1:a:71:ILE:HG12	2.17	0.44
1:a:359:TRP:HB3	14:a:1103:CLA:HAC1	2.00	0.44
1:a:360:HIS:CD2	14:a:1103:CLA:HBC1	2.53	0.44
1:a:419:ALA:O	1:a:423:MET:HG2	2.17	0.44
1:a:458:LEU:O	1:a:462:SER:OG	2.20	0.44
1:a:490:GLN:NE2	1:a:495:GLN:HE22	2.14	0.44
1:a:774:VAL:HG22	18:a:4011:BCR:HC21	1.98	0.44
14:a:1135:CLA:H3A	14:a:1135:CLA:HBA1	1.46	0.44
14:b:1021:CLA:H112	14:b:1021:CLA:H151	1.45	0.44
14:b:1021:CLA:H141	14:b:1021:CLA:H162	1.74	0.44
15:b:1230:F6C:O1D	8:j:37:GLY:HA2	2.17	0.44
4:d:38:LYS:NZ	10:l:124:ASP:HB2	2.33	0.44
7:i:21:MET:HA	7:i:24:LEU:HB2	1.98	0.44
7:i:44:GLU:HG2	10:l:111:GLN:OE1	2.16	0.44
1:A:406:TRP:HB3	14:A:1126:CLA:HMC2	1.98	0.44
14:A:1138:CLA:H91	14:A:1138:CLA:H111	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:HIS:HE1	14:B:1234:CLA:HBC1	1.82	0.44
14:B:1210:CLA:H171	14:B:1215:CLA:HBB2	1.99	0.44
14:B:1222:CLA:H91	14:B:1222:CLA:H111	1.80	0.44
10:L:147:MET:HG3	18:L:4022:BCR:H382	2.00	0.44
1:G:487:ILE:HD11	14:G:1132:CLA:HED1	1.99	0.44
2:H:500:TRP:CD1	14:H:1231:CLA:HED1	2.52	0.44
14:H:1214:CLA:H71	14:H:1214:CLA:H112	1.68	0.44
4:O:29:PHE:HZ	4:O:32:SER:HB2	1.83	0.44
18:a:4008:BCR:H351	18:a:4008:BCR:H15C	1.65	0.44
2:b:468:GLN:HG2	2:b:516:PHE:CD1	2.51	0.44
5:e:34:ARG:HE	5:e:34:ARG:HB3	1.57	0.44
1:A:67:ILE:O	1:A:71:ILE:HG12	2.17	0.44
1:A:193:GLN:HG3	1:A:314:TYR:HB3	2.00	0.44
1:A:419:ALA:O	1:A:423:MET:HG2	2.17	0.44
2:B:362:TYR:OH	14:B:1225:CLA:OBD	2.29	0.44
2:B:667:SER:HB3	2:B:718:HIS:HB2	1.99	0.44
14:G:1104:CLA:H161	14:G:1104:CLA:H193	1.72	0.44
10:U:41:ASN:HB3	14:U:1501:CLA:HAC1	2.00	0.44
1:a:310:ALA:HB2	14:a:1119:CLA:HBC2	2.00	0.44
1:a:707:LEU:HD12	14:a:1107:CLA:HAC1	1.99	0.44
1:a:731:GLN:NE2	1:a:754:ALA:H	2.14	0.44
14:a:1103:CLA:H42	18:a:4003:BCR:H272	2.00	0.44
14:a:1138:CLA:HBA2	2:b:428:TRP:HD1	1.83	0.44
2:b:669:MET:HE1	14:b:1239:CLA:HBC3	1.99	0.44
2:b:727:TYR:HB2	14:b:1021:CLA:HED3	1.98	0.44
14:b:1203:CLA:HMA3	14:b:1203:CLA:H52	2.00	0.44
14:b:1221:CLA:H162	14:b:1221:CLA:H141	1.75	0.44
18:b:4010:BCR:H371	18:b:4010:BCR:H24C	1.65	0.44
2:B:601:TRP:CD1	14:B:1234:CLA:HBC2	2.53	0.44
2:B:624:MET:O	2:B:628:ARG:N	2.44	0.44
14:B:1222:CLA:H72	14:B:1234:CLA:H92	1.99	0.44
6:F:141:GLU:HB3	6:F:147:LEU:HB2	2.00	0.44
12:X:96:TYR:CG	14:X:1701:CLA:HED1	2.53	0.44
1:G:359:TRP:HB3	14:G:1103:CLA:HAC1	2.00	0.44
1:G:377:ILE:HD13	14:G:1127:CLA:HHD	1.98	0.44
1:G:480:ASP:OD1	1:G:480:ASP:N	2.50	0.44
2:H:601:TRP:CD1	14:H:1234:CLA:HBC2	2.53	0.44
18:H:4013:BCR:H371	18:H:4013:BCR:H24C	1.78	0.44
1:a:716:PHE:CG	13:a:1011:CL0:H5	2.52	0.44
2:b:460:GLU:OE1	6:f:69:ARG:HD3	2.18	0.44
14:b:1229:CLA:H62	14:b:1229:CLA:H41	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:74:ARG:HD2	12:x:97:PHE:HB3	1.98	0.44
1:A:13:VAL:HG11	14:A:1108:CLA:HAA2	1.99	0.44
1:A:359:TRP:HB3	14:A:1103:CLA:HAC1	2.00	0.44
1:A:360:HIS:CD2	14:A:1103:CLA:HBC1	2.53	0.44
14:A:1112:CLA:H61	14:A:1112:CLA:H2	1.64	0.44
2:B:375:LEU:HD11	14:B:1225:CLA:HED3	1.99	0.44
2:B:557:LYS:HE2	2:B:577:ILE:HG12	1.99	0.44
14:B:1203:CLA:HMA3	14:B:1203:CLA:H52	2.00	0.44
14:B:1204:CLA:H111	14:B:1204:CLA:H72	1.65	0.44
1:G:280:PHE:HE2	14:G:1134:CLA:HED1	1.82	0.44
1:G:310:ALA:HB2	14:G:1119:CLA:HBC2	2.00	0.44
2:H:322:PRO:O	2:H:411:VAL:N	2.50	0.44
2:H:432:PHE:CE2	14:H:1235:CLA:HAB	2.53	0.44
14:H:1023:CLA:HMB3	14:H:1023:CLA:H52	2.00	0.44
12:W:96:TYR:CG	14:W:1701:CLA:HED1	2.53	0.44
1:a:82:VAL:HG11	14:a:1103:CLA:H41	1.99	0.44
1:a:616:ARG:HA	3:c:77:MET:HA	1.99	0.44
2:b:266:GLN:HG3	2:b:367:LYS:NZ	2.33	0.44
5:e:18:PHE:O	6:f:155:PRO:HA	2.17	0.44
10:l:41:ASN:HB3	14:l:1501:CLA:HAC1	2.00	0.44
1:A:684:ARG:NH2	2:B:644:PRO:HD3	2.33	0.44
16:A:2001:PQN:H292	8:J:17:ALA:HB1	1.99	0.44
18:A:4001:BCR:H353	9:K:73:ALA:HB1	2.00	0.44
2:B:322:PRO:O	2:B:411:VAL:N	2.50	0.44
2:B:551:SER:OG	2:B:552:LYS:N	2.51	0.44
14:B:1022:CLA:H61	14:B:1022:CLA:H41	1.59	0.44
6:F:54:LEU:HA	6:F:57:TYR:CD1	2.49	0.44
1:G:237:LEU:HD23	1:G:237:LEU:HA	1.88	0.44
1:G:684:ARG:NH2	2:H:644:PRO:HD3	2.32	0.44
1:G:707:LEU:HD12	14:G:1107:CLA:HAC1	1.99	0.44
14:H:1211:CLA:H93	18:H:4006:BCR:H362	1.99	0.44
14:H:1229:CLA:H93	14:H:1229:CLA:H112	1.80	0.44
1:a:32:HIS:HA	1:a:38:ALA:HB2	2.00	0.44
1:a:193:GLN:HG3	1:a:314:TYR:HB3	2.00	0.44
14:a:1118:CLA:H41	14:a:1118:CLA:H62	1.84	0.44
16:a:2001:PQN:H292	8:j:17:ALA:HB1	1.99	0.44
18:a:4008:BCR:H371	18:a:4008:BCR:H24C	1.75	0.44
14:b:1022:CLA:H61	14:b:1022:CLA:H41	1.59	0.44
4:d:100:ILE:HD12	4:d:113:HIS:CD2	2.52	0.44
10:l:64:TYR:CD1	10:l:153:ALA:HB2	2.53	0.44
11:m:10:ILE:HD11	21:A:6001:LMT:H72	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:HG23	18:A:4002:BCR:H312	1.99	0.44
1:A:194:SER:O	1:A:198:HIS:ND1	2.39	0.44
2:B:610:GLN:NE2	2:B:738:LYS:HG2	2.33	0.44
14:B:1239:CLA:H203	14:B:1239:CLA:H161	1.77	0.44
4:D:32:SER:OG	4:D:33:THR:N	2.49	0.44
10:L:122:SER:HB3	10:L:130:ARG:NH1	2.32	0.44
11:M:9:TYR:HB3	18:M:4021:BCR:H401	1.99	0.44
14:G:1136:CLA:H102	14:G:1136:CLA:H61	1.82	0.43
2:H:334:LEU:HD23	2:H:334:LEU:HA	1.82	0.43
2:H:551:SER:OG	2:H:552:LYS:N	2.51	0.43
2:H:605:HIS:HE1	14:H:1234:CLA:HBC1	1.82	0.43
14:H:1204:CLA:H72	18:R:4018:BCR:HC31	2.00	0.43
1:a:280:PHE:HE2	14:a:1134:CLA:HED1	1.82	0.43
14:a:1104:CLA:H161	14:a:1104:CLA:H193	1.72	0.43
14:a:1111:CLA:HBA2	14:a:1111:CLA:H12	1.79	0.43
14:a:1115:CLA:H71	14:a:1115:CLA:H112	1.76	0.43
14:a:1136:CLA:H41	14:a:1136:CLA:H62	1.50	0.43
14:b:1023:CLA:H202	14:b:1023:CLA:H162	1.82	0.43
4:d:29:PHE:CZ	4:d:32:SER:HB2	2.53	0.43
6:f:54:LEU:HA	6:f:57:TYR:CD1	2.49	0.43
1:A:323:SER:OG	1:A:326:GLU:HG3	2.17	0.43
1:A:714:PHE:CG	18:A:4011:BCR:H363	2.53	0.43
14:A:1117:CLA:H62	14:A:1117:CLA:H2	1.73	0.43
2:B:68:VAL:HG23	2:B:135:LEU:HD13	1.99	0.43
6:F:121:VAL:HG23	6:F:122:PRO:HD3	2.00	0.43
18:G:4002:BCR:H24C	18:G:4002:BCR:H371	1.82	0.43
2:H:266:GLN:HG3	2:H:367:LYS:NZ	2.33	0.43
2:H:610:GLN:NE2	2:H:738:LYS:HG2	2.33	0.43
14:H:1203:CLA:H193	14:H:1203:CLA:H161	1.74	0.43
5:P:12:ARG:HG2	5:P:14:GLU:HG2	1.99	0.43
1:a:684:ARG:NH2	2:b:644:PRO:HD3	2.33	0.43
1:a:714:PHE:CG	18:a:4011:BCR:H363	2.54	0.43
14:a:1120:CLA:C3D	18:a:4001:BCR:H312	2.48	0.43
14:b:1211:CLA:H93	18:b:4006:BCR:H362	1.99	0.43
5:e:12:ARG:HD2	5:e:15:SER:HB2	2.00	0.43
6:f:121:VAL:HG23	6:f:122:PRO:HD3	2.00	0.43
10:l:85:LEU:HD22	10:L:159:ASN:HB3	2.00	0.43
10:l:147:MET:HG3	18:l:4022:BCR:H382	2.00	0.43
14:A:1111:CLA:H12	14:A:1111:CLA:HBA2	1.79	0.43
14:A:1115:CLA:H112	14:A:1115:CLA:H71	1.76	0.43
2:B:460:GLU:OE1	6:F:69:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ARG:HG2	5:E:14:GLU:HG2	1.99	0.43
6:F:53:PRO:HB3	8:J:37:GLY:HA3	2.00	0.43
18:I:4018:BCR:H371	18:I:4018:BCR:H24C	1.71	0.43
10:L:41:ASN:HB3	14:L:1501:CLA:HAC1	2.00	0.43
1:G:347:GLY:O	1:G:436:VAL:N	2.52	0.43
18:G:4008:BCR:H371	18:G:4008:BCR:H24C	1.75	0.43
18:H:4010:BCR:H24C	18:H:4010:BCR:H371	1.65	0.43
4:O:29:PHE:CZ	4:O:32:SER:HB2	2.53	0.43
10:U:64:TYR:CD1	10:U:153:ALA:HB2	2.53	0.43
1:a:200:LEU:HD21	14:a:1119:CLA:C3B	2.49	0.43
1:a:708:MET:HG3	1:a:777:TRP:HZ3	1.82	0.43
13:a:1011:CL0:H72	13:a:1011:CL0:H10	1.62	0.43
14:a:1131:CLA:HMD2	14:a:1136:CLA:H141	2.00	0.43
2:b:86:PRO:HB3	2:b:121:TYR:CG	2.54	0.43
2:b:174:ARG:HB3	14:b:1221:CLA:HMD1	2.00	0.43
12:x:96:TYR:CG	14:x:1701:CLA:HED1	2.53	0.43
1:A:505:ILE:HD13	1:A:541:PRO:HB3	1.99	0.43
1:A:734:ILE:HG22	1:A:738:VAL:HG23	2.01	0.43
14:A:1013:CLA:CGA	14:A:1013:CLA:H3A	2.46	0.43
14:B:1201:CLA:HMA3	11:M:29:LEU:HD13	2.01	0.43
14:B:1221:CLA:H71	14:B:1223:CLA:H42	1.99	0.43
14:B:1229:CLA:H62	14:B:1229:CLA:H41	1.76	0.43
10:L:64:TYR:CD1	10:L:153:ALA:HB2	2.53	0.43
1:G:193:GLN:HG3	1:G:314:TYR:HB3	2.00	0.43
1:G:737:ILE:O	1:G:741:HIS:ND1	2.39	0.43
14:G:1013:CLA:H91	14:G:1013:CLA:H111	1.82	0.43
14:G:1106:CLA:H3A	14:G:1106:CLA:HBA2	1.32	0.43
2:H:26:ALA:HB2	20:H:5002:LMG:H132	2.01	0.43
2:H:666:VAL:N	14:H:1023:CLA:HAB	2.33	0.43
18:H:4009:BCR:H371	18:H:4009:BCR:H24C	1.73	0.43
18:R:4020:BCR:H15C	18:R:4020:BCR:H351	1.63	0.43
2:b:32:GLU:CD	2:b:335:HIS:HE2	2.26	0.43
2:b:432:PHE:CE2	14:b:1235:CLA:HAB	2.53	0.43
2:b:605:HIS:HE1	14:b:1234:CLA:HBC1	1.82	0.43
2:b:666:VAL:N	14:b:1023:CLA:HAB	2.33	0.43
14:b:1221:CLA:H71	14:b:1223:CLA:H42	1.99	0.43
6:f:61:LEU:HD12	6:f:71:ALA:HB3	2.00	0.43
1:A:32:HIS:HA	1:A:38:ALA:HB2	2.00	0.43
2:B:468:GLN:HG2	2:B:516:PHE:CD1	2.51	0.43
14:B:1211:CLA:H142	14:B:1211:CLA:H112	1.72	0.43
20:L:5007:LMG:H391	20:L:5007:LMG:H422	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:THR:HG23	18:G:4002:BCR:H312	1.99	0.43
1:G:299:HIS:HB2	14:G:1116:CLA:CHB	2.49	0.43
1:G:384:MET:SD	14:G:1116:CLA:HBD	2.59	0.43
14:G:1103:CLA:H42	18:G:4003:BCR:H272	2.00	0.43
14:G:1138:CLA:HBA2	2:H:428:TRP:HD1	1.83	0.43
14:G:1139:CLA:HAA1	16:G:2001:PQN:H241	2.01	0.43
2:H:667:SER:HB3	2:H:718:HIS:HB2	1.99	0.43
14:H:1203:CLA:HMA3	14:H:1203:CLA:H52	2.00	0.43
14:H:1210:CLA:H142	14:H:1210:CLA:H112	1.73	0.43
6:Q:61:LEU:HD12	6:Q:71:ALA:HB3	2.00	0.43
20:R:5006:LMG:H112	20:l:5007:LMG:H401	2.00	0.43
1:a:381:MET:HE2	1:a:381:MET:HB3	1.86	0.43
1:a:430:GLU:HA	4:d:57:VAL:HG11	2.00	0.43
14:a:1102:CLA:HBA1	14:a:1102:CLA:H3A	1.81	0.43
14:a:1119:CLA:H152	14:a:1129:CLA:HAC1	2.00	0.43
14:a:1125:CLA:H141	14:a:1125:CLA:H162	1.71	0.43
2:b:26:ALA:HB2	20:b:5002:LMG:H132	2.01	0.43
2:b:232:ALA:HA	2:b:235:GLN:HE21	1.84	0.43
14:b:1023:CLA:HMB3	14:b:1023:CLA:H52	2.00	0.43
7:i:24:LEU:HD23	7:i:24:LEU:HA	1.89	0.43
8:j:12:SER:OG	8:j:13:ALA:N	2.51	0.43
1:A:373:LEU:HD13	14:A:1125:CLA:H42	2.00	0.43
14:A:1114:CLA:HBA1	14:A:1114:CLA:H3A	1.88	0.43
14:A:1139:CLA:HAA1	16:A:2001:PQN:H241	2.01	0.43
14:B:1023:CLA:H52	14:B:1023:CLA:HMB3	2.00	0.43
14:B:1211:CLA:H51	14:B:1211:CLA:H12	1.70	0.43
14:B:1216:CLA:H41	14:B:1216:CLA:H62	1.74	0.43
1:G:69:ARG:HH21	1:G:185:LYS:HA	1.84	0.43
2:H:232:ALA:HA	2:H:235:GLN:HE21	1.84	0.43
2:H:460:GLU:OE1	6:Q:69:ARG:HD3	2.18	0.43
2:H:669:MET:HE1	14:H:1239:CLA:HBC3	1.99	0.43
14:H:1206:CLA:H3A	14:H:1206:CLA:HBA2	1.61	0.43
16:H:2002:PQN:H141	16:H:2002:PQN:H161	1.82	0.43
1:a:69:ARG:HH21	1:a:185:LYS:HA	1.84	0.43
18:a:4001:BCR:H323	9:k:74:PHE:CD1	2.53	0.43
2:b:334:LEU:HD23	2:b:334:LEU:HA	1.82	0.43
14:b:1201:CLA:H11	18:m:4021:BCR:HC21	2.01	0.43
14:b:1225:CLA:H3A	14:b:1225:CLA:HBA2	1.51	0.43
6:f:52:LYS:HB2	6:f:53:PRO:HD3	2.00	0.43
14:A:1106:CLA:H93	14:A:1106:CLA:H61	1.75	0.43
2:B:86:PRO:HB3	2:B:121:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:SER:O	2:B:396:ILE:HD12	2.19	0.43
2:B:666:VAL:N	14:B:1023:CLA:HAB	2.33	0.43
2:B:701:ASP:OD1	2:B:701:ASP:N	2.52	0.43
3:C:29:VAL:HG21	4:D:129:LYS:HG2	2.00	0.43
18:L:4022:BCR:H351	18:L:4022:BCR:H15C	1.61	0.43
2:H:304:MET:HE3	14:H:1216:CLA:HED3	2.01	0.43
2:H:468:GLN:HG2	2:H:516:PHE:CD1	2.51	0.43
6:Q:115:LYS:NZ	6:Q:120:ASP:HB2	2.28	0.43
1:a:480:ASP:OD1	1:a:480:ASP:N	2.50	0.43
1:a:497:LEU:HB3	1:a:501:HIS:CE1	2.54	0.43
1:a:613:GLY:HA3	3:c:51:CYS:O	2.18	0.43
14:a:1126:CLA:H41	14:a:1126:CLA:H62	1.73	0.43
2:b:319:PHE:CD2	14:b:1220:CLA:HMB3	2.54	0.43
2:b:557:LYS:HE2	2:b:577:ILE:HG12	1.99	0.43
18:b:4005:BCR:H15C	18:b:4005:BCR:H351	1.78	0.43
1:A:497:LEU:HB3	1:A:501:HIS:CE1	2.54	0.43
2:B:232:ALA:HA	2:B:235:GLN:HE21	1.84	0.43
10:L:137:GLN:OE1	10:L:137:GLN:N	2.51	0.43
2:H:392:SER:O	2:H:396:ILE:HD12	2.19	0.43
14:H:1217:CLA:HBA2	14:H:1217:CLA:H3A	1.49	0.43
1:a:149:ALA:O	1:a:214:HIS:NE2	2.46	0.43
1:a:384:MET:SD	14:a:1116:CLA:HBD	2.59	0.43
14:a:1140:CLA:HBA2	14:a:1140:CLA:H3A	1.64	0.43
16:a:2001:PQN:H162	16:a:2001:PQN:H192	1.69	0.43
16:a:2001:PQN:H243	16:a:2001:PQN:H261	1.73	0.43
2:b:392:SER:O	2:b:396:ILE:HD12	2.19	0.43
2:b:610:GLN:NE2	2:b:738:LYS:HG2	2.33	0.43
14:b:1210:CLA:H202	14:b:1210:CLA:H162	1.77	0.43
14:b:1214:CLA:H112	14:b:1214:CLA:H71	1.68	0.43
14:b:1239:CLA:H92	14:b:1239:CLA:H62	1.81	0.43
1:A:299:HIS:HB2	14:A:1116:CLA:CHB	2.49	0.43
1:A:326:GLU:HA	1:A:329:ASP:HB2	2.01	0.43
14:B:1213:CLA:H141	14:B:1213:CLA:H161	1.83	0.43
4:D:38:LYS:NZ	10:L:124:ASP:HB2	2.33	0.43
5:E:12:ARG:HD2	5:E:15:SER:HB2	2.00	0.43
6:F:74:ARG:HD2	12:X:97:PHE:HB3	2.00	0.43
1:G:32:HIS:HA	1:G:38:ALA:HB2	2.00	0.43
1:G:148:ALA:HB2	1:G:388:PRO:HD3	2.01	0.43
1:G:714:PHE:CG	18:G:4011:BCR:H363	2.54	0.43
14:H:1205:CLA:O1A	14:H:1224:CLA:HBD	2.19	0.43
14:H:1215:CLA:H112	14:H:1215:CLA:H91	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:52:LYS:HB2	6:Q:53:PRO:HD3	2.00	0.43
10:U:137:GLN:OE1	10:U:137:GLN:N	2.51	0.43
1:a:326:GLU:HA	1:a:329:ASP:HB2	2.01	0.43
14:a:1106:CLA:H91	14:a:1106:CLA:H112	1.76	0.43
14:a:1111:CLA:H71	14:a:1111:CLA:H112	1.74	0.43
2:b:356:MET:HE3	2:b:356:MET:HB3	1.76	0.43
2:b:377:THR:HG23	2:b:598:THR:HG21	2.01	0.43
14:b:1201:CLA:HMA3	11:m:29:LEU:HD13	2.01	0.43
14:b:1202:CLA:H3A	14:b:1202:CLA:HBA1	1.60	0.43
14:b:1224:CLA:H11	14:b:1224:CLA:H51	1.64	0.43
16:b:2002:PQN:H141	16:b:2002:PQN:H161	1.83	0.43
1:A:148:ALA:HB2	1:A:388:PRO:HD3	2.01	0.43
14:A:1104:CLA:H112	14:A:1104:CLA:H71	1.85	0.43
14:A:1117:CLA:HBB1	14:A:1117:CLA:HMB1	2.01	0.43
2:B:428:TRP:CD1	14:B:1229:CLA:HED2	2.54	0.43
14:B:1203:CLA:H152	14:B:1203:CLA:H112	1.47	0.43
6:F:61:LEU:HD12	6:F:71:ALA:HB3	2.00	0.43
8:J:12:SER:OG	8:J:13:ALA:N	2.51	0.43
1:G:480:ASP:HB3	14:G:1132:CLA:HED3	2.01	0.43
1:G:497:LEU:HB3	1:G:501:HIS:CE1	2.54	0.43
14:G:1120:CLA:C3D	18:G:4001:BCR:H312	2.48	0.43
21:G:6001:LMT:O3'	21:G:6001:LMT:O2B	2.32	0.43
2:H:21:ILE:O	2:H:25:ILE:HG12	2.19	0.43
14:H:1221:CLA:H2	14:H:1221:CLA:H61	1.65	0.43
14:H:1228:CLA:H93	14:H:1228:CLA:H62	1.79	0.43
6:Q:54:LEU:HA	6:Q:57:TYR:CD1	2.49	0.43
8:S:12:SER:OG	8:S:13:ALA:N	2.51	0.43
14:a:1135:CLA:H12	14:a:1135:CLA:H51	1.82	0.43
2:b:44:GLN:OE1	2:b:162:ARG:HD3	2.19	0.43
14:b:1023:CLA:H161	14:b:1023:CLA:H141	1.74	0.43
14:b:1203:CLA:H193	14:b:1203:CLA:H161	1.75	0.43
14:b:1222:CLA:HBA2	14:b:1222:CLA:H3A	1.63	0.43
14:b:1224:CLA:H92	14:b:1224:CLA:H61	1.74	0.43
7:i:22:ILE:O	7:i:26:PHE:HB2	2.19	0.43
1:A:200:LEU:HD21	14:A:1119:CLA:C3B	2.49	0.43
1:A:384:MET:SD	14:A:1116:CLA:HBD	2.59	0.43
14:A:1103:CLA:H42	18:A:4003:BCR:H272	2.00	0.43
2:B:32:GLU:CD	2:B:335:HIS:HE2	2.26	0.43
14:B:1203:CLA:H62	14:B:1203:CLA:H41	1.57	0.43
14:B:1223:CLA:H72	14:B:1223:CLA:H111	1.62	0.43
14:B:1239:CLA:H92	14:B:1239:CLA:H62	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:ARG:HG3	5:E:28:GLU:OE1	2.19	0.43
7:I:22:ILE:O	7:I:26:PHE:HB2	2.19	0.43
1:G:26:LYS:HD2	14:G:1109:CLA:HAA2	2.01	0.42
1:G:734:ILE:HG22	1:G:738:VAL:HG23	2.01	0.42
2:H:377:THR:HG23	2:H:598:THR:HG21	2.01	0.42
14:H:1222:CLA:H93	14:H:1222:CLA:H61	1.79	0.42
3:N:73:THR:H	3:N:76:SER:HG	1.63	0.42
1:a:298:HIS:HB3	14:a:1116:CLA:HMB2	2.01	0.42
1:a:634:TRP:HH2	14:a:1012:CLA:CAB	2.31	0.42
14:b:1204:CLA:H192	14:b:1204:CLA:H162	1.83	0.42
14:b:1205:CLA:H2	14:b:1205:CLA:H61	1.65	0.42
14:b:1222:CLA:H51	14:b:1234:CLA:H2	2.01	0.42
10:l:117:SER:CB	10:l:127:ARG:HD2	2.49	0.42
1:A:69:ARG:HH21	1:A:185:LYS:HA	1.84	0.42
1:A:149:ALA:O	1:A:214:HIS:NE2	2.46	0.42
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.75	0.42
14:A:1119:CLA:H152	14:A:1129:CLA:HAC1	2.00	0.42
14:A:1120:CLA:C3D	18:A:4001:BCR:H312	2.48	0.42
2:B:174:ARG:HB3	14:B:1221:CLA:HMD1	2.00	0.42
2:B:266:GLN:HG3	2:B:367:LYS:NZ	2.33	0.42
18:B:4005:BCR:H351	18:B:4005:BCR:H15C	1.78	0.42
1:G:211:TRP:HD1	1:G:300:HIS:CD2	2.37	0.42
1:G:326:GLU:HA	1:G:329:ASP:HB2	2.01	0.42
2:H:585:LEU:HD23	2:H:585:LEU:HA	1.89	0.42
14:H:1023:CLA:H111	14:H:1023:CLA:H143	1.74	0.42
1:a:347:GLY:O	1:a:436:VAL:N	2.52	0.42
14:a:1139:CLA:HAA1	16:a:2001:PQN:H241	2.01	0.42
14:b:1216:CLA:H61	14:b:1216:CLA:H92	1.71	0.42
14:b:1221:CLA:HMA1	14:b:1221:CLA:H92	2.01	0.42
3:c:29:VAL:HG21	4:d:129:LYS:HG2	2.00	0.42
14:l:1502:CLA:H111	14:l:1502:CLA:H91	1.82	0.42
1:A:423:MET:O	1:A:594:ARG:NH1	2.44	0.42
14:A:1102:CLA:HBA1	14:A:1102:CLA:H3A	1.81	0.42
14:A:1119:CLA:H161	14:A:1119:CLA:H122	1.74	0.42
14:B:1228:CLA:HAC1	14:B:1236:CLA:HBC3	2.01	0.42
18:B:4009:BCR:H24C	18:B:4010:BCR:H23C	2.02	0.42
4:D:29:PHE:CZ	4:D:32:SER:HB2	2.53	0.42
18:L:4019:BCR:H371	18:L:4019:BCR:H24C	1.77	0.42
2:H:174:ARG:HB3	14:H:1221:CLA:HMD1	2.00	0.42
2:H:290:MET:HE1	14:H:1216:CLA:C3D	2.50	0.42
2:H:428:TRP:CD1	14:H:1229:CLA:HED2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:1023:CLA:H141	14:H:1023:CLA:H161	1.74	0.42
14:H:1228:CLA:HAC1	14:H:1236:CLA:HBC3	2.01	0.42
18:H:4005:BCR:H15C	18:H:4005:BCR:H351	1.78	0.42
7:R:22:ILE:O	7:R:26:PHE:HB2	2.19	0.42
1:a:428:ASP:HB3	1:a:431:GLN:HG2	2.02	0.42
1:a:734:ILE:HG22	1:a:738:VAL:HG23	2.01	0.42
1:A:310:ALA:HB2	14:A:1119:CLA:HBC2	2.00	0.42
14:A:1112:CLA:HBA1	14:A:1112:CLA:H3A	1.94	0.42
2:B:44:GLN:OE1	2:B:162:ARG:HD3	2.19	0.42
14:B:1215:CLA:H91	14:B:1215:CLA:H112	1.76	0.42
6:F:52:LYS:HB2	6:F:53:PRO:HD3	2.00	0.42
1:G:373:LEU:HD11	14:G:1117:CLA:H72	2.02	0.42
1:G:373:LEU:HD13	14:G:1125:CLA:H42	2.01	0.42
14:G:1117:CLA:H2	14:G:1117:CLA:H62	1.73	0.42
18:G:4001:BCR:H353	9:T:73:ALA:HB1	2.00	0.42
2:H:482:LEU:HD13	14:H:1231:CLA:HMD2	2.02	0.42
14:H:1022:CLA:H61	14:H:1022:CLA:H41	1.59	0.42
14:H:1222:CLA:H91	14:H:1222:CLA:H111	1.81	0.42
14:H:1222:CLA:H51	14:H:1234:CLA:H2	2.01	0.42
18:H:4006:BCR:H351	18:H:4006:BCR:H15C	1.67	0.42
14:b:1201:CLA:H3A	11:m:29:LEU:HD13	2.01	0.42
14:b:1208:CLA:H12	14:b:1208:CLA:H52	1.65	0.42
18:b:4014:BCR:H321	6:f:88:PHE:HB2	2.01	0.42
1:A:298:HIS:HB3	14:A:1116:CLA:HMB2	2.01	0.42
1:A:635:MET:HE3	1:A:635:MET:HB3	1.94	0.42
14:A:1012:CLA:H62	14:A:1012:CLA:H92	1.79	0.42
14:A:1140:CLA:H41	14:A:1140:CLA:H62	1.57	0.42
2:B:21:ILE:O	2:B:25:ILE:HG12	2.19	0.42
2:B:464:ALA:HB1	14:B:1234:CLA:HBD	2.01	0.42
14:B:1023:CLA:H111	14:B:1023:CLA:H143	1.74	0.42
10:L:117:SER:CB	10:L:127:ARG:HD2	2.49	0.42
14:G:1116:CLA:H62	14:G:1116:CLA:H41	1.57	0.42
2:H:32:GLU:CD	2:H:335:HIS:HE2	2.26	0.42
2:H:319:PHE:CD2	14:H:1220:CLA:HMB3	2.54	0.42
2:H:631:LEU:O	2:H:635:SER:OG	2.22	0.42
2:H:656:MET:HA	2:H:659:PHE:HB3	2.01	0.42
14:H:1203:CLA:H112	14:H:1203:CLA:H152	1.47	0.42
14:H:1210:CLA:H62	14:H:1210:CLA:H41	1.85	0.42
14:H:1236:CLA:HHC	14:H:1236:CLA:HBB1	2.02	0.42
18:H:4017:BCR:H343	18:H:4017:BCR:HC7	1.85	0.42
1:a:299:HIS:HB2	14:a:1116:CLA:CHB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:a:4011:BCR:H343	18:a:4011:BCR:HC7	1.87	0.42
2:b:464:ALA:HB1	14:b:1234:CLA:HBD	2.00	0.42
2:b:656:MET:HA	2:b:659:PHE:HB3	2.01	0.42
14:b:1203:CLA:H62	14:b:1203:CLA:H41	1.57	0.42
14:b:1236:CLA:HHC	14:b:1236:CLA:HBB1	2.02	0.42
7:i:12:TYR:OH	7:i:18:PRO:HG2	2.20	0.42
1:A:393:ASP:OD2	1:A:396:THR:OG1	2.28	0.42
1:A:480:ASP:HB3	14:A:1132:CLA:HED3	2.01	0.42
1:A:634:TRP:HH2	14:A:1012:CLA:CAB	2.31	0.42
2:B:26:ALA:HB2	20:B:5002:LMG:H132	2.01	0.42
1:G:298:HIS:HB3	14:G:1116:CLA:HMB2	2.01	0.42
14:G:1122:CLA:HED2	14:G:1122:CLA:H2A	2.01	0.42
2:H:142:LEU:HD23	2:H:142:LEU:HA	1.87	0.42
6:Q:121:VAL:HG23	6:Q:122:PRO:HD3	2.00	0.42
7:R:12:TYR:OH	7:R:18:PRO:HG2	2.20	0.42
10:U:117:SER:CB	10:U:127:ARG:HD2	2.49	0.42
1:a:775:THR:HG23	13:a:1011:CL0:H28	2.02	0.42
14:a:1116:CLA:HBA2	14:a:1116:CLA:H3A	1.48	0.42
14:b:1215:CLA:H112	14:b:1215:CLA:H91	1.76	0.42
2:B:142:LEU:HG	18:B:4006:BCR:H382	2.01	0.42
2:B:319:PHE:CD2	14:B:1220:CLA:HMB3	2.54	0.42
2:B:377:THR:HG23	2:B:598:THR:HG21	2.01	0.42
14:B:1210:CLA:H91	14:B:1221:CLA:H11	2.02	0.42
14:B:1222:CLA:H93	14:B:1222:CLA:H61	1.79	0.42
14:B:1236:CLA:HHC	14:B:1236:CLA:HBB1	2.02	0.42
3:C:2:SER:O	3:C:2:SER:OG	2.37	0.42
4:D:52:SER:HB3	4:D:68:MET:HE2	2.01	0.42
18:I:4020:BCR:HC32	18:I:4020:BCR:H312	1.76	0.42
1:G:428:ASP:HB3	1:G:431:GLN:HG2	2.02	0.42
14:G:1115:CLA:H11	14:G:1115:CLA:H52	1.72	0.42
14:G:1124:CLA:HAB	18:G:4008:BCR:H311	2.01	0.42
14:G:1135:CLA:H12	14:G:1135:CLA:H51	1.82	0.42
2:H:44:GLN:OE1	2:H:162:ARG:HD3	2.19	0.42
14:H:1213:CLA:H91	14:H:1213:CLA:H112	1.93	0.42
14:H:1222:CLA:HBA2	14:H:1222:CLA:H3A	1.63	0.42
18:H:4009:BCR:H24C	18:H:4010:BCR:H23C	2.01	0.42
5:P:12:ARG:HD2	5:P:15:SER:HB2	2.00	0.42
1:a:148:ALA:HB2	1:a:388:PRO:HD3	2.01	0.42
2:b:21:ILE:O	2:b:25:ILE:HG12	2.19	0.42
14:b:1023:CLA:H122	18:i:4018:BCR:H281	2.02	0.42
14:b:1205:CLA:O1A	14:b:1224:CLA:HBD	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ILE:HG23	2:B:113:VAL:HB	2.02	0.42
2:B:555:PRO:HD2	3:C:62:PHE:CE1	2.55	0.42
2:B:663:ALA:O	2:B:718:HIS:HB3	2.19	0.42
14:G:1119:CLA:H152	14:G:1129:CLA:HAC1	2.00	0.42
14:G:1135:CLA:H142	14:G:1135:CLA:H112	1.79	0.42
14:G:1136:CLA:H112	14:G:1136:CLA:H142	1.83	0.42
2:H:356:MET:HE1	14:H:1225:CLA:O1D	2.20	0.42
2:H:555:PRO:HD2	3:N:62:PHE:CE1	2.55	0.42
14:H:1221:CLA:HMA1	14:H:1221:CLA:H92	2.01	0.42
18:H:4014:BCR:H321	6:Q:88:PHE:HB2	2.01	0.42
14:a:1106:CLA:H61	14:a:1106:CLA:H41	1.90	0.42
2:b:290:MET:HE1	14:b:1216:CLA:C3D	2.50	0.42
2:b:304:MET:HE3	14:b:1216:CLA:HED3	2.01	0.42
14:b:1205:CLA:HAB	14:b:1206:CLA:CGA	2.50	0.42
14:b:1216:CLA:H162	14:b:1216:CLA:H122	1.34	0.42
14:b:1239:CLA:H203	14:b:1239:CLA:H161	1.77	0.42
1:A:430:GLU:HA	4:D:57:VAL:HG11	2.00	0.42
1:A:473:ARG:NH2	2:B:644:PRO:HG3	2.35	0.42
2:B:203:ARG:HD3	2:B:250:ALA:HB1	2.02	0.42
16:B:2002:PQN:H141	16:B:2002:PQN:H161	1.82	0.42
1:G:51:HIS:HB2	19:G:5001:LHG:H102	2.01	0.42
1:G:731:GLN:O	1:G:735:GLU:HG3	2.20	0.42
14:G:1136:CLA:H62	14:G:1136:CLA:H41	1.50	0.42
18:G:4011:BCR:H15C	18:G:4011:BCR:H351	1.75	0.42
2:H:86:PRO:HB3	2:H:121:TYR:CG	2.54	0.42
2:H:348:ALA:HB2	14:H:1221:CLA:H41	2.02	0.42
2:H:663:ALA:O	2:H:718:HIS:HB3	2.19	0.42
14:H:1204:CLA:H162	14:H:1204:CLA:H192	1.83	0.42
18:H:4004:BCR:H351	18:H:4004:BCR:H15C	1.69	0.42
10:U:88:LEU:O	10:U:92:ILE:HG12	2.20	0.42
1:a:211:TRP:HD1	1:a:300:HIS:CD2	2.37	0.42
14:a:1126:CLA:H62	14:a:1126:CLA:H92	1.82	0.42
14:a:1128:CLA:H61	14:a:1128:CLA:H41	1.79	0.42
18:a:4011:BCR:H15C	18:a:4011:BCR:H351	1.75	0.42
2:b:377:THR:HB	14:b:1224:CLA:HMB1	2.02	0.42
2:b:428:TRP:CD1	14:b:1229:CLA:HED2	2.54	0.42
14:b:1223:CLA:H72	14:b:1223:CLA:H111	1.62	0.42
18:b:4005:BCR:H24C	18:b:4005:BCR:H371	1.77	0.42
1:A:428:ASP:HB3	1:A:431:GLN:HG2	2.02	0.42
18:A:4002:BCR:H371	18:A:4002:BCR:H24C	1.82	0.42
19:A:5001:LHG:H142	19:A:5001:LHG:H111	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:LEU:HD22	4:D:148:PHE:HZ	1.85	0.42
2:B:356:MET:HE1	14:B:1225:CLA:O1D	2.20	0.42
2:B:482:LEU:HD13	14:B:1231:CLA:HMD2	2.01	0.42
2:B:689:HIS:NE2	2:B:697:GLY:O	2.34	0.42
14:B:1205:CLA:HAB	14:B:1206:CLA:CGA	2.50	0.42
14:B:1205:CLA:O1A	14:B:1224:CLA:HBD	2.19	0.42
5:E:9:ARG:NH2	6:F:152:GLU:O	2.53	0.42
7:I:12:TYR:OH	7:I:18:PRO:HG2	2.20	0.42
14:G:1117:CLA:HBB1	14:G:1117:CLA:HMB1	2.01	0.42
2:H:464:ALA:HB1	14:H:1234:CLA:HBD	2.01	0.42
14:H:1202:CLA:HBA1	14:H:1202:CLA:H3A	1.60	0.42
14:H:1205:CLA:HAB	14:H:1206:CLA:CGA	2.50	0.42
14:H:1210:CLA:H91	14:H:1221:CLA:H11	2.02	0.42
14:U:1503:CLA:HBC1	18:L:4022:BCR:H341	2.02	0.42
1:a:255:ALA:HB3	1:a:257:TRP:NE1	2.35	0.42
1:a:280:PHE:HD1	14:a:1116:CLA:HMB3	1.85	0.42
1:a:715:ILE:HG21	1:a:770:LEU:HD23	2.02	0.42
2:b:203:ARG:HD3	2:b:250:ALA:HB1	2.01	0.42
2:b:504:TRP:CD1	2:b:505:LEU:HD12	2.55	0.42
2:b:533:GLY:O	2:b:537:THR:HG22	2.20	0.42
2:b:723:TYR:CE2	14:b:1021:CLA:HED1	2.55	0.42
18:b:4014:BCR:H24C	18:b:4014:BCR:H371	1.68	0.42
14:A:1115:CLA:H162	14:A:1115:CLA:H193	1.75	0.42
16:A:2001:PQN:H211	16:A:2001:PQN:H191	1.75	0.42
2:B:304:MET:HE3	14:B:1216:CLA:HED3	2.01	0.42
2:B:334:LEU:HA	2:B:334:LEU:HD23	1.82	0.42
1:G:200:LEU:HD21	14:G:1119:CLA:C3B	2.49	0.41
14:G:1106:CLA:H142	14:G:1106:CLA:H111	1.80	0.41
14:H:1219:CLA:H3A	14:H:1219:CLA:HBA2	1.71	0.41
4:O:52:SER:HB3	4:O:68:MET:HE2	2.01	0.41
18:R:4020:BCR:H24C	18:R:4020:BCR:H371	1.73	0.41
10:U:102:ILE:HD13	10:U:102:ILE:HG21	1.85	0.41
1:a:51:HIS:HB2	19:a:5001:LHG:H102	2.02	0.41
1:a:373:LEU:HD13	14:a:1125:CLA:H42	2.00	0.41
2:b:663:ALA:O	2:b:718:HIS:HB3	2.19	0.41
14:b:1221:CLA:H13	14:b:1221:CLA:H102	1.82	0.41
18:b:4009:BCR:H24C	18:b:4010:BCR:H23C	2.01	0.41
1:A:731:GLN:O	1:A:735:GLU:HG3	2.20	0.41
14:B:1208:CLA:H12	14:B:1208:CLA:H52	1.65	0.41
14:B:1222:CLA:H51	14:B:1234:CLA:H2	2.01	0.41
18:I:4020:BCR:H393	18:I:4020:BCR:H281	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:88:LEU:O	10:L:92:ILE:HG12	2.20	0.41
14:X:1701:CLA:HBA2	14:X:1701:CLA:H3A	1.93	0.41
1:G:255:ALA:HB3	1:G:257:TRP:NE1	2.35	0.41
1:G:672:PHE:O	1:G:676:SER:OG	2.37	0.41
14:G:1131:CLA:H143	14:G:1131:CLA:H111	1.80	0.41
2:H:689:HIS:NE2	2:H:697:GLY:O	2.34	0.41
1:a:119:ILE:O	1:a:122:GLN:HG2	2.20	0.41
1:a:635:MET:HE3	1:a:635:MET:HB3	1.94	0.41
2:b:348:ALA:HB2	14:b:1221:CLA:H41	2.02	0.41
2:b:356:MET:HE1	14:b:1225:CLA:O1D	2.20	0.41
2:b:421:ALA:O	2:b:425:HIS:ND1	2.52	0.41
14:b:1208:CLA:HBA2	14:b:1208:CLA:H102	2.02	0.41
1:A:211:TRP:HD1	1:A:300:HIS:CD2	2.37	0.41
1:A:215:LEU:HA	1:A:219:SER:HB2	2.02	0.41
1:A:715:ILE:HG21	1:A:770:LEU:HD23	2.02	0.41
14:A:1106:CLA:H142	14:A:1106:CLA:H111	1.81	0.41
14:A:1138:CLA:HBA2	2:B:428:TRP:HD1	1.83	0.41
2:B:290:MET:HE1	14:B:1216:CLA:C3D	2.50	0.41
2:B:533:GLY:O	2:B:537:THR:HG22	2.20	0.41
2:B:656:MET:HA	2:B:659:PHE:HB3	2.01	0.41
14:B:1213:CLA:H61	14:B:1213:CLA:H41	1.50	0.41
14:B:1222:CLA:CHB	14:B:1236:CLA:HAA2	2.50	0.41
5:E:18:PHE:O	6:F:155:PRO:HA	2.20	0.41
1:G:280:PHE:CE2	14:G:1134:CLA:HED1	2.56	0.41
1:G:715:ILE:HG21	1:G:770:LEU:HD23	2.02	0.41
2:H:17:THR:OG1	2:H:19:ARG:HG2	2.21	0.41
14:H:1205:CLA:H2	14:H:1205:CLA:H61	1.65	0.41
14:H:1222:CLA:CHB	14:H:1236:CLA:HAA2	2.50	0.41
6:Q:79:VAL:O	6:Q:83:ILE:HG12	2.21	0.41
14:U:1503:CLA:H41	14:U:1503:CLA:H61	1.68	0.41
14:a:1115:CLA:H162	14:a:1115:CLA:H193	1.75	0.41
14:a:1122:CLA:HED2	14:a:1122:CLA:H2A	2.01	0.41
2:b:17:THR:OG1	2:b:19:ARG:HG2	2.21	0.41
2:b:45:ARG:NH1	14:b:1201:CLA:HED2	2.36	0.41
2:b:87:ILE:HG23	2:b:113:VAL:HB	2.02	0.41
2:b:701:ASP:OD1	2:b:701:ASP:N	2.51	0.41
1:A:26:LYS:HD2	14:A:1109:CLA:HAA2	2.01	0.41
1:A:373:LEU:HD11	14:A:1117:CLA:H72	2.02	0.41
14:A:1131:CLA:HAB	14:A:1132:CLA:HHB	2.02	0.41
14:A:1135:CLA:H142	14:A:1135:CLA:H112	1.79	0.41
14:A:1136:CLA:H142	14:A:1136:CLA:H112	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:LEU:HD21	19:B:5004:LHG:HC5	2.02	0.41
14:B:1216:CLA:H92	14:B:1216:CLA:H61	1.71	0.41
1:G:490:GLN:HE21	1:G:495:GLN:HE22	1.68	0.41
1:G:775:THR:HG23	13:G:1011:CL0:H28	2.02	0.41
2:H:377:THR:HB	14:H:1224:CLA:HMB1	2.02	0.41
18:V:4021:BCR:H371	18:V:4021:BCR:H24C	1.82	0.41
1:a:26:LYS:HD2	14:a:1109:CLA:HAA2	2.01	0.41
14:a:1109:CLA:H111	14:a:1109:CLA:H91	1.62	0.41
14:a:1124:CLA:HAB	18:a:4008:BCR:H311	2.01	0.41
2:b:42:LEU:HD22	4:d:148:PHE:HZ	1.85	0.41
2:b:362:TYR:OH	14:b:1225:CLA:OBD	2.29	0.41
14:b:1216:CLA:H3A	14:b:1216:CLA:HBA2	1.55	0.41
18:l:4022:BCR:H24C	18:l:4022:BCR:H371	1.69	0.41
1:A:347:GLY:O	1:A:436:VAL:N	2.52	0.41
1:A:625:TRP:NE1	14:A:1128:CLA:HMD3	2.36	0.41
16:A:2001:PQN:H192	16:A:2001:PQN:H162	1.69	0.41
2:B:17:THR:OG1	2:B:19:ARG:HG2	2.21	0.41
2:B:45:ARG:NH1	14:B:1201:CLA:HED2	2.35	0.41
2:B:421:ALA:O	2:B:425:HIS:ND1	2.52	0.41
2:B:723:TYR:CE2	14:B:1021:CLA:HED1	2.55	0.41
14:B:1201:CLA:H62	14:B:1201:CLA:H41	1.78	0.41
14:G:1111:CLA:H93	14:G:1111:CLA:H62	1.86	0.41
2:H:142:LEU:HG	18:H:4006:BCR:H382	2.01	0.41
2:H:182:LEU:HD13	14:H:1210:CLA:HHB	2.02	0.41
2:H:343:ALA:HB2	18:H:4010:BCR:H372	2.02	0.41
2:H:504:TRP:CD1	2:H:505:LEU:HD12	2.55	0.41
2:H:639:ILE:HD13	14:H:1021:CLA:HBC1	2.03	0.41
1:a:480:ASP:HB3	14:a:1132:CLA:HED3	2.01	0.41
1:a:755:LEU:N	16:a:2001:PQN:O4	2.49	0.41
14:a:1131:CLA:HAB	14:a:1132:CLA:HHB	2.02	0.41
2:b:142:LEU:HG	18:b:4006:BCR:H382	2.01	0.41
2:b:534:LEU:HD12	14:b:1236:CLA:HED3	2.03	0.41
2:b:639:ILE:HD13	14:b:1021:CLA:HBC1	2.03	0.41
18:i:4020:BCR:HC41	10:l:93:TYR:CD1	2.55	0.41
2:B:348:ALA:HB2	14:B:1221:CLA:H41	2.02	0.41
14:B:1023:CLA:H161	14:B:1023:CLA:H141	1.74	0.41
14:B:1222:CLA:HMD3	14:B:1234:CLA:HBB2	2.03	0.41
1:G:625:TRP:NE1	14:G:1128:CLA:HMD3	2.36	0.41
14:G:1140:CLA:H161	14:G:1140:CLA:H141	1.71	0.41
2:H:701:ASP:OD1	2:H:701:ASP:N	2.52	0.41
14:H:1213:CLA:H41	14:H:1213:CLA:H61	1.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:2002:PQN:H222	16:H:2002:PQN:H261	1.65	0.41
7:R:37:LEU:HD21	18:U:4019:BCR:H312	2.02	0.41
10:U:124:ASP:N	10:U:130:ARG:HH22	2.11	0.41
1:a:304:ALA:O	1:a:308:ILE:HG13	2.21	0.41
2:b:140:LEU:HD22	11:m:14:VAL:HG11	2.03	0.41
2:b:482:LEU:HD13	14:b:1231:CLA:HMD2	2.02	0.41
14:A:1136:CLA:H62	14:A:1136:CLA:H41	1.49	0.41
16:B:2002:PQN:H261	16:B:2002:PQN:H222	1.65	0.41
18:B:4013:BCR:H371	18:B:4013:BCR:H24C	1.78	0.41
10:L:53:MET:HE1	14:L:1501:CLA:HED3	2.03	0.41
1:G:119:ILE:O	1:G:122:GLN:HG2	2.20	0.41
14:G:1118:CLA:H62	14:G:1118:CLA:H41	1.84	0.41
2:H:87:ILE:HG23	2:H:113:VAL:HB	2.02	0.41
2:H:321:LEU:HD21	19:H:5004:LHG:HC5	2.03	0.41
2:H:533:GLY:O	2:H:537:THR:HG22	2.20	0.41
3:N:6:LYS:HE3	4:O:133:ASN:OD1	2.21	0.41
4:O:61:PRO:HG3	4:O:86:LEU:HB2	2.03	0.41
1:a:625:TRP:NE1	14:a:1128:CLA:HMD3	2.36	0.41
1:a:731:GLN:O	1:a:735:GLU:HG3	2.20	0.41
14:a:1117:CLA:HMB1	14:a:1117:CLA:HBB1	2.01	0.41
18:a:4008:BCR:H312	18:a:4008:BCR:HC32	1.91	0.41
14:b:1222:CLA:CHB	14:b:1236:CLA:HAA2	2.50	0.41
18:i:4020:BCR:H351	18:i:4020:BCR:H15C	1.63	0.41
1:A:51:HIS:HB2	19:A:5001:LHG:H102	2.01	0.41
1:A:460:PHE:O	1:A:464:ALA:HB3	2.21	0.41
14:A:1122:CLA:HED2	14:A:1122:CLA:H2A	2.01	0.41
14:A:1124:CLA:HAB	18:A:4008:BCR:H311	2.01	0.41
14:B:1202:CLA:H3A	14:B:1202:CLA:HBA1	1.60	0.41
14:B:1221:CLA:HMA1	14:B:1221:CLA:H92	2.01	0.41
14:B:1239:CLA:H162	7:I:31:PHE:HZ	1.86	0.41
18:B:4014:BCR:H321	6:F:88:PHE:HB2	2.01	0.41
9:K:72:MET:HE3	9:K:73:ALA:N	2.36	0.41
14:L:1503:CLA:HBB1	14:L:1503:CLA:HMB1	2.03	0.41
1:G:42:LYS:HA	6:Q:113:GLU:OE2	2.20	0.41
1:G:304:ALA:O	1:G:308:ILE:HG13	2.21	0.41
14:H:1208:CLA:H102	14:H:1208:CLA:HBA2	2.02	0.41
14:U:1503:CLA:HMB1	14:U:1503:CLA:HBB1	2.03	0.41
1:a:731:GLN:HE22	1:a:753:ARG:HA	1.86	0.41
18:a:4003:BCR:H351	18:a:4003:BCR:H15C	1.68	0.41
14:b:1220:CLA:HBC1	18:b:4010:BCR:H292	2.02	0.41
1:A:280:PHE:CE2	14:A:1134:CLA:HED1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:628:ARG:HG3	2:B:629:ASP:OD2	2.21	0.41
2:B:639:ILE:HD13	14:B:1021:CLA:HBC1	2.03	0.41
14:B:1220:CLA:HBC1	18:B:4010:BCR:H292	2.02	0.41
4:D:113:HIS:HA	4:D:114:PRO:HA	1.94	0.41
5:E:34:ARG:HE	5:E:34:ARG:HB3	1.57	0.41
1:G:194:SER:O	1:G:198:HIS:ND1	2.39	0.41
1:G:473:ARG:NH2	2:H:644:PRO:HG3	2.35	0.41
14:G:1111:CLA:H12	14:G:1111:CLA:HBA2	1.79	0.41
2:H:658:LEU:HD12	2:H:658:LEU:HA	1.90	0.41
2:H:723:TYR:CE2	14:H:1021:CLA:HED1	2.55	0.41
14:H:1210:CLA:H202	14:H:1210:CLA:H162	1.77	0.41
14:H:1227:CLA:H3A	14:H:1227:CLA:HBA2	1.48	0.41
9:T:72:MET:HE3	9:T:73:ALA:N	2.36	0.41
20:U:5007:LMG:H361	7:I:19:TRP:CE3	2.55	0.41
1:a:42:LYS:HA	6:f:113:GLU:OE2	2.20	0.41
1:a:258:GLY:H	1:a:262:GLY:HA3	1.86	0.41
1:a:473:ARG:NH2	2:b:644:PRO:HG3	2.35	0.41
1:a:634:TRP:HE1	14:b:1023:CLA:C1D	2.34	0.41
14:a:1012:CLA:H92	14:a:1012:CLA:H62	1.79	0.41
14:a:1136:CLA:H111	14:a:1136:CLA:H91	1.89	0.41
2:b:182:LEU:HD13	14:b:1210:CLA:HHB	2.02	0.41
2:b:655:TRP:CZ3	18:b:4017:BCR:HC21	2.56	0.41
14:b:1201:CLA:H62	14:b:1201:CLA:H41	1.78	0.41
18:b:4014:BCR:H343	6:f:88:PHE:CD1	2.56	0.41
3:c:31:TRP:N	3:c:37:GLY:O	2.48	0.41
18:i:4020:BCR:HC32	18:i:4020:BCR:H312	1.76	0.41
18:i:4020:BCR:H371	18:i:4020:BCR:H24C	1.72	0.41
10:l:88:LEU:O	10:l:92:ILE:HG12	2.20	0.41
1:A:42:LYS:HA	6:F:113:GLU:OE2	2.20	0.41
1:A:119:ILE:O	1:A:122:GLN:HG2	2.20	0.41
1:A:255:ALA:HB3	1:A:257:TRP:NE1	2.35	0.41
1:A:731:GLN:HE22	1:A:753:ARG:HA	1.86	0.41
14:A:1124:CLA:HBA1	14:A:1125:CLA:HED2	2.03	0.41
2:B:140:LEU:HD22	11:M:14:VAL:HG11	2.03	0.41
2:B:182:LEU:HD13	14:B:1210:CLA:HHB	2.02	0.41
2:B:377:THR:HB	14:B:1224:CLA:HMB1	2.02	0.41
2:B:537:THR:HB	2:B:589:TRP:HB3	2.03	0.41
18:B:4009:BCR:H351	18:B:4009:BCR:H15C	1.53	0.41
6:F:75:LEU:HA	6:F:78:ALA:HB2	2.03	0.41
6:F:79:VAL:O	6:F:83:ILE:HG12	2.21	0.41
14:X:1701:CLA:H52	14:X:1701:CLA:H11	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:381:MET:HE2	1:G:381:MET:HB3	1.86	0.41
2:H:45:ARG:NH1	14:H:1201:CLA:HED2	2.35	0.41
2:H:628:ARG:HG3	2:H:629:ASP:OD2	2.21	0.41
14:H:1231:CLA:HBA1	14:H:1231:CLA:H3A	1.92	0.41
14:H:1239:CLA:H203	14:H:1239:CLA:H161	1.77	0.41
18:R:4018:BCR:H24C	18:R:4018:BCR:H371	1.71	0.41
1:a:280:PHE:CE2	14:a:1134:CLA:HED1	2.56	0.41
1:a:680:ASN:O	1:a:684:ARG:HG2	2.21	0.41
14:a:1112:CLA:HBA1	14:a:1112:CLA:H3A	1.94	0.41
2:b:343:ALA:HB2	18:b:4010:BCR:H372	2.02	0.41
2:b:537:THR:HB	2:b:589:TRP:HB3	2.03	0.41
14:b:1023:CLA:H111	14:b:1023:CLA:H143	1.74	0.41
14:b:1210:CLA:H91	14:b:1221:CLA:H11	2.02	0.41
2:B:343:ALA:HB2	18:B:4010:BCR:H372	2.02	0.41
2:B:376:TYR:CE2	2:B:380:GLN:HG3	2.56	0.41
14:B:1202:CLA:H101	14:B:1210:CLA:CAD	2.51	0.41
14:B:1221:CLA:H141	14:B:1221:CLA:H162	1.75	0.41
18:B:4014:BCR:H343	6:F:88:PHE:CD1	2.56	0.41
3:C:31:TRP:N	3:C:37:GLY:O	2.48	0.41
18:I:4020:BCR:HC41	10:L:93:TYR:CD1	2.55	0.41
1:G:200:LEU:HD23	1:G:200:LEU:HA	1.75	0.40
14:H:1220:CLA:HBC1	18:H:4010:BCR:H292	2.02	0.40
5:P:34:ARG:HE	5:P:34:ARG:HB3	1.57	0.40
1:a:373:LEU:HD11	14:a:1117:CLA:H72	2.01	0.40
2:b:628:ARG:HG3	2:b:629:ASP:OD2	2.21	0.40
14:b:1202:CLA:H101	14:b:1210:CLA:CAD	2.51	0.40
14:b:1222:CLA:HMD3	14:b:1234:CLA:HBB2	2.03	0.40
18:b:4014:BCR:H15C	18:b:4014:BCR:H351	1.74	0.40
14:B:1208:CLA:HBA2	14:B:1208:CLA:H102	2.02	0.40
20:L:5007:LMG:H342	20:L:5007:LMG:H311	1.89	0.40
1:G:86:LEU:HD23	1:G:86:LEU:HA	1.89	0.40
1:G:209:LEU:HG	14:G:1113:CLA:HBB2	2.03	0.40
1:G:560:MET:SD	1:G:666:HIS:HE1	2.44	0.40
2:H:58:PHE:HE1	2:H:149:PHE:CE2	2.40	0.40
14:H:1205:CLA:H43	14:H:1224:CLA:H51	2.03	0.40
19:H:5004:LHG:HC61	12:W:78:ARG:HE	1.85	0.40
10:U:53:MET:HE1	14:U:1501:CLA:HED3	2.03	0.40
1:a:209:LEU:HG	14:a:1113:CLA:HBB2	2.03	0.40
1:a:215:LEU:HA	1:a:219:SER:HB2	2.03	0.40
2:b:376:TYR:CE2	2:b:380:GLN:HG3	2.56	0.40
10:l:122:SER:C	10:l:123:LYS:HG3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ALA:O	1:A:308:ILE:HG13	2.21	0.40
1:A:634:TRP:HE1	14:B:1023:CLA:C1D	2.34	0.40
2:B:567:ASP:OD1	3:C:66:ARG:NH2	2.51	0.40
1:G:26:LYS:HB2	14:G:1109:CLA:HBA1	2.03	0.40
1:G:258:GLY:H	1:G:262:GLY:HA3	1.86	0.40
1:G:303:ILE:HD13	1:G:303:ILE:HA	1.95	0.40
1:G:406:TRP:HB3	14:G:1126:CLA:HMC3	2.04	0.40
1:G:608:ARG:HG3	1:G:625:TRP:CG	2.57	0.40
1:G:755:LEU:N	16:G:2001:PQN:O4	2.49	0.40
2:H:203:ARG:HD3	2:H:250:ALA:HB1	2.01	0.40
14:H:1226:CLA:H203	14:H:1226:CLA:H161	1.99	0.40
1:a:490:GLN:HE21	1:a:495:GLN:HE22	1.68	0.40
14:a:1110:CLA:HED2	14:a:1111:CLA:HAC1	2.04	0.40
14:a:1124:CLA:HBA1	14:a:1125:CLA:HED2	2.03	0.40
2:b:278:LEU:HD13	14:b:1212:CLA:HMC3	2.04	0.40
14:b:1228:CLA:HAC1	14:b:1236:CLA:HBC3	2.01	0.40
3:c:73:THR:H	3:c:76:SER:HG	1.65	0.40
4:d:61:PRO:HG3	4:d:86:LEU:HB2	2.03	0.40
7:i:35:ALA:HB1	10:l:104:ILE:HG21	2.04	0.40
9:k:72:MET:HE3	9:k:73:ALA:N	2.36	0.40
10:l:51:PRO:HB2	10:l:137:GLN:HB2	2.04	0.40
10:l:137:GLN:OE1	10:l:137:GLN:N	2.51	0.40
14:l:1503:CLA:HMB1	14:l:1503:CLA:HBB1	2.03	0.40
1:A:280:PHE:HD1	14:A:1116:CLA:HMB3	1.85	0.40
1:A:299:HIS:HB2	14:A:1116:CLA:C1B	2.52	0.40
1:A:490:GLN:HE21	1:A:495:GLN:HE22	1.68	0.40
10:L:49:LEU:HD23	10:L:49:LEU:HA	1.93	0.40
2:H:11:ASP:HB2	3:N:71:ALA:HB2	2.02	0.40
2:H:445:ASP:OD1	2:H:622:TYR:HB2	2.22	0.40
2:H:536:VAL:O	2:H:540:ILE:HG13	2.21	0.40
14:H:1216:CLA:H92	14:H:1216:CLA:H61	1.71	0.40
14:H:1222:CLA:HMD3	14:H:1234:CLA:HBB2	2.03	0.40
4:O:141:PRO:HD2	4:O:153:THR:O	2.22	0.40
2:b:89:HIS:ND1	2:b:90:ALA:O	2.54	0.40
14:b:1227:CLA:HAB	14:b:1236:CLA:CBB	2.52	0.40
4:d:52:SER:HB3	4:d:68:MET:HE2	2.01	0.40
1:A:299:HIS:HD2	1:A:300:HIS:ND1	2.19	0.40
14:A:1140:CLA:H93	14:A:1140:CLA:H61	1.94	0.40
2:B:11:ASP:HB2	3:C:71:ALA:HB2	2.03	0.40
2:B:534:LEU:HD12	14:B:1236:CLA:HED3	2.03	0.40
14:B:1205:CLA:H43	14:B:1224:CLA:H51	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:407:ILE:HD12	14:G:1104:CLA:H143	2.04	0.40
2:H:494:PRO:HG3	14:H:1233:CLA:C1D	2.52	0.40
2:H:534:LEU:HD12	14:H:1236:CLA:HED3	2.03	0.40
2:H:655:TRP:CZ3	18:H:4017:BCR:HC21	2.56	0.40
14:H:1202:CLA:H101	14:H:1210:CLA:CAD	2.51	0.40
14:H:1203:CLA:H62	14:H:1203:CLA:H41	1.57	0.40
1:a:307:PHE:CZ	14:a:1117:CLA:H142	2.57	0.40
19:a:5001:LHG:H142	19:a:5001:LHG:H111	1.77	0.40
2:b:536:VAL:O	2:b:540:ILE:HG13	2.21	0.40
2:b:694:LEU:HB2	18:i:4020:BCR:H282	2.04	0.40
4:d:141:PRO:HD2	4:d:153:THR:O	2.22	0.40
7:i:23:PRO:HB3	7:i:27:TYR:OH	2.22	0.40
10:l:53:MET:HE1	14:l:1501:CLA:HED3	2.03	0.40
1:A:680:ASN:O	1:A:684:ARG:HG2	2.22	0.40
1:A:755:LEU:N	16:A:2001:PQN:O4	2.49	0.40
1:A:775:THR:HG23	13:A:1011:CL0:H28	2.02	0.40
2:B:655:TRP:CZ3	18:B:4017:BCR:HC21	2.56	0.40
2:B:719:PHE:O	2:B:723:TYR:HB2	2.22	0.40
14:B:1204:CLA:H162	14:B:1204:CLA:H192	1.83	0.40
14:B:1224:CLA:H112	14:B:1224:CLA:H91	1.77	0.40
7:I:23:PRO:HB3	7:I:27:TYR:OH	2.22	0.40
18:I:4020:BCR:H371	18:I:4020:BCR:H24C	1.72	0.40
10:L:122:SER:C	10:L:123:LYS:HG3	2.47	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	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
1	G	747/788 (95%)	707 (95%)	40 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	747/788 (95%)	707 (95%)	40 (5%)	0	100	100
2	B	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	H	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	b	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	26
3	N	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	26
3	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	O	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
4	d	137/159 (86%)	129 (94%)	8 (6%)	0	100	100
5	E	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	P	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
5	e	60/72 (83%)	57 (95%)	3 (5%)	0	100	100
6	F	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	37
6	Q	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	37
6	f	133/159 (84%)	118 (89%)	14 (10%)	1 (1%)	16	37
7	I	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	R	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
7	i	40/67 (60%)	36 (90%)	4 (10%)	0	100	100
8	J	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	4	13
8	S	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	4	13
8	j	41/48 (85%)	32 (78%)	8 (20%)	1 (2%)	4	13
9	K	17/49 (35%)	17 (100%)	0	0	100	100
9	T	17/49 (35%)	17 (100%)	0	0	100	100
9	k	17/49 (35%)	17 (100%)	0	0	100	100
10	L	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	U	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
10	l	161/174 (92%)	150 (93%)	11 (7%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	W	27/101 (27%)	27 (100%)	0	0	100 100
12	X	27/101 (27%)	27 (100%)	0	0	100 100
12	x	27/101 (27%)	27 (100%)	0	0	100 100
All	All	6621/7410 (89%)	6240 (94%)	373 (6%)	8 (0%)	49 72

All (8) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	613/641 (96%)	607 (99%)	6 (1%)	68 82
1	G	613/641 (96%)	607 (99%)	6 (1%)	68 82
1	a	613/641 (96%)	607 (99%)	6 (1%)	68 82
2	B	595/597 (100%)	590 (99%)	5 (1%)	73 85
2	H	595/597 (100%)	590 (99%)	5 (1%)	73 85
2	b	595/597 (100%)	590 (99%)	5 (1%)	73 85
3	C	68/69 (99%)	64 (94%)	4 (6%)	18 41
3	N	68/69 (99%)	64 (94%)	4 (6%)	18 41
3	c	68/69 (99%)	64 (94%)	4 (6%)	18 41
4	D	115/132 (87%)	111 (96%)	4 (4%)	32 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	115/132 (87%)	111 (96%)	4 (4%)	32	57
4	d	115/132 (87%)	111 (96%)	4 (4%)	32	57
5	E	54/60 (90%)	51 (94%)	3 (6%)	19	43
5	P	54/60 (90%)	51 (94%)	3 (6%)	19	43
5	e	54/60 (90%)	51 (94%)	3 (6%)	19	43
6	F	115/134 (86%)	107 (93%)	8 (7%)	14	34
6	Q	115/134 (86%)	107 (93%)	8 (7%)	14	34
6	f	115/134 (86%)	107 (93%)	8 (7%)	14	34
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%)	33 (92%)	3 (8%)	10	27
8	S	36/42 (86%)	33 (92%)	3 (8%)	10	27
8	j	36/42 (86%)	33 (92%)	3 (8%)	10	27
9	K	12/16 (75%)	11 (92%)	1 (8%)	10	27
9	T	12/16 (75%)	11 (92%)	1 (8%)	10	27
9	k	12/16 (75%)	11 (92%)	1 (8%)	10	27
10	L	128/138 (93%)	125 (98%)	3 (2%)	44	67
10	U	128/138 (93%)	125 (98%)	3 (2%)	44	67
10	l	128/138 (93%)	125 (98%)	3 (2%)	44	67
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	5469/5997 (91%)	5358 (98%)	111 (2%)	48	71

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	45	THR
1	G	95	ARG

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Mol	Chain	Res	Type
1	G	170	LEU
1	G	364	SER
1	G	480	ASP
1	G	641	MET
2	H	37	MET
2	H	110	ARG
2	H	296	ARG
2	H	297	ILE
2	H	387	MET
3	N	15	THR
3	N	19	ARG
3	N	49	VAL
3	N	73	THR
4	O	22	LEU
4	O	41	GLU
4	O	131	ARG
4	O	154	TYR
5	P	23	THR
5	P	34	ARG
5	P	58	GLU
6	Q	27	THR
6	Q	38	VAL
6	Q	48	TYR
6	Q	54	LEU
6	Q	62	CYS
6	Q	115	LYS
6	Q	146	GLU
6	Q	153	GLU
8	S	24	ILE
8	S	34	LEU
8	S	38	LEU
9	T	72	MET
10	U	14	LYS
10	U	123	LYS
10	U	132	ARG
1	a	45	THR
1	a	95	ARG
1	a	170	LEU
1	a	364	SER
1	a	480	ASP
1	a	641	MET
2	b	37	MET

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Mol	Chain	Res	Type
2	b	110	ARG
2	b	296	ARG
2	b	297	ILE
2	b	387	MET
3	c	15	THR
3	c	19	ARG
3	c	49	VAL
3	c	73	THR
4	d	22	LEU
4	d	41	GLU
4	d	131	ARG
4	d	154	TYR
5	e	23	THR
5	e	34	ARG
5	e	58	GLU
6	f	27	THR
6	f	38	VAL
6	f	48	TYR
6	f	54	LEU
6	f	62	CYS
6	f	115	LYS
6	f	146	GLU
6	f	153	GLU
8	j	24	ILE
8	j	34	LEU
8	j	38	LEU
9	k	72	MET
10	l	14	LYS
10	l	123	LYS
10	l	132	ARG
1	A	45	THR
1	A	95	ARG
1	A	170	LEU
1	A	364	SER
1	A	480	ASP
1	A	641	MET
2	B	37	MET
2	B	110	ARG
2	B	296	ARG
2	B	297	ILE
2	B	387	MET
3	C	15	THR

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Mol	Chain	Res	Type
3	C	19	ARG
3	C	49	VAL
3	C	73	THR
4	D	22	LEU
4	D	41	GLU
4	D	131	ARG
4	D	154	TYR
5	E	23	THR
5	E	34	ARG
5	E	58	GLU
6	F	27	THR
6	F	38	VAL
6	F	48	TYR
6	F	54	LEU
6	F	62	CYS
6	F	115	LYS
6	F	146	GLU
6	F	153	GLU
8	J	24	ILE
8	J	34	LEU
8	J	38	LEU
9	K	72	MET
10	L	14	LYS
10	L	123	LYS
10	L	132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	25	GLN
1	G	51	HIS
1	G	78	HIS
1	G	105	ASN
1	G	144	GLN
1	G	193	GLN
1	G	273	HIS
1	G	299	HIS
1	G	366	ASN
1	G	379	HIS
1	G	434	ASN
1	G	435	ASN
1	G	490	GLN

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Mol	Chain	Res	Type
1	G	539	HIS
1	G	604	ASN
1	G	731	GLN
1	G	751	GLN
2	H	34	HIS
2	H	53	HIS
2	H	67	HIS
2	H	95	GLN
2	H	132	ASN
2	H	211	ASN
2	H	235	GLN
2	H	242	HIS
2	H	332	ASN
2	H	444	ASN
2	H	610	GLN
2	H	691	GLN
4	O	25	GLN
4	O	70	GLN
5	P	19	GLN
6	Q	104	GLN
10	U	40	ASN
12	W	98	HIS
1	a	25	GLN
1	a	51	HIS
1	a	78	HIS
1	a	105	ASN
1	a	144	GLN
1	a	193	GLN
1	a	273	HIS
1	a	299	HIS
1	a	366	ASN
1	a	379	HIS
1	a	434	ASN
1	a	435	ASN
1	a	490	GLN
1	a	539	HIS
1	a	604	ASN
1	a	731	GLN
1	a	751	GLN
2	b	34	HIS
2	b	53	HIS
2	b	67	HIS

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Mol	Chain	Res	Type
2	b	95	GLN
2	b	111	ASN
2	b	206	HIS
2	b	235	GLN
2	b	242	HIS
2	b	332	ASN
2	b	444	ASN
2	b	610	GLN
2	b	691	GLN
4	d	25	GLN
4	d	70	GLN
5	e	19	GLN
6	f	104	GLN
10	l	40	ASN
10	l	81	HIS
12	x	98	HIS
1	A	25	GLN
1	A	51	HIS
1	A	78	HIS
1	A	105	ASN
1	A	144	GLN
1	A	193	GLN
1	A	273	HIS
1	A	299	HIS
1	A	366	ASN
1	A	379	HIS
1	A	434	ASN
1	A	435	ASN
1	A	490	GLN
1	A	539	HIS
1	A	604	ASN
1	A	731	GLN
1	A	751	GLN
2	B	34	HIS
2	B	53	HIS
2	B	67	HIS
2	B	95	GLN
2	B	111	ASN
2	B	211	ASN
2	B	235	GLN
2	B	242	HIS
2	B	332	ASN

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Mol	Chain	Res	Type
2	B	444	ASN
2	B	610	GLN
2	B	691	GLN
3	C	16	GLN
4	D	25	GLN
4	D	70	GLN
5	E	19	GLN
10	L	40	ASN
12	X	98	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
15	F6C	B	1230	-	52,54,74	3.04	27 (51%)	59,90,114	3.65	30 (50%)
14	CLA	b	1220	-	59,63,73	2.38	20 (33%)	70,101,113	2.74	26 (37%)
14	CLA	A	1113	-	49,53,73	2.48	20 (40%)	58,89,113	2.76	25 (43%)
14	CLA	G	1013	-	64,68,73	2.28	21 (32%)	76,107,113	2.60	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	1226	-	69,73,73	2.23	19 (27%)	82,113,113	2.35	27 (32%)
14	CLA	G	1118	-	59,63,73	2.38	21 (35%)	70,101,113	2.65	30 (42%)
16	PQN	A	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	A	1136	-	69,73,73	2.19	20 (28%)	82,113,113	2.49	25 (30%)
21	LMT	A	6001	-	32,32,36	1.25	5 (15%)	43,43,47	1.06	2 (4%)
16	PQN	B	2002	-	34,34,34	1.50	2 (5%)	43,45,45	1.28	3 (6%)
18	BCR	A	4008	-	41,41,41	2.90	7 (17%)	56,56,56	6.61	20 (35%)
14	CLA	b	1224	-	69,73,73	2.20	20 (28%)	82,113,113	2.47	24 (29%)
14	CLA	H	1217	-	59,63,73	2.36	20 (33%)	70,101,113	2.67	24 (34%)
14	CLA	a	1132	-	69,73,73	2.18	20 (28%)	82,113,113	2.61	27 (32%)
14	CLA	G	1132	-	69,73,73	2.19	20 (28%)	82,113,113	2.62	27 (32%)
19	LHG	B	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.14	3 (6%)
15	F6C	B	1207	-	72,74,74	2.66	26 (36%)	83,114,114	3.33	33 (39%)
19	LHG	A	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.12	3 (6%)
14	CLA	a	1133	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	26 (34%)
14	CLA	a	1134	-	49,53,73	2.57	21 (42%)	58,89,113	2.75	25 (43%)
14	CLA	b	1235	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	28 (36%)
14	CLA	a	1124	-	59,63,73	2.37	19 (32%)	70,101,113	2.74	28 (40%)
14	CLA	H	1225	-	69,73,73	2.23	19 (27%)	82,113,113	2.34	22 (26%)
14	CLA	L	1503	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	27 (32%)
15	F6C	B	1238	-	72,74,74	2.63	23 (31%)	83,114,114	3.21	34 (40%)
14	CLA	H	1219	-	49,53,73	2.52	22 (44%)	58,89,113	2.76	23 (39%)
14	CLA	G	1138	-	64,68,73	2.31	20 (31%)	76,107,113	2.52	27 (35%)
18	BCR	H	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	24 (42%)
14	CLA	a	1111	-	64,68,73	2.27	20 (31%)	76,107,113	4.44	29 (38%)
14	CLA	A	1115	-	69,73,73	2.20	20 (28%)	82,113,113	2.59	28 (34%)
14	CLA	b	1222	-	69,73,73	2.21	20 (28%)	82,113,113	2.54	29 (35%)
18	BCR	R	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
15	F6C	G	1121	-	52,54,74	3.04	24 (46%)	59,90,114	3.58	32 (54%)
14	CLA	G	1113	-	49,53,73	2.48	20 (40%)	58,89,113	2.76	25 (43%)
18	BCR	L	4019	-	41,41,41	2.75	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	a	1128	-	64,68,73	2.31	19 (29%)	76,107,113	2.51	26 (34%)
14	CLA	B	1217	-	59,63,73	2.36	20 (33%)	70,101,113	2.68	24 (34%)
14	CLA	b	1215	-	64,68,73	2.26	19 (29%)	76,107,113	2.48	24 (31%)
14	CLA	H	1221	-	69,73,73	2.19	20 (28%)	82,113,113	2.42	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	H	1213	-	69,73,73	2.21	20 (28%)	82,113,113	2.50	24 (29%)
14	CLA	H	1021	-	69,73,73	2.17	21 (30%)	82,113,113	2.43	26 (31%)
18	BCR	H	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
18	BCR	I	4018	-	41,41,41	2.84	7 (17%)	56,56,56	6.73	25 (44%)
14	CLA	a	1126	-	64,68,73	2.30	19 (29%)	76,107,113	2.55	29 (38%)
14	CLA	W	1701	-	59,63,73	2.37	20 (33%)	70,101,113	2.62	26 (37%)
18	BCR	b	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	G	1124	-	59,63,73	2.38	21 (35%)	70,101,113	2.74	28 (40%)
14	CLA	B	1221	-	69,73,73	2.19	20 (28%)	82,113,113	2.43	27 (32%)
14	CLA	a	1102	-	64,68,73	2.29	20 (31%)	76,107,113	2.58	26 (34%)
14	CLA	a	1107	1	49,53,73	2.49	19 (38%)	58,89,113	2.71	23 (39%)
14	CLA	G	1120	-	49,53,73	2.45	19 (38%)	58,89,113	2.81	22 (37%)
14	CLA	H	1216	-	69,73,73	2.21	22 (31%)	82,113,113	2.42	28 (34%)
14	CLA	a	1122	-	59,63,73	2.36	20 (33%)	70,101,113	2.65	28 (40%)
14	CLA	b	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.53	24 (29%)
14	CLA	b	1232	-	49,53,73	2.50	19 (38%)	58,89,113	2.70	23 (39%)
14	CLA	H	1239	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	34 (41%)
19	LHG	G	5001	-	41,41,48	1.00	2 (4%)	44,47,54	1.11	3 (6%)
20	LMG	H	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
18	BCR	H	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.90	20 (35%)
14	CLA	B	1205	-	69,73,73	2.16	20 (28%)	82,113,113	2.51	25 (30%)
14	CLA	a	1106	-	64,68,73	2.26	20 (31%)	76,107,113	2.66	27 (35%)
14	CLA	H	1214	-	69,73,73	2.23	21 (30%)	82,113,113	2.46	31 (37%)
14	CLA	H	1226	-	69,73,73	2.23	19 (27%)	82,113,113	2.35	27 (32%)
14	CLA	b	1023	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
18	BCR	a	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
13	CL0	a	1011	-	58,73,73	3.06	21 (36%)	60,113,113	2.96	21 (35%)
14	CLA	A	1117	-	69,73,73	2.17	20 (28%)	82,113,113	2.52	28 (34%)
14	CLA	a	1112	-	59,63,73	2.38	20 (33%)	70,101,113	2.66	27 (38%)
15	F6C	b	1230	-	52,54,74	3.04	27 (51%)	59,90,114	3.65	30 (50%)
14	CLA	a	1129	-	54,58,73	2.49	20 (37%)	64,95,113	2.74	24 (37%)
14	CLA	G	1102	-	64,68,73	2.29	20 (31%)	76,107,113	2.57	26 (34%)
14	CLA	G	1115	-	69,73,73	2.20	20 (28%)	82,113,113	2.59	28 (34%)
14	CLA	A	1013	-	64,68,73	2.28	21 (32%)	76,107,113	2.61	27 (35%)
14	CLA	a	1117	-	69,73,73	2.18	20 (28%)	82,113,113	2.51	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.71	24 (41%)
14	CLA	G	1111	-	64,68,73	2.27	20 (31%)	76,107,113	4.44	29 (38%)
14	CLA	H	1223	-	69,73,73	2.18	20 (28%)	82,113,113	2.55	29 (35%)
14	CLA	G	1135	-	64,68,73	2.28	20 (31%)	76,107,113	2.55	27 (35%)
14	CLA	B	1208	-	69,73,73	2.20	20 (28%)	82,113,113	2.44	27 (32%)
14	CLA	G	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.51	27 (35%)
18	BCR	H	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	19 (33%)
14	CLA	A	1105	-	49,53,73	2.50	20 (40%)	58,89,113	2.80	23 (39%)
14	CLA	H	1022	-	69,73,73	2.19	20 (28%)	82,113,113	2.53	29 (35%)
14	CLA	H	1231	2	59,63,73	2.37	20 (33%)	70,101,113	2.62	25 (35%)
14	CLA	x	1701	-	59,63,73	2.38	20 (33%)	70,101,113	2.63	26 (37%)
19	LHG	b	5004	-	43,43,48	0.97	2 (4%)	46,49,54	1.14	3 (6%)
14	CLA	H	1220	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	26 (37%)
18	BCR	i	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
20	LMG	U	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
17	SF4	A	3001	1,2	0,12,12	-	-	-		
14	CLA	B	1212	-	49,53,73	2.46	19 (38%)	58,89,113	2.73	20 (34%)
14	CLA	A	1128	-	64,68,73	2.31	19 (29%)	76,107,113	2.50	27 (35%)
14	CLA	a	1109	-	69,73,73	2.19	20 (28%)	82,113,113	2.51	27 (32%)
18	BCR	H	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)
14	CLA	b	1204	-	69,73,73	2.22	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	G	1129	-	54,58,73	2.49	20 (37%)	64,95,113	2.74	24 (37%)
19	LHG	H	5004	-	43,43,48	0.96	2 (4%)	46,49,54	1.14	3 (6%)
14	CLA	H	1224	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	24 (29%)
14	CLA	G	1107	1	49,53,73	2.49	19 (38%)	58,89,113	2.71	23 (39%)
14	CLA	H	1202	-	64,68,73	2.22	20 (31%)	76,107,113	2.59	28 (36%)
14	CLA	A	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.61	28 (40%)
15	F6C	b	1238	-	72,74,74	2.63	23 (31%)	83,114,114	3.21	34 (40%)
14	CLA	b	1201	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	25 (35%)
14	CLA	G	1106	-	64,68,73	2.26	20 (31%)	76,107,113	2.66	27 (35%)
14	CLA	a	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	24 (29%)
14	CLA	H	1210	-	69,73,73	2.22	22 (31%)	82,113,113	2.64	30 (36%)
18	BCR	a	4003	-	41,41,41	2.69	6 (14%)	56,56,56	6.70	22 (39%)
14	CLA	H	1205	-	69,73,73	2.17	20 (28%)	82,113,113	2.51	26 (31%)
18	BCR	m	4021	-	41,41,41	2.76	7 (17%)	56,56,56	6.81	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	b	1217	-	59,63,73	2.35	20 (33%)	70,101,113	2.67	24 (34%)
21	LMT	a	6001	-	32,32,36	1.24	5 (15%)	43,43,47	1.06	2 (4%)
14	CLA	b	1022	-	69,73,73	2.18	20 (28%)	82,113,113	2.53	29 (35%)
15	F6C	H	1207	-	72,74,74	2.66	26 (36%)	83,114,114	3.33	33 (39%)
14	CLA	G	1122	-	59,63,73	2.36	20 (33%)	70,101,113	2.66	28 (40%)
14	CLA	B	1233	-	49,53,73	2.51	20 (40%)	58,89,113	2.76	22 (37%)
18	BCR	a	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	a	1110	-	49,53,73	2.48	19 (38%)	58,89,113	2.72	22 (37%)
18	BCR	V	4021	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	16 (28%)
14	CLA	H	1222	-	69,73,73	2.21	20 (28%)	82,113,113	2.54	29 (35%)
14	CLA	a	1119	-	69,73,73	2.21	22 (31%)	82,113,113	2.47	25 (30%)
14	CLA	B	1225	-	69,73,73	2.23	19 (27%)	82,113,113	2.34	23 (28%)
14	CLA	H	1232	-	49,53,73	2.50	19 (38%)	58,89,113	2.70	23 (39%)
14	CLA	H	1215	-	64,68,73	2.26	19 (29%)	76,107,113	2.48	24 (31%)
15	F6C	b	1207	-	72,74,74	2.67	26 (36%)	83,114,114	3.33	33 (39%)
14	CLA	A	1122	-	59,63,73	2.36	20 (33%)	70,101,113	2.66	28 (40%)
18	BCR	B	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
18	BCR	G	4008	-	41,41,41	2.90	7 (17%)	56,56,56	6.61	20 (35%)
14	CLA	a	1130	-	59,63,73	2.39	19 (32%)	70,101,113	2.61	28 (40%)
18	BCR	H	4006	-	41,41,41	2.67	6 (14%)	56,56,56	6.76	21 (37%)
20	LMG	A	5005	-	46,46,55	1.38	5 (10%)	54,54,63	1.10	2 (3%)
14	CLA	H	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.53	24 (29%)
14	CLA	b	1209	-	49,53,73	2.49	21 (42%)	58,89,113	2.84	23 (39%)
14	CLA	H	1234	-	69,73,73	2.17	20 (28%)	82,113,113	2.45	24 (29%)
14	CLA	G	1110	-	49,53,73	2.49	19 (38%)	58,89,113	2.73	22 (37%)
14	CLA	B	1236	-	49,53,73	2.47	20 (40%)	58,89,113	2.78	22 (37%)
14	CLA	B	1229	-	64,68,73	2.29	21 (32%)	76,107,113	2.62	27 (35%)
14	CLA	A	1133	-	64,68,73	2.29	20 (31%)	76,107,113	2.61	26 (34%)
14	CLA	G	1119	-	69,73,73	2.20	22 (31%)	82,113,113	2.47	24 (29%)
14	CLA	A	1114	-	49,53,73	2.52	21 (42%)	58,89,113	2.72	21 (36%)
14	CLA	A	1102	-	64,68,73	2.29	20 (31%)	76,107,113	2.58	26 (34%)
14	CLA	G	1134	-	49,53,73	2.56	21 (42%)	58,89,113	2.75	24 (41%)
18	BCR	B	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.90	20 (35%)
13	CL0	A	1011	-	58,73,73	3.06	21 (36%)	60,113,113	2.96	21 (35%)
14	CLA	A	1111	-	64,68,73	2.27	20 (31%)	76,107,113	4.44	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	1216	-	69,73,73	2.20	22 (31%)	82,113,113	2.41	28 (34%)
14	CLA	b	1208	-	69,73,73	2.21	20 (28%)	82,113,113	2.44	27 (32%)
14	CLA	G	1012	-	69,73,73	2.20	19 (27%)	82,113,113	2.54	29 (35%)
14	CLA	b	1234	-	69,73,73	2.18	20 (28%)	82,113,113	2.45	24 (29%)
15	F6C	a	1121	-	52,54,74	3.05	24 (46%)	59,90,114	3.57	32 (54%)
14	CLA	b	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.76	21 (36%)
14	CLA	H	1236	-	49,53,73	2.48	20 (40%)	58,89,113	2.77	22 (37%)
14	CLA	G	1103	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	B	1213	-	69,73,73	2.20	20 (28%)	82,113,113	2.50	24 (29%)
14	CLA	b	1212	-	49,53,73	2.46	19 (38%)	58,89,113	2.74	20 (34%)
14	CLA	H	1201	-	59,63,73	2.37	20 (33%)	70,101,113	2.75	25 (35%)
14	CLA	b	1214	-	69,73,73	2.23	21 (30%)	82,113,113	2.46	31 (37%)
14	CLA	U	1502	-	64,68,73	2.24	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	G	1101	-	49,53,73	2.45	20 (40%)	58,89,113	2.81	22 (37%)
14	CLA	k	1401	-	49,53,73	2.52	22 (44%)	58,89,113	2.80	23 (39%)
14	CLA	H	1218	-	49,53,73	2.53	19 (38%)	58,89,113	2.65	21 (36%)
14	CLA	G	1133	-	64,68,73	2.29	20 (31%)	76,107,113	2.61	26 (34%)
14	CLA	G	1104	-	69,73,73	2.15	20 (28%)	82,113,113	2.62	25 (30%)
18	BCR	a	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	B	1022	-	69,73,73	2.18	20 (28%)	82,113,113	2.53	29 (35%)
14	CLA	A	1116	-	59,63,73	2.40	20 (33%)	70,101,113	2.69	30 (42%)
18	BCR	M	4021	-	41,41,41	2.77	7 (17%)	56,56,56	6.82	16 (28%)
21	LMT	A	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
14	CLA	A	1135	-	64,68,73	2.28	20 (31%)	76,107,113	2.54	27 (35%)
17	SF4	C	3003	3	0,12,12	-	-	-		
14	CLA	B	1231	2	59,63,73	2.38	20 (33%)	70,101,113	2.63	25 (35%)
14	CLA	G	1128	-	64,68,73	2.30	19 (29%)	76,107,113	2.50	26 (34%)
14	CLA	b	1223	-	69,73,73	2.18	20 (28%)	82,113,113	2.54	29 (35%)
14	CLA	A	1127	-	69,73,73	2.19	20 (28%)	82,113,113	2.46	24 (29%)
14	CLA	B	1202	-	64,68,73	2.22	20 (31%)	76,107,113	2.58	28 (36%)
14	CLA	a	1137	-	54,58,73	2.47	20 (37%)	64,95,113	2.89	27 (42%)
18	BCR	A	4003	-	41,41,41	2.69	7 (17%)	56,56,56	6.71	22 (39%)
14	CLA	b	1218	-	49,53,73	2.53	19 (38%)	58,89,113	2.65	21 (36%)
18	BCR	G	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	b	1231	2	59,63,73	2.38	20 (33%)	70,101,113	2.63	25 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	G	1131	-	64,68,73	2.29	20 (31%)	76,107,113	2.55	24 (31%)
14	CLA	G	1112	-	59,63,73	2.39	20 (33%)	70,101,113	2.66	27 (38%)
14	CLA	a	1115	-	69,73,73	2.20	20 (28%)	82,113,113	2.59	28 (34%)
14	CLA	B	1206	2	49,53,73	2.48	18 (36%)	58,89,113	2.60	23 (39%)
14	CLA	b	1227	-	49,53,73	2.54	20 (40%)	58,89,113	2.70	23 (39%)
14	CLA	b	1211	-	69,73,73	2.20	21 (30%)	82,113,113	2.50	25 (30%)
14	CLA	G	1117	-	69,73,73	2.18	20 (28%)	82,113,113	2.52	28 (34%)
18	BCR	B	4006	-	41,41,41	2.66	6 (14%)	56,56,56	6.77	21 (37%)
14	CLA	b	1205	-	69,73,73	2.17	20 (28%)	82,113,113	2.50	25 (30%)
14	CLA	a	1118	-	59,63,73	2.38	21 (35%)	70,101,113	2.65	30 (42%)
20	LMG	L	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
14	CLA	a	1101	-	49,53,73	2.45	19 (38%)	58,89,113	2.81	22 (37%)
14	CLA	a	1138	-	64,68,73	2.31	20 (31%)	76,107,113	2.51	25 (32%)
14	CLA	A	1118	-	59,63,73	2.38	21 (35%)	70,101,113	2.65	30 (42%)
14	CLA	B	1220	-	59,63,73	2.37	20 (33%)	70,101,113	2.74	26 (37%)
14	CLA	b	1206	2	49,53,73	2.49	18 (36%)	58,89,113	2.61	23 (39%)
15	F6C	H	1237	-	72,74,74	2.60	23 (31%)	83,114,114	3.18	33 (39%)
14	CLA	A	1125	-	69,73,73	2.17	20 (28%)	82,113,113	2.56	26 (31%)
17	SF4	c	3002	3	0,12,12	-	-	-		
14	CLA	a	1104	-	69,73,73	2.15	20 (28%)	82,113,113	2.62	25 (30%)
18	BCR	B	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
14	CLA	b	1229	-	64,68,73	2.29	20 (31%)	76,107,113	2.62	27 (35%)
14	CLA	A	1120	-	49,53,73	2.45	19 (38%)	58,89,113	2.81	22 (37%)
14	CLA	B	1224	-	69,73,73	2.20	20 (28%)	82,113,113	2.47	24 (29%)
14	CLA	B	1228	-	59,63,73	2.38	22 (37%)	70,101,113	2.65	28 (40%)
16	PQN	b	2002	-	34,34,34	1.51	2 (5%)	43,45,45	1.28	3 (6%)
18	BCR	a	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
20	LMG	R	5006	-	37,37,55	1.14	3 (8%)	45,45,63	1.21	4 (8%)
18	BCR	b	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	a	1116	-	59,63,73	2.40	20 (33%)	70,101,113	2.68	30 (42%)
14	CLA	G	1140	-	69,73,73	2.20	21 (30%)	82,113,113	2.42	26 (31%)
14	CLA	l	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.41	25 (30%)
14	CLA	B	1210	-	69,73,73	2.21	21 (30%)	82,113,113	2.64	29 (35%)
18	BCR	B	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	24 (42%)
18	BCR	B	4013	-	41,41,41	2.62	6 (14%)	56,56,56	6.87	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	H	1209	-	49,53,73	2.50	21 (42%)	58,89,113	2.85	23 (39%)
14	CLA	a	1131	-	64,68,73	2.29	20 (31%)	76,107,113	2.54	23 (30%)
14	CLA	A	1138	-	64,68,73	2.31	20 (31%)	76,107,113	2.52	27 (35%)
17	SF4	C	3002	3	0,12,12	-	-	-		
15	F6C	A	1121	-	52,54,74	3.05	24 (46%)	59,90,114	3.57	32 (54%)
14	CLA	A	1101	-	49,53,73	2.45	19 (38%)	58,89,113	2.80	22 (37%)
17	SF4	N	3002	3	0,12,12	-	-	-		
18	BCR	G	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	B	1222	-	69,73,73	2.22	20 (28%)	82,113,113	2.54	29 (35%)
18	BCR	U	4019	-	41,41,41	2.75	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	G	1136	-	69,73,73	2.19	20 (28%)	82,113,113	2.48	25 (30%)
18	BCR	B	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	18 (32%)
14	CLA	A	1104	-	69,73,73	2.15	20 (28%)	82,113,113	2.62	25 (30%)
18	BCR	b	4014	-	41,41,41	2.81	8 (19%)	56,56,56	6.59	25 (44%)
14	CLA	L	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
17	SF4	c	3003	3	0,12,12	-	-	-		
14	CLA	B	1215	-	64,68,73	2.26	19 (29%)	76,107,113	2.48	24 (31%)
14	CLA	H	1212	-	49,53,73	2.46	19 (38%)	58,89,113	2.74	20 (34%)
14	CLA	A	1124	-	59,63,73	2.38	19 (32%)	70,101,113	2.74	28 (40%)
14	CLA	b	1221	-	69,73,73	2.18	20 (28%)	82,113,113	2.42	27 (32%)
18	BCR	H	4005	-	41,41,41	2.77	8 (19%)	56,56,56	6.74	24 (42%)
18	BCR	b	4009	-	41,41,41	2.75	7 (17%)	56,56,56	6.58	20 (35%)
14	CLA	B	1219	-	49,53,73	2.53	22 (44%)	58,89,113	2.76	23 (39%)
18	BCR	G	4003	-	41,41,41	2.69	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	B	1232	-	49,53,73	2.50	19 (38%)	58,89,113	2.71	22 (37%)
14	CLA	H	1204	-	69,73,73	2.22	20 (28%)	82,113,113	2.48	29 (35%)
14	CLA	B	1214	-	69,73,73	2.23	21 (30%)	82,113,113	2.46	31 (37%)
14	CLA	b	1225	-	69,73,73	2.23	19 (27%)	82,113,113	2.34	23 (28%)
14	CLA	a	1140	-	69,73,73	2.19	21 (30%)	82,113,113	2.42	25 (30%)
14	CLA	B	1021	-	69,73,73	2.17	21 (30%)	82,113,113	2.44	25 (30%)
18	BCR	l	4022	-	41,41,41	2.85	7 (17%)	56,56,56	6.65	22 (39%)
14	CLA	a	1105	-	49,53,73	2.50	21 (42%)	58,89,113	2.79	23 (39%)
14	CLA	H	1208	-	69,73,73	2.21	20 (28%)	82,113,113	2.44	26 (31%)
18	BCR	A	4001	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	23 (41%)
14	CLA	H	1206	2	49,53,73	2.49	18 (36%)	58,89,113	2.61	23 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	1131	-	64,68,73	2.29	20 (31%)	76,107,113	2.54	24 (31%)
18	BCR	b	4017	-	41,41,41	2.79	7 (17%)	56,56,56	6.89	20 (35%)
14	CLA	B	1209	-	49,53,73	2.50	20 (40%)	58,89,113	2.85	23 (39%)
14	CLA	B	1023	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
14	CLA	A	1126	-	64,68,73	2.31	20 (31%)	76,107,113	2.56	29 (38%)
17	SF4	a	3001	1,2	0,12,12	-	-	-		
14	CLA	G	1125	-	69,73,73	2.17	20 (28%)	82,113,113	2.56	26 (31%)
14	CLA	G	1130	-	59,63,73	2.38	19 (32%)	70,101,113	2.61	29 (41%)
14	CLA	B	1223	-	69,73,73	2.18	20 (28%)	82,113,113	2.55	30 (36%)
18	BCR	H	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	a	1108	-	49,53,73	2.51	20 (40%)	58,89,113	2.73	24 (41%)
14	CLA	B	1226	-	69,73,73	2.22	19 (27%)	82,113,113	2.35	27 (32%)
15	F6C	B	1237	-	72,74,74	2.60	23 (31%)	83,114,114	3.18	33 (39%)
14	CLA	G	1105	-	49,53,73	2.50	21 (42%)	58,89,113	2.80	23 (39%)
14	CLA	G	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.71	24 (41%)
14	CLA	b	1228	-	59,63,73	2.38	22 (37%)	70,101,113	2.65	28 (40%)
18	BCR	B	4005	-	41,41,41	2.77	7 (17%)	56,56,56	6.74	23 (41%)
14	CLA	a	1103	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	25 (32%)
18	BCR	l	4019	-	41,41,41	2.76	6 (14%)	56,56,56	7.19	28 (50%)
14	CLA	A	1140	-	69,73,73	2.19	21 (30%)	82,113,113	2.41	25 (30%)
14	CLA	A	1112	-	59,63,73	2.38	20 (33%)	70,101,113	2.65	27 (38%)
14	CLA	A	1129	-	54,58,73	2.48	20 (37%)	64,95,113	2.73	24 (37%)
15	F6C	H	1238	-	72,74,74	2.63	23 (31%)	83,114,114	3.21	34 (40%)
18	BCR	b	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	X	1701	-	59,63,73	2.38	20 (33%)	70,101,113	2.63	26 (37%)
18	BCR	b	4005	-	41,41,41	2.77	7 (17%)	56,56,56	6.74	24 (42%)
14	CLA	A	1139	-	49,53,73	2.49	20 (40%)	58,89,113	2.71	24 (41%)
14	CLA	G	1108	-	49,53,73	2.51	20 (40%)	58,89,113	2.73	24 (41%)
14	CLA	B	1239	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	34 (41%)
18	BCR	I	4020	-	41,41,41	2.94	8 (19%)	56,56,56	6.92	22 (39%)
14	CLA	G	1126	-	64,68,73	2.30	19 (29%)	76,107,113	2.57	29 (38%)
18	BCR	B	4004	-	41,41,41	2.67	7 (17%)	56,56,56	6.65	25 (44%)
14	CLA	H	1227	-	49,53,73	2.54	20 (40%)	58,89,113	2.70	23 (39%)
16	PQN	G	2001	-	34,34,34	1.47	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	A	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.50	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	a	1113	-	49,53,73	2.47	20 (40%)	58,89,113	2.76	24 (41%)
18	BCR	A	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
20	LMG	a	5005	-	46,46,55	1.38	5 (10%)	54,54,63	1.10	2 (3%)
15	F6C	H	1230	-	52,54,74	3.04	27 (51%)	59,90,114	3.65	30 (50%)
18	BCR	b	4016	-	41,41,41	2.74	6 (14%)	56,56,56	6.81	19 (33%)
14	CLA	U	1503	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	28 (34%)
14	CLA	H	1023	-	69,73,73	2.19	21 (30%)	82,113,113	2.65	29 (35%)
21	LMT	G	6001	-	32,32,36	1.25	5 (15%)	43,43,47	1.06	2 (4%)
14	CLA	a	1012	-	69,73,73	2.20	19 (27%)	82,113,113	2.54	29 (35%)
14	CLA	H	1235	-	64,68,73	2.29	20 (31%)	76,107,113	2.56	28 (36%)
14	CLA	a	1114	-	49,53,73	2.52	21 (42%)	58,89,113	2.73	22 (37%)
14	CLA	A	1107	1	49,53,73	2.48	19 (38%)	58,89,113	2.71	23 (39%)
14	CLA	U	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.41	25 (30%)
18	BCR	R	4018	-	41,41,41	2.83	7 (17%)	56,56,56	6.73	25 (44%)
18	BCR	U	4022	-	41,41,41	2.85	7 (17%)	56,56,56	6.64	22 (39%)
20	LMG	i	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	4 (8%)
18	BCR	A	4002	-	41,41,41	2.74	6 (14%)	56,56,56	6.43	28 (50%)
14	CLA	b	1021	-	69,73,73	2.17	21 (30%)	82,113,113	2.44	25 (30%)
14	CLA	A	1106	-	64,68,73	2.26	20 (31%)	76,107,113	2.66	27 (35%)
20	LMG	G	5005	-	46,46,55	1.37	5 (10%)	54,54,63	1.10	2 (3%)
18	BCR	A	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)
14	CLA	a	1123	-	64,68,73	2.30	20 (31%)	76,107,113	2.50	27 (35%)
14	CLA	A	1109	-	69,73,73	2.19	20 (28%)	82,113,113	2.51	26 (31%)
14	CLA	b	1236	-	49,53,73	2.47	20 (40%)	58,89,113	2.77	22 (37%)
14	CLA	a	1135	-	64,68,73	2.29	20 (31%)	76,107,113	2.55	27 (35%)
14	CLA	G	1114	-	49,53,73	2.52	21 (42%)	58,89,113	2.72	21 (36%)
14	CLA	A	1110	-	49,53,73	2.49	19 (38%)	58,89,113	2.72	22 (37%)
18	BCR	i	4018	-	41,41,41	2.84	7 (17%)	56,56,56	6.73	25 (44%)
14	CLA	L	1501	10	69,73,73	2.19	20 (28%)	82,113,113	2.41	25 (30%)
14	CLA	A	1119	-	69,73,73	2.21	22 (31%)	82,113,113	2.47	26 (31%)
18	BCR	L	4022	-	41,41,41	2.85	6 (14%)	56,56,56	6.64	22 (39%)
14	CLA	b	1210	-	69,73,73	2.22	22 (31%)	82,113,113	2.64	30 (36%)
14	CLA	b	1239	-	69,73,73	2.23	20 (28%)	82,113,113	2.57	34 (41%)
14	CLA	H	1229	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	27 (35%)
14	CLA	A	1134	-	49,53,73	2.56	21 (42%)	58,89,113	2.76	24 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	l	1502	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	24 (31%)
14	CLA	b	1216	-	69,73,73	2.21	22 (31%)	82,113,113	2.42	28 (34%)
14	CLA	B	1204	-	69,73,73	2.22	20 (28%)	82,113,113	2.47	29 (35%)
14	CLA	H	1233	-	49,53,73	2.51	21 (42%)	58,89,113	2.76	22 (37%)
14	CLA	B	1235	-	64,68,73	2.29	20 (31%)	76,107,113	2.57	28 (36%)
14	CLA	A	1012	-	69,73,73	2.20	19 (27%)	82,113,113	2.53	29 (35%)
18	BCR	G	4007	-	41,41,41	2.87	8 (19%)	56,56,56	6.72	24 (42%)
13	CL0	G	1011	-	58,73,73	3.06	21 (36%)	60,113,113	2.96	21 (35%)
15	F6C	b	1237	-	72,74,74	2.59	24 (33%)	83,114,114	3.17	33 (39%)
16	PQN	a	2001	-	34,34,34	1.46	2 (5%)	43,45,45	1.28	6 (13%)
14	CLA	a	1136	-	69,73,73	2.19	19 (27%)	82,113,113	2.48	26 (31%)
14	CLA	B	1234	-	69,73,73	2.17	20 (28%)	82,113,113	2.45	24 (29%)
14	CLA	A	1103	-	64,68,73	2.25	20 (31%)	76,107,113	2.60	25 (32%)
14	CLA	b	1213	-	69,73,73	2.21	20 (28%)	82,113,113	2.50	24 (29%)
21	LMT	a	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
17	SF4	G	3001	1,2	0,12,12	-	-	-		
14	CLA	G	1116	-	59,63,73	2.39	20 (33%)	70,101,113	2.67	30 (42%)
14	CLA	T	1401	-	49,53,73	2.52	22 (44%)	58,89,113	2.81	23 (39%)
14	CLA	l	1503	-	69,73,73	2.21	20 (28%)	82,113,113	2.47	27 (32%)
14	CLA	b	1219	-	49,53,73	2.52	22 (44%)	58,89,113	2.76	23 (39%)
14	CLA	H	1211	-	69,73,73	2.20	21 (30%)	82,113,113	2.50	25 (30%)
14	CLA	G	1109	-	69,73,73	2.19	20 (28%)	82,113,113	2.51	26 (31%)
18	BCR	a	4008	-	41,41,41	2.90	6 (14%)	56,56,56	6.61	20 (35%)
16	PQN	H	2002	-	34,34,34	1.51	2 (5%)	43,45,45	1.28	4 (9%)
14	CLA	B	1201	-	59,63,73	2.37	20 (33%)	70,101,113	2.75	25 (35%)
20	LMG	I	5006	-	37,37,55	1.13	3 (8%)	45,45,63	1.21	4 (8%)
14	CLA	A	1137	-	54,58,73	2.47	20 (37%)	64,95,113	2.88	27 (42%)
14	CLA	K	1401	-	49,53,73	2.53	22 (44%)	58,89,113	2.81	23 (39%)
21	LMT	G	6002	-	29,29,36	1.36	6 (20%)	40,40,47	1.18	4 (10%)
14	CLA	a	1013	-	64,68,73	2.28	21 (32%)	76,107,113	2.61	26 (34%)
14	CLA	B	1203	-	69,73,73	2.17	20 (28%)	82,113,113	2.53	23 (28%)
14	CLA	b	1202	-	64,68,73	2.22	21 (32%)	76,107,113	2.59	28 (36%)
17	SF4	N	3003	3	0,12,12	-	-	-		
20	LMG	B	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
14	CLA	A	1132	-	69,73,73	2.19	20 (28%)	82,113,113	2.61	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	LHG	a	5001	-	41,41,48	0.99	2 (4%)	44,47,54	1.11	3 (6%)
14	CLA	a	1125	-	69,73,73	2.18	20 (28%)	82,113,113	2.56	26 (31%)
14	CLA	G	1127	-	69,73,73	2.20	20 (28%)	82,113,113	2.46	24 (29%)
20	LMG	l	5007	-	50,50,55	1.45	7 (14%)	58,58,63	1.10	2 (3%)
18	BCR	H	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.84	20 (35%)
14	CLA	a	1120	-	49,53,73	2.46	19 (38%)	58,89,113	2.82	22 (37%)
14	CLA	B	1218	-	49,53,73	2.54	19 (38%)	58,89,113	2.66	21 (36%)
14	CLA	A	1108	-	49,53,73	2.51	20 (40%)	58,89,113	2.74	24 (41%)
14	CLA	G	1137	-	54,58,73	2.47	20 (37%)	64,95,113	2.89	27 (42%)
20	LMG	b	5002	-	46,46,55	1.34	5 (10%)	54,54,63	1.27	4 (7%)
18	BCR	b	4006	-	41,41,41	2.67	6 (14%)	56,56,56	6.76	21 (37%)
14	CLA	B	1227	-	49,53,73	2.54	20 (40%)	58,89,113	2.70	24 (41%)
14	CLA	B	1211	-	69,73,73	2.20	21 (30%)	82,113,113	2.49	25 (30%)
14	CLA	H	1228	-	59,63,73	2.38	22 (37%)	70,101,113	2.66	28 (40%)
18	BCR	G	4011	-	41,41,41	2.80	7 (17%)	56,56,56	6.69	28 (50%)

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
15	F6C	B	1230	-	1/1/6/16	8/17/73/97	-
14	CLA	b	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	A	1113	-	1/1/11/20	9/15/91/115	-
14	CLA	G	1013	-	1/1/14/20	12/33/109/115	-
14	CLA	b	1226	-	1/1/15/20	11/39/115/115	-
14	CLA	G	1118	-	1/1/13/20	10/27/103/115	-
16	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	A	1136	-	1/1/15/20	19/39/115/115	-
21	LMT	A	6001	-	-	6/17/57/61	0/2/2/2
16	PQN	B	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	A	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	b	1224	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1217	-	1/1/13/20	13/27/103/115	-
14	CLA	a	1132	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	1132	-	1/1/15/20	14/39/115/115	-
19	LHG	B	5004	-	-	25/48/48/53	-
15	F6C	B	1207	-	1/1/10/16	20/41/97/97	-
19	LHG	A	5001	-	-	23/46/46/53	-
14	CLA	a	1133	-	1/1/14/20	9/33/109/115	-
14	CLA	a	1134	-	1/1/11/20	5/15/91/115	-
14	CLA	b	1235	-	1/1/14/20	12/33/109/115	-
14	CLA	a	1124	-	1/1/13/20	11/27/103/115	-
14	CLA	H	1225	-	1/1/15/20	15/39/115/115	-
14	CLA	L	1503	-	1/1/15/20	15/39/115/115	-
15	F6C	B	1238	-	1/1/10/16	16/41/97/97	-
14	CLA	H	1219	-	1/1/11/20	5/15/91/115	-
14	CLA	G	1138	-	1/1/14/20	15/33/109/115	-
18	BCR	H	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	a	1111	-	1/1/14/20	13/33/109/115	-
14	CLA	A	1115	-	1/1/15/20	20/39/115/115	-
14	CLA	b	1222	-	1/1/15/20	17/39/115/115	-
18	BCR	R	4020	-	-	12/29/63/63	0/2/2/2
15	F6C	G	1121	-	1/1/6/16	9/17/73/97	-
14	CLA	G	1113	-	1/1/11/20	9/15/91/115	-
18	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	B	1217	-	1/1/13/20	13/27/103/115	-
14	CLA	b	1215	-	1/1/14/20	18/33/109/115	-
14	CLA	H	1221	-	1/1/15/20	11/39/115/115	-
14	CLA	H	1213	-	1/1/15/20	16/39/115/115	-
14	CLA	H	1021	-	1/1/15/20	20/39/115/115	-
18	BCR	H	4009	-	-	8/29/63/63	0/2/2/2
18	BCR	I	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	a	1126	-	1/1/14/20	21/33/109/115	-
14	CLA	W	1701	-	1/1/13/20	11/27/103/115	-
18	BCR	b	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	G	1124	-	1/1/13/20	11/27/103/115	-
14	CLA	B	1221	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1102	-	1/1/14/20	14/33/109/115	-
14	CLA	a	1107	1	1/1/11/20	5/15/91/115	-
14	CLA	G	1120	-	1/1/11/20	9/15/91/115	-
14	CLA	H	1216	-	1/1/15/20	21/39/115/115	-
14	CLA	a	1122	-	1/1/13/20	13/27/103/115	-
14	CLA	b	1203	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	H	1239	-	1/1/15/20	22/39/115/115	-
19	LHG	G	5001	-	-	23/46/46/53	-
20	LMG	H	5002	-	-	12/41/61/70	0/1/1/1
18	BCR	H	4017	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1205	-	1/1/15/20	10/39/115/115	-
14	CLA	a	1106	-	1/1/14/20	13/33/109/115	-
14	CLA	H	1214	-	1/1/15/20	17/39/115/115	-
14	CLA	H	1226	-	1/1/15/20	11/39/115/115	-
14	CLA	b	1023	-	1/1/15/20	15/39/115/115	-
18	BCR	a	4007	-	-	12/29/63/63	0/2/2/2
13	CL0	a	1011	-	3/3/20/25	10/37/135/135	-
14	CLA	A	1117	-	1/1/15/20	19/39/115/115	-
14	CLA	a	1112	-	1/1/13/20	14/27/103/115	-
15	F6C	b	1230	-	1/1/6/16	8/17/73/97	-
14	CLA	a	1129	-	1/1/12/20	7/21/97/115	-
14	CLA	G	1102	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1115	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1013	-	1/1/14/20	12/33/109/115	-
14	CLA	a	1117	-	1/1/15/20	19/39/115/115	-
14	CLA	a	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1111	-	1/1/14/20	13/33/109/115	-
14	CLA	H	1223	-	1/1/15/20	17/39/115/115	-
14	CLA	G	1135	-	1/1/14/20	14/33/109/115	-
14	CLA	B	1208	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1123	-	1/1/14/20	13/33/109/115	-
18	BCR	H	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	A	1105	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1022	-	1/1/15/20	19/39/115/115	-
14	CLA	H	1231	2	1/1/13/20	7/27/103/115	-
14	CLA	x	1701	-	1/1/13/20	11/27/103/115	-
19	LHG	b	5004	-	-	25/48/48/53	-
14	CLA	H	1220	-	1/1/13/20	10/27/103/115	-
18	BCR	i	4020	-	-	12/29/63/63	0/2/2/2
20	LMG	U	5007	-	-	14/45/65/70	0/1/1/1
17	SF4	A	3001	1,2	-	-	0/6/5/5
14	CLA	B	1212	-	1/1/11/20	4/15/91/115	-
14	CLA	A	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	a	1109	-	1/1/15/20	19/39/115/115	-
18	BCR	H	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	b	1204	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1129	-	1/1/12/20	7/21/97/115	-
19	LHG	H	5004	-	-	25/48/48/53	-
14	CLA	H	1224	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1107	1	1/1/11/20	5/15/91/115	-
14	CLA	H	1202	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1130	-	1/1/13/20	9/27/103/115	-
15	F6C	b	1238	-	1/1/10/16	16/41/97/97	-
14	CLA	b	1201	-	1/1/13/20	7/27/103/115	-
14	CLA	G	1106	-	1/1/14/20	13/33/109/115	-
14	CLA	a	1127	-	1/1/15/20	13/39/115/115	-
14	CLA	H	1210	-	1/1/15/20	14/39/115/115	-
18	BCR	a	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	H	1205	-	1/1/15/20	10/39/115/115	-
18	BCR	m	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	b	1217	-	1/1/13/20	13/27/103/115	-
21	LMT	a	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	b	1022	-	1/1/15/20	19/39/115/115	-
15	F6C	H	1207	-	1/1/10/16	20/41/97/97	-
14	CLA	G	1122	-	1/1/13/20	12/27/103/115	-
14	CLA	B	1233	-	1/1/11/20	7/15/91/115	-
18	BCR	a	4011	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	1110	-	1/1/11/20	7/15/91/115	-
18	BCR	V	4021	-	-	18/29/63/63	0/2/2/2
14	CLA	H	1222	-	1/1/15/20	17/39/115/115	-
14	CLA	a	1119	-	1/1/15/20	9/39/115/115	-
14	CLA	B	1225	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	H	1215	-	1/1/14/20	18/33/109/115	-
15	F6C	b	1207	-	1/1/10/16	20/41/97/97	-
14	CLA	A	1122	-	1/1/13/20	13/27/103/115	-
18	BCR	B	4010	-	-	10/29/63/63	0/2/2/2
18	BCR	G	4008	-	-	12/29/63/63	0/2/2/2
14	CLA	a	1130	-	1/1/13/20	9/27/103/115	-
18	BCR	H	4006	-	-	10/29/63/63	0/2/2/2
20	LMG	A	5005	-	-	19/41/61/70	0/1/1/1
14	CLA	H	1203	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1209	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1234	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1110	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1236	-	1/1/11/20	3/15/91/115	-
14	CLA	B	1229	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1133	-	1/1/14/20	9/33/109/115	-
14	CLA	G	1119	-	1/1/15/20	9/39/115/115	-
14	CLA	A	1114	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1102	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1134	-	1/1/11/20	5/15/91/115	-
18	BCR	B	4017	-	-	13/29/63/63	0/2/2/2
13	CL0	A	1011	-	3/3/20/25	10/37/135/135	-
14	CLA	A	1111	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1216	-	1/1/15/20	21/39/115/115	-
14	CLA	b	1208	-	1/1/15/20	16/39/115/115	-
14	CLA	G	1012	-	1/1/15/20	11/39/115/115	-
14	CLA	b	1234	-	1/1/15/20	18/39/115/115	-
15	F6C	a	1121	-	1/1/6/16	9/17/73/97	-
14	CLA	b	1233	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	1236	-	1/1/11/20	3/15/91/115	-
14	CLA	G	1103	-	1/1/14/20	13/33/109/115	-
14	CLA	B	1213	-	1/1/15/20	16/39/115/115	-
14	CLA	b	1212	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1201	-	1/1/13/20	7/27/103/115	-
14	CLA	b	1214	-	1/1/15/20	17/39/115/115	-
14	CLA	U	1502	-	1/1/14/20	11/33/109/115	-
14	CLA	G	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	k	1401	-	1/1/11/20	9/15/91/115	-
14	CLA	H	1218	-	1/1/11/20	6/15/91/115	-
14	CLA	G	1133	-	1/1/14/20	9/33/109/115	-
14	CLA	G	1104	-	1/1/15/20	9/39/115/115	-
18	BCR	a	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1022	-	1/1/15/20	19/39/115/115	-
14	CLA	A	1116	-	1/1/13/20	12/27/103/115	-
18	BCR	M	4021	-	-	18/29/63/63	0/2/2/2
21	LMT	A	6002	-	-	8/14/54/61	0/2/2/2
14	CLA	A	1135	-	1/1/14/20	14/33/109/115	-
17	SF4	C	3003	3	-	-	0/6/5/5
14	CLA	B	1231	2	1/1/13/20	7/27/103/115	-
14	CLA	G	1128	-	1/1/14/20	15/33/109/115	-
14	CLA	b	1223	-	1/1/15/20	17/39/115/115	-
14	CLA	A	1127	-	1/1/15/20	13/39/115/115	-
14	CLA	B	1202	-	1/1/14/20	14/33/109/115	-
14	CLA	a	1137	-	1/1/12/20	5/21/97/115	-
18	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	b	1218	-	1/1/11/20	6/15/91/115	-
18	BCR	G	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	b	1231	2	1/1/13/20	7/27/103/115	-
14	CLA	G	1131	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1112	-	1/1/13/20	14/27/103/115	-
14	CLA	a	1115	-	1/1/15/20	20/39/115/115	-
14	CLA	B	1206	2	1/1/11/20	5/15/91/115	-
14	CLA	b	1227	-	1/1/11/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1211	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1117	-	1/1/15/20	19/39/115/115	-
18	BCR	B	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	b	1205	-	1/1/15/20	10/39/115/115	-
14	CLA	a	1118	-	1/1/13/20	10/27/103/115	-
20	LMG	L	5007	-	-	15/45/65/70	0/1/1/1
14	CLA	a	1101	-	1/1/11/20	8/15/91/115	-
14	CLA	a	1138	-	1/1/14/20	15/33/109/115	-
14	CLA	A	1118	-	1/1/13/20	10/27/103/115	-
14	CLA	B	1220	-	1/1/13/20	10/27/103/115	-
14	CLA	b	1206	2	1/1/11/20	5/15/91/115	-
15	F6C	H	1237	-	1/1/10/16	18/41/97/97	-
14	CLA	A	1125	-	1/1/15/20	18/39/115/115	-
17	SF4	c	3002	3	-	-	0/6/5/5
14	CLA	a	1104	-	1/1/15/20	9/39/115/115	-
18	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	b	1229	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1120	-	1/1/11/20	9/15/91/115	-
14	CLA	B	1224	-	1/1/15/20	16/39/115/115	-
14	CLA	B	1228	-	1/1/13/20	14/27/103/115	-
16	PQN	b	2002	-	-	12/23/43/43	0/2/2/2
18	BCR	a	4002	-	-	6/29/63/63	0/2/2/2
20	LMG	R	5006	-	-	10/32/52/70	0/1/1/1
18	BCR	b	4010	-	-	10/29/63/63	0/2/2/2
14	CLA	a	1116	-	1/1/13/20	12/27/103/115	-
14	CLA	G	1140	-	1/1/15/20	21/39/115/115	-
14	CLA	l	1501	10	1/1/15/20	12/39/115/115	-
14	CLA	B	1210	-	1/1/15/20	14/39/115/115	-
18	BCR	B	4014	-	-	7/29/63/63	0/2/2/2
18	BCR	B	4013	-	-	11/29/63/63	0/2/2/2
14	CLA	H	1209	-	1/1/11/20	5/15/91/115	-
14	CLA	a	1131	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1138	-	1/1/14/20	15/33/109/115	-
17	SF4	C	3002	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	F6C	A	1121	-	1/1/6/16	9/17/73/97	-
14	CLA	A	1101	-	1/1/11/20	8/15/91/115	-
17	SF4	N	3002	3	-	-	0/6/5/5
18	BCR	G	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	B	1222	-	1/1/15/20	17/39/115/115	-
18	BCR	U	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	G	1136	-	1/1/15/20	19/39/115/115	-
18	BCR	B	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	A	1104	-	1/1/15/20	9/39/115/115	-
18	BCR	b	4014	-	-	7/29/63/63	0/2/2/2
14	CLA	L	1502	-	1/1/14/20	11/33/109/115	-
17	SF4	c	3003	3	-	-	0/6/5/5
14	CLA	B	1215	-	1/1/14/20	18/33/109/115	-
14	CLA	H	1212	-	1/1/11/20	4/15/91/115	-
14	CLA	A	1124	-	1/1/13/20	11/27/103/115	-
14	CLA	b	1221	-	1/1/15/20	10/39/115/115	-
18	BCR	H	4005	-	-	4/29/63/63	0/2/2/2
18	BCR	b	4009	-	-	8/29/63/63	0/2/2/2
14	CLA	B	1219	-	1/1/11/20	5/15/91/115	-
18	BCR	G	4003	-	-	14/29/63/63	0/2/2/2
14	CLA	B	1232	-	1/1/11/20	2/15/91/115	-
14	CLA	H	1204	-	1/1/15/20	16/39/115/115	-
14	CLA	B	1214	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1225	-	1/1/15/20	15/39/115/115	-
14	CLA	a	1140	-	1/1/15/20	21/39/115/115	-
14	CLA	B	1021	-	1/1/15/20	20/39/115/115	-
18	BCR	l	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	a	1105	-	1/1/11/20	4/15/91/115	-
14	CLA	H	1208	-	1/1/15/20	16/39/115/115	-
18	BCR	A	4001	-	-	14/29/63/63	0/2/2/2
14	CLA	H	1206	2	1/1/11/20	5/15/91/115	-
14	CLA	A	1131	-	1/1/14/20	14/33/109/115	-
18	BCR	b	4017	-	-	13/29/63/63	0/2/2/2
14	CLA	B	1209	-	1/1/11/20	5/15/91/115	-

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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	A	1126	-	1/1/14/20	21/33/109/115	-
17	SF4	a	3001	1,2	-	-	0/6/5/5
14	CLA	G	1125	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1130	-	1/1/13/20	9/27/103/115	-
14	CLA	B	1223	-	1/1/15/20	17/39/115/115	-
18	BCR	H	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	a	1108	-	1/1/11/20	4/15/91/115	-
14	CLA	B	1226	-	1/1/15/20	11/39/115/115	-
15	F6C	B	1237	-	1/1/10/16	18/41/97/97	-
14	CLA	G	1105	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	b	1228	-	1/1/13/20	14/27/103/115	-
18	BCR	B	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	a	1103	-	1/1/14/20	13/33/109/115	-
18	BCR	l	4019	-	-	12/29/63/63	0/2/2/2
14	CLA	A	1140	-	1/1/15/20	21/39/115/115	-
14	CLA	A	1112	-	1/1/13/20	14/27/103/115	-
14	CLA	A	1129	-	1/1/12/20	7/21/97/115	-
15	F6C	H	1238	-	1/1/10/16	16/41/97/97	-
18	BCR	b	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	X	1701	-	1/1/13/20	11/27/103/115	-
18	BCR	b	4005	-	-	4/29/63/63	0/2/2/2
14	CLA	A	1139	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1108	-	1/1/11/20	4/15/91/115	-
14	CLA	B	1239	-	1/1/15/20	22/39/115/115	-
18	BCR	I	4020	-	-	12/29/63/63	0/2/2/2
14	CLA	G	1126	-	1/1/14/20	21/33/109/115	-
18	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	CLA	H	1227	-	1/1/11/20	7/15/91/115	-
16	PQN	G	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	A	1123	-	1/1/14/20	13/33/109/115	-
14	CLA	a	1113	-	1/1/11/20	9/15/91/115	-
18	BCR	A	4007	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	a	5005	-	-	19/41/61/70	0/1/1/1
15	F6C	H	1230	-	1/1/6/16	8/17/73/97	-
18	BCR	b	4016	-	-	10/29/63/63	0/2/2/2
14	CLA	U	1503	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1023	-	1/1/15/20	15/39/115/115	-
21	LMT	G	6001	-	-	7/17/57/61	0/2/2/2
14	CLA	a	1012	-	1/1/15/20	11/39/115/115	-
14	CLA	H	1235	-	1/1/14/20	12/33/109/115	-
14	CLA	a	1114	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1107	1	1/1/11/20	5/15/91/115	-
14	CLA	U	1501	10	1/1/15/20	12/39/115/115	-
18	BCR	R	4018	-	-	8/29/63/63	0/2/2/2
18	BCR	U	4022	-	-	6/29/63/63	0/2/2/2
20	LMG	i	5006	-	-	10/32/52/70	0/1/1/1
18	BCR	A	4002	-	-	6/29/63/63	0/2/2/2
14	CLA	b	1021	-	1/1/15/20	20/39/115/115	-
14	CLA	A	1106	-	1/1/14/20	13/33/109/115	-
20	LMG	G	5005	-	-	19/41/61/70	0/1/1/1
18	BCR	A	4011	-	-	17/29/63/63	0/2/2/2
14	CLA	a	1123	-	1/1/14/20	13/33/109/115	-
14	CLA	A	1109	-	1/1/15/20	19/39/115/115	-
14	CLA	b	1236	-	1/1/11/20	3/15/91/115	-
14	CLA	a	1135	-	1/1/14/20	14/33/109/115	-
14	CLA	G	1114	-	1/1/11/20	11/15/91/115	-
14	CLA	A	1110	-	1/1/11/20	7/15/91/115	-
18	BCR	i	4018	-	-	8/29/63/63	0/2/2/2
14	CLA	L	1501	10	1/1/15/20	12/39/115/115	-
14	CLA	A	1119	-	1/1/15/20	9/39/115/115	-
18	BCR	L	4022	-	-	6/29/63/63	0/2/2/2
14	CLA	b	1210	-	1/1/15/20	14/39/115/115	-
14	CLA	b	1239	-	1/1/15/20	22/39/115/115	-
14	CLA	H	1229	-	1/1/14/20	14/33/109/115	-
14	CLA	A	1134	-	1/1/11/20	5/15/91/115	-
14	CLA	l	1502	-	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	1216	-	1/1/15/20	21/39/115/115	-
14	CLA	B	1204	-	1/1/15/20	15/39/115/115	-
14	CLA	H	1233	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1235	-	1/1/14/20	12/33/109/115	-
14	CLA	A	1012	-	1/1/15/20	11/39/115/115	-
18	BCR	G	4007	-	-	12/29/63/63	0/2/2/2
13	CL0	G	1011	-	3/3/20/25	10/37/135/135	-
15	F6C	b	1237	-	1/1/10/16	18/41/97/97	-
16	PQN	a	2001	-	-	9/23/43/43	0/2/2/2
14	CLA	a	1136	-	1/1/15/20	19/39/115/115	-
14	CLA	B	1234	-	1/1/15/20	18/39/115/115	-
14	CLA	A	1103	-	1/1/14/20	13/33/109/115	-
14	CLA	b	1213	-	1/1/15/20	16/39/115/115	-
21	LMT	a	6002	-	-	8/14/54/61	0/2/2/2
17	SF4	G	3001	1,2	-	-	0/6/5/5
14	CLA	G	1116	-	1/1/13/20	12/27/103/115	-
14	CLA	T	1401	-	1/1/11/20	9/15/91/115	-
14	CLA	l	1503	-	1/1/15/20	15/39/115/115	-
14	CLA	b	1219	-	1/1/11/20	5/15/91/115	-
14	CLA	H	1211	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1109	-	1/1/15/20	19/39/115/115	-
18	BCR	a	4008	-	-	12/29/63/63	0/2/2/2
16	PQN	H	2002	-	-	12/23/43/43	0/2/2/2
14	CLA	B	1201	-	1/1/13/20	7/27/103/115	-
20	LMG	I	5006	-	-	10/32/52/70	0/1/1/1
14	CLA	A	1137	-	1/1/12/20	5/21/97/115	-
14	CLA	K	1401	-	1/1/11/20	9/15/91/115	-
21	LMT	G	6002	-	-	7/14/54/61	0/2/2/2
14	CLA	a	1013	-	1/1/14/20	12/33/109/115	-
14	CLA	B	1203	-	1/1/15/20	17/39/115/115	-
14	CLA	b	1202	-	1/1/14/20	14/33/109/115	-
20	LMG	B	5002	-	-	13/41/61/70	0/1/1/1
17	SF4	N	3003	3	-	-	0/6/5/5
14	CLA	A	1132	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	a	5001	-	-	23/46/46/53	-
14	CLA	a	1125	-	1/1/15/20	18/39/115/115	-
14	CLA	G	1127	-	1/1/15/20	13/39/115/115	-
20	LMG	l	5007	-	-	14/45/65/70	0/1/1/1
18	BCR	H	4010	-	-	10/29/63/63	0/2/2/2
14	CLA	a	1120	-	1/1/11/20	9/15/91/115	-
14	CLA	B	1218	-	1/1/11/20	6/15/91/115	-
14	CLA	A	1108	-	1/1/11/20	4/15/91/115	-
14	CLA	G	1137	-	1/1/12/20	5/21/97/115	-
20	LMG	b	5002	-	-	13/41/61/70	0/1/1/1
18	BCR	b	4006	-	-	10/29/63/63	0/2/2/2
14	CLA	B	1227	-	1/1/11/20	7/15/91/115	-
14	CLA	B	1211	-	1/1/15/20	18/39/115/115	-
14	CLA	H	1228	-	1/1/13/20	14/27/103/115	-
18	BCR	G	4011	-	-	17/29/63/63	0/2/2/2

All (6019) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1230	F6C	C1A-CHA	9.56	1.50	1.35
15	B	1230	F6C	C1A-CHA	9.54	1.50	1.35
15	H	1230	F6C	C1A-CHA	9.53	1.50	1.35
15	b	1207	F6C	C1A-CHA	9.52	1.50	1.35
15	H	1207	F6C	C1A-CHA	9.51	1.50	1.35
15	B	1207	F6C	C1A-CHA	9.51	1.50	1.35
15	A	1121	F6C	C1A-CHA	9.37	1.50	1.35
15	a	1121	F6C	C1A-CHA	9.36	1.50	1.35
15	G	1121	F6C	C1A-CHA	9.33	1.50	1.35
15	H	1237	F6C	C1A-CHA	9.27	1.50	1.35
15	B	1237	F6C	C1A-CHA	9.25	1.50	1.35
15	b	1237	F6C	C1A-CHA	9.21	1.50	1.35
15	B	1238	F6C	C1A-CHA	9.03	1.50	1.35
15	H	1238	F6C	C1A-CHA	9.00	1.49	1.35
15	b	1238	F6C	C1A-CHA	8.99	1.49	1.35
18	I	4020	BCR	C8-C9	-8.92	1.26	1.46
18	V	4021	BCR	C8-C9	-8.92	1.26	1.46
18	i	4020	BCR	C8-C9	-8.91	1.26	1.46
18	M	4021	BCR	C8-C9	-8.91	1.26	1.46
18	m	4021	BCR	C8-C9	-8.90	1.26	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	1121	F6C	MG-NA	8.88	2.23	2.05
18	R	4020	BCR	C8-C9	-8.87	1.27	1.46
15	G	1121	F6C	MG-NA	8.85	2.23	2.05
15	a	1121	F6C	MG-NA	8.84	2.23	2.05
18	L	4022	BCR	C8-C9	-8.83	1.27	1.46
18	I	4018	BCR	C8-C9	-8.82	1.27	1.46
18	G	4007	BCR	C8-C9	-8.82	1.27	1.46
18	l	4022	BCR	C8-C9	-8.81	1.27	1.46
18	A	4007	BCR	C8-C9	-8.80	1.27	1.46
18	A	4008	BCR	C8-C9	-8.80	1.27	1.46
18	U	4022	BCR	C8-C9	-8.79	1.27	1.46
18	i	4018	BCR	C8-C9	-8.79	1.27	1.46
18	G	4011	BCR	C8-C9	-8.79	1.27	1.46
18	a	4007	BCR	C8-C9	-8.78	1.27	1.46
18	R	4018	BCR	C8-C9	-8.78	1.27	1.46
18	a	4008	BCR	C8-C9	-8.77	1.27	1.46
18	a	4011	BCR	C8-C9	-8.76	1.27	1.46
18	b	4010	BCR	C8-C9	-8.76	1.27	1.46
18	B	4010	BCR	C8-C9	-8.76	1.27	1.46
18	b	4016	BCR	C8-C9	-8.75	1.27	1.46
18	B	4016	BCR	C8-C9	-8.74	1.27	1.46
18	G	4008	BCR	C8-C9	-8.73	1.27	1.46
18	A	4011	BCR	C8-C9	-8.73	1.27	1.46
18	H	4016	BCR	C8-C9	-8.73	1.27	1.46
18	H	4010	BCR	C8-C9	-8.73	1.27	1.46
15	H	1207	F6C	MG-NA	8.71	2.23	2.05
15	B	1207	F6C	MG-NA	8.71	2.23	2.05
15	b	1207	F6C	MG-NA	8.69	2.23	2.05
15	H	1230	F6C	MG-NA	8.67	2.23	2.05
15	b	1230	F6C	MG-NA	8.66	2.23	2.05
15	B	1238	F6C	MG-NA	8.65	2.22	2.05
15	b	1238	F6C	MG-NA	8.64	2.22	2.05
15	B	1230	F6C	MG-NA	8.64	2.22	2.05
18	B	4017	BCR	C8-C9	-8.61	1.27	1.46
15	H	1238	F6C	MG-NA	8.60	2.22	2.05
18	B	4010	BCR	C11-C10	-8.59	1.16	1.43
18	a	4001	BCR	C8-C9	-8.59	1.27	1.46
18	A	4008	BCR	C11-C10	-8.59	1.16	1.43
18	G	4008	BCR	C11-C10	-8.59	1.16	1.43
18	b	4017	BCR	C8-C9	-8.59	1.27	1.46
18	a	4008	BCR	C11-C10	-8.59	1.16	1.43
18	G	4001	BCR	C8-C9	-8.59	1.27	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4001	BCR	C8-C9	-8.58	1.27	1.46
18	b	4014	BCR	C8-C9	-8.58	1.27	1.46
18	B	4014	BCR	C8-C9	-8.58	1.27	1.46
18	H	4017	BCR	C8-C9	-8.58	1.27	1.46
18	L	4019	BCR	C8-C9	-8.57	1.27	1.46
18	H	4010	BCR	C11-C10	-8.57	1.16	1.43
18	H	4014	BCR	C8-C9	-8.56	1.27	1.46
18	l	4019	BCR	C8-C9	-8.56	1.27	1.46
18	a	4002	BCR	C8-C9	-8.56	1.27	1.46
18	b	4010	BCR	C11-C10	-8.55	1.16	1.43
18	A	4002	BCR	C8-C9	-8.55	1.27	1.46
18	U	4019	BCR	C8-C9	-8.53	1.27	1.46
18	G	4002	BCR	C8-C9	-8.53	1.27	1.46
18	i	4020	BCR	C11-C10	-8.52	1.16	1.43
18	a	4007	BCR	C11-C10	-8.50	1.16	1.43
18	G	4007	BCR	C11-C10	-8.49	1.16	1.43
18	b	4009	BCR	C8-C9	-8.49	1.27	1.46
18	B	4009	BCR	C8-C9	-8.49	1.27	1.46
18	A	4007	BCR	C11-C10	-8.48	1.16	1.43
18	H	4009	BCR	C8-C9	-8.48	1.27	1.46
18	I	4020	BCR	C11-C10	-8.48	1.16	1.43
18	R	4020	BCR	C11-C10	-8.47	1.16	1.43
13	A	1011	CL0	C1A-CHA	8.47	1.49	1.40
13	G	1011	CL0	C1A-CHA	8.44	1.49	1.40
18	b	4006	BCR	C8-C9	-8.42	1.27	1.46
13	a	1011	CL0	C1A-CHA	8.41	1.49	1.40
18	a	4003	BCR	C8-C9	-8.40	1.28	1.46
18	H	4004	BCR	C8-C9	-8.38	1.28	1.46
18	l	4022	BCR	C11-C10	-8.38	1.17	1.43
18	A	4003	BCR	C8-C9	-8.38	1.28	1.46
18	L	4022	BCR	C11-C10	-8.37	1.17	1.43
18	B	4006	BCR	C8-C9	-8.37	1.28	1.46
18	b	4014	BCR	C11-C10	-8.37	1.17	1.43
18	H	4006	BCR	C8-C9	-8.37	1.28	1.46
18	U	4022	BCR	C11-C10	-8.36	1.17	1.43
18	H	4014	BCR	C11-C10	-8.36	1.17	1.43
18	G	4003	BCR	C8-C9	-8.35	1.28	1.46
18	b	4004	BCR	C8-C9	-8.34	1.28	1.46
18	B	4014	BCR	C11-C10	-8.34	1.17	1.43
18	B	4005	BCR	C8-C9	-8.32	1.28	1.46
18	b	4005	BCR	C8-C9	-8.31	1.28	1.46
18	B	4004	BCR	C8-C9	-8.31	1.28	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	I	4018	BCR	C11-C10	-8.30	1.17	1.43
18	H	4005	BCR	C8-C9	-8.30	1.28	1.46
18	H	4013	BCR	C8-C9	-8.30	1.28	1.46
18	R	4018	BCR	C11-C10	-8.29	1.17	1.43
18	i	4018	BCR	C11-C10	-8.28	1.17	1.43
18	V	4021	BCR	C11-C10	-8.27	1.17	1.43
18	B	4005	BCR	C11-C10	-8.27	1.17	1.43
18	B	4013	BCR	C8-C9	-8.26	1.28	1.46
18	b	4013	BCR	C8-C9	-8.26	1.28	1.46
18	G	4011	BCR	C11-C10	-8.25	1.17	1.43
18	B	4009	BCR	C11-C10	-8.25	1.17	1.43
15	B	1237	F6C	MG-NA	8.25	2.22	2.05
18	b	4009	BCR	C11-C10	-8.25	1.17	1.43
18	H	4009	BCR	C11-C10	-8.24	1.17	1.43
18	H	4005	BCR	C11-C10	-8.24	1.17	1.43
18	m	4021	BCR	C11-C10	-8.24	1.17	1.43
18	M	4021	BCR	C11-C10	-8.23	1.17	1.43
18	b	4005	BCR	C11-C10	-8.23	1.17	1.43
18	B	4017	BCR	C11-C10	-8.23	1.17	1.43
18	H	4017	BCR	C11-C10	-8.22	1.17	1.43
15	H	1237	F6C	MG-NA	8.22	2.22	2.05
18	a	4011	BCR	C11-C10	-8.22	1.17	1.43
15	b	1237	F6C	MG-NA	8.21	2.22	2.05
18	l	4019	BCR	C11-C10	-8.21	1.17	1.43
18	A	4011	BCR	C11-C10	-8.21	1.17	1.43
18	U	4019	BCR	C11-C10	-8.20	1.17	1.43
18	G	4001	BCR	C11-C10	-8.19	1.17	1.43
18	L	4019	BCR	C11-C10	-8.19	1.17	1.43
18	b	4017	BCR	C11-C10	-8.19	1.17	1.43
18	a	4001	BCR	C11-C10	-8.19	1.17	1.43
18	A	4001	BCR	C11-C10	-8.17	1.17	1.43
18	B	4016	BCR	C11-C10	-8.10	1.18	1.43
18	b	4016	BCR	C11-C10	-8.10	1.18	1.43
18	H	4016	BCR	C11-C10	-8.09	1.18	1.43
18	b	4006	BCR	C11-C10	-8.06	1.18	1.43
18	H	4006	BCR	C11-C10	-8.05	1.18	1.43
18	B	4006	BCR	C11-C10	-8.03	1.18	1.43
18	a	4003	BCR	C11-C10	-8.02	1.18	1.43
18	A	4003	BCR	C11-C10	-8.01	1.18	1.43
18	G	4003	BCR	C11-C10	-8.01	1.18	1.43
18	R	4020	BCR	C20-C21	-7.99	1.18	1.43
18	I	4020	BCR	C20-C21	-7.99	1.18	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	i	4020	BCR	C20-C21	-7.98	1.18	1.43
18	B	4013	BCR	C11-C10	-7.97	1.18	1.43
18	A	4002	BCR	C11-C10	-7.97	1.18	1.43
18	a	4002	BCR	C11-C10	-7.96	1.18	1.43
18	G	4002	BCR	C11-C10	-7.96	1.18	1.43
18	b	4013	BCR	C11-C10	-7.96	1.18	1.43
18	H	4013	BCR	C11-C10	-7.94	1.18	1.43
18	H	4004	BCR	C11-C10	-7.93	1.18	1.43
18	b	4004	BCR	C11-C10	-7.92	1.18	1.43
18	B	4004	BCR	C11-C10	-7.92	1.18	1.43
18	U	4022	BCR	C20-C21	-7.91	1.18	1.43
18	G	4008	BCR	C20-C21	-7.91	1.18	1.43
18	A	4008	BCR	C20-C21	-7.91	1.18	1.43
18	a	4008	BCR	C20-C21	-7.90	1.18	1.43
18	l	4022	BCR	C20-C21	-7.89	1.18	1.43
18	L	4022	BCR	C20-C21	-7.88	1.18	1.43
18	R	4020	BCR	C16-C17	-7.86	1.18	1.43
18	I	4020	BCR	C16-C17	-7.85	1.18	1.43
18	A	4011	BCR	C20-C21	-7.85	1.18	1.43
18	a	4011	BCR	C20-C21	-7.84	1.18	1.43
18	G	4011	BCR	C20-C21	-7.84	1.18	1.43
18	i	4020	BCR	C16-C17	-7.84	1.18	1.43
18	H	4010	BCR	C16-C17	-7.80	1.19	1.43
18	b	4010	BCR	C16-C17	-7.78	1.19	1.43
18	a	4008	BCR	C16-C17	-7.78	1.19	1.43
18	l	4022	BCR	C16-C17	-7.77	1.19	1.43
18	L	4022	BCR	C16-C17	-7.77	1.19	1.43
18	A	4008	BCR	C16-C17	-7.77	1.19	1.43
18	B	4010	BCR	C16-C17	-7.76	1.19	1.43
18	G	4008	BCR	C16-C17	-7.76	1.19	1.43
18	U	4022	BCR	C16-C17	-7.73	1.19	1.43
18	I	4018	BCR	C20-C21	-7.72	1.19	1.43
18	i	4018	BCR	C20-C21	-7.72	1.19	1.43
18	R	4018	BCR	C20-C21	-7.71	1.19	1.43
18	B	4014	BCR	C16-C17	-7.66	1.19	1.43
18	B	4017	BCR	C20-C21	-7.65	1.19	1.43
18	U	4019	BCR	C20-C21	-7.64	1.19	1.43
18	l	4019	BCR	C20-C21	-7.64	1.19	1.43
18	H	4017	BCR	C20-C21	-7.64	1.19	1.43
18	H	4014	BCR	C16-C17	-7.64	1.19	1.43
18	b	4017	BCR	C20-C21	-7.64	1.19	1.43
18	B	4010	BCR	C20-C21	-7.63	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	4019	BCR	C20-C21	-7.63	1.19	1.43
18	b	4009	BCR	C20-C21	-7.63	1.19	1.43
18	b	4014	BCR	C16-C17	-7.63	1.19	1.43
18	H	4010	BCR	C20-C21	-7.62	1.19	1.43
18	G	4007	BCR	C16-C17	-7.62	1.19	1.43
18	a	4007	BCR	C16-C17	-7.61	1.19	1.43
18	b	4010	BCR	C20-C21	-7.61	1.19	1.43
18	B	4009	BCR	C20-C21	-7.61	1.19	1.43
18	H	4014	BCR	C20-C21	-7.61	1.19	1.43
18	b	4014	BCR	C20-C21	-7.60	1.19	1.43
18	B	4014	BCR	C20-C21	-7.60	1.19	1.43
18	H	4009	BCR	C20-C21	-7.60	1.19	1.43
18	A	4007	BCR	C16-C17	-7.60	1.19	1.43
18	G	4007	BCR	C20-C21	-7.60	1.19	1.43
18	b	4017	BCR	C16-C17	-7.59	1.19	1.43
18	b	4005	BCR	C20-C21	-7.58	1.19	1.43
18	a	4007	BCR	C20-C21	-7.58	1.19	1.43
18	H	4017	BCR	C16-C17	-7.57	1.19	1.43
18	A	4007	BCR	C20-C21	-7.56	1.19	1.43
18	I	4018	BCR	C16-C17	-7.56	1.19	1.43
18	H	4005	BCR	C20-C21	-7.56	1.19	1.43
18	B	4017	BCR	C16-C17	-7.56	1.19	1.43
18	B	4005	BCR	C20-C21	-7.55	1.19	1.43
18	b	4016	BCR	C20-C21	-7.54	1.19	1.43
14	K	1401	CLA	MG-NA	7.53	2.24	2.06
13	a	1011	CL0	C3B-C4B	7.53	1.48	1.41
18	G	4002	BCR	C20-C21	-7.53	1.19	1.43
18	a	4002	BCR	C20-C21	-7.53	1.19	1.43
18	R	4018	BCR	C16-C17	-7.52	1.19	1.43
18	A	4002	BCR	C20-C21	-7.52	1.19	1.43
18	i	4018	BCR	C16-C17	-7.52	1.19	1.43
18	H	4016	BCR	C16-C17	-7.52	1.19	1.43
14	T	1401	CLA	MG-NA	7.51	2.24	2.06
18	H	4016	BCR	C20-C21	-7.51	1.19	1.43
18	B	4016	BCR	C20-C21	-7.50	1.19	1.43
18	B	4016	BCR	C16-C17	-7.50	1.19	1.43
13	A	1011	CL0	C3B-C4B	7.50	1.48	1.41
18	b	4016	BCR	C16-C17	-7.49	1.20	1.43
14	k	1401	CLA	MG-NA	7.49	2.24	2.06
18	G	4003	BCR	C20-C21	-7.49	1.20	1.43
18	b	4005	BCR	C16-C17	-7.49	1.20	1.43
18	V	4021	BCR	C20-C21	-7.48	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4009	BCR	C16-C17	-7.48	1.20	1.43
18	A	4003	BCR	C20-C21	-7.48	1.20	1.43
18	B	4009	BCR	C16-C17	-7.48	1.20	1.43
14	a	1123	CLA	MG-NA	7.47	2.24	2.06
14	G	1134	CLA	MG-NA	7.47	2.24	2.06
18	L	4019	BCR	C16-C17	-7.47	1.20	1.43
18	U	4019	BCR	C16-C17	-7.47	1.20	1.43
18	B	4005	BCR	C16-C17	-7.47	1.20	1.43
13	G	1011	CL0	C3B-C4B	7.47	1.48	1.41
18	a	4003	BCR	C20-C21	-7.47	1.20	1.43
14	A	1123	CLA	MG-NA	7.46	2.24	2.06
18	l	4019	BCR	C16-C17	-7.46	1.20	1.43
18	M	4021	BCR	C20-C21	-7.46	1.20	1.43
18	G	4011	BCR	C16-C17	-7.46	1.20	1.43
14	A	1134	CLA	MG-NA	7.46	2.24	2.06
18	H	4005	BCR	C16-C17	-7.46	1.20	1.43
18	m	4021	BCR	C20-C21	-7.45	1.20	1.43
14	b	1214	CLA	MG-NA	7.45	2.24	2.06
18	a	4011	BCR	C16-C17	-7.44	1.20	1.43
14	a	1134	CLA	MG-NA	7.44	2.23	2.06
18	A	4011	BCR	C16-C17	-7.44	1.20	1.43
18	b	4009	BCR	C16-C17	-7.43	1.20	1.43
14	G	1123	CLA	MG-NA	7.43	2.23	2.06
18	H	4004	BCR	C20-C21	-7.43	1.20	1.43
18	b	4004	BCR	C20-C21	-7.42	1.20	1.43
18	B	4004	BCR	C20-C21	-7.42	1.20	1.43
18	H	4006	BCR	C20-C21	-7.41	1.20	1.43
18	b	4006	BCR	C20-C21	-7.41	1.20	1.43
14	H	1214	CLA	MG-NA	7.41	2.23	2.06
13	A	1011	CL0	C1D-C2D	7.41	1.48	1.39
14	H	1239	CLA	MG-NA	7.40	2.23	2.06
14	b	1232	CLA	MG-NA	7.40	2.23	2.06
14	B	1214	CLA	MG-NA	7.39	2.23	2.06
14	H	1232	CLA	MG-NA	7.39	2.23	2.06
18	B	4006	BCR	C20-C21	-7.39	1.20	1.43
14	B	1232	CLA	MG-NA	7.38	2.23	2.06
14	b	1239	CLA	MG-NA	7.37	2.23	2.06
13	G	1011	CL0	C3A-C2A	-7.37	1.48	1.54
18	G	4001	BCR	C20-C21	-7.37	1.20	1.43
18	A	4001	BCR	C20-C21	-7.36	1.20	1.43
14	b	1233	CLA	MG-NA	7.36	2.23	2.06
14	B	1239	CLA	MG-NA	7.36	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	4002	BCR	C16-C17	-7.36	1.20	1.43
18	a	4001	BCR	C20-C21	-7.36	1.20	1.43
18	G	4002	BCR	C16-C17	-7.35	1.20	1.43
18	A	4003	BCR	C16-C17	-7.35	1.20	1.43
14	b	1218	CLA	MG-NA	7.35	2.23	2.06
18	a	4002	BCR	C16-C17	-7.35	1.20	1.43
14	H	1213	CLA	MG-NA	7.34	2.23	2.06
14	H	1233	CLA	MG-NA	7.34	2.23	2.06
14	B	1233	CLA	MG-NA	7.34	2.23	2.06
18	a	4003	BCR	C16-C17	-7.34	1.20	1.43
13	a	1011	CL0	C1D-C2D	7.34	1.47	1.39
18	G	4003	BCR	C16-C17	-7.34	1.20	1.43
14	B	1213	CLA	MG-NA	7.33	2.23	2.06
14	b	1213	CLA	MG-NA	7.32	2.23	2.06
18	H	4006	BCR	C16-C17	-7.32	1.20	1.43
14	G	1140	CLA	MG-NA	7.32	2.23	2.06
13	G	1011	CL0	C1D-C2D	7.32	1.47	1.39
14	B	1219	CLA	MG-NA	7.32	2.23	2.06
18	M	4021	BCR	C16-C17	-7.32	1.20	1.43
14	H	1218	CLA	MG-NA	7.31	2.23	2.06
18	b	4006	BCR	C16-C17	-7.31	1.20	1.43
18	V	4021	BCR	C16-C17	-7.31	1.20	1.43
18	B	4004	BCR	C16-C17	-7.30	1.20	1.43
13	a	1011	CL0	C3A-C2A	-7.30	1.48	1.54
18	B	4006	BCR	C16-C17	-7.30	1.20	1.43
14	X	1701	CLA	MG-NA	7.30	2.23	2.06
14	x	1701	CLA	MG-NA	7.29	2.23	2.06
14	W	1701	CLA	MG-NA	7.29	2.23	2.06
18	A	4001	BCR	C16-C17	-7.29	1.20	1.43
14	b	1219	CLA	MG-NA	7.28	2.23	2.06
14	H	1219	CLA	MG-NA	7.28	2.23	2.06
18	m	4021	BCR	C16-C17	-7.28	1.20	1.43
18	G	4001	BCR	C16-C17	-7.28	1.20	1.43
14	B	1218	CLA	MG-NA	7.28	2.23	2.06
18	b	4004	BCR	C16-C17	-7.28	1.20	1.43
14	H	1209	CLA	MG-NA	7.28	2.23	2.06
18	H	4004	BCR	C16-C17	-7.28	1.20	1.43
13	A	1011	CL0	C3A-C2A	-7.27	1.48	1.54
18	a	4001	BCR	C16-C17	-7.27	1.20	1.43
18	b	4013	BCR	C20-C21	-7.27	1.20	1.43
14	a	1139	CLA	MG-NA	7.25	2.23	2.06
14	B	1209	CLA	MG-NA	7.25	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4013	BCR	C16-C17	-7.25	1.20	1.43
14	A	1140	CLA	MG-NA	7.25	2.23	2.06
14	H	1223	CLA	MG-NA	7.24	2.23	2.06
14	a	1135	CLA	MG-NA	7.24	2.23	2.06
14	G	1139	CLA	MG-NA	7.24	2.23	2.06
14	A	1135	CLA	MG-NA	7.24	2.23	2.06
14	B	1223	CLA	MG-NA	7.24	2.23	2.06
14	a	1127	CLA	MG-NA	7.24	2.23	2.06
14	a	1140	CLA	MG-NA	7.24	2.23	2.06
14	b	1223	CLA	MG-NA	7.24	2.23	2.06
14	b	1209	CLA	MG-NA	7.24	2.23	2.06
18	B	4013	BCR	C20-C21	-7.23	1.20	1.43
16	H	2002	PQN	C3-C2	7.23	1.48	1.35
14	G	1135	CLA	MG-NA	7.23	2.23	2.06
14	A	1139	CLA	MG-NA	7.23	2.23	2.06
14	G	1113	CLA	MG-NA	7.23	2.23	2.06
16	b	2002	PQN	C3-C2	7.23	1.48	1.35
14	A	1127	CLA	MG-NA	7.23	2.23	2.06
18	b	4013	BCR	C16-C17	-7.22	1.20	1.43
18	H	4013	BCR	C20-C21	-7.22	1.20	1.43
14	b	1217	CLA	MG-NA	7.22	2.23	2.06
14	G	1127	CLA	MG-NA	7.22	2.23	2.06
14	B	1217	CLA	MG-NA	7.22	2.23	2.06
14	G	1114	CLA	MG-NA	7.21	2.23	2.06
14	b	1229	CLA	MG-NA	7.21	2.23	2.06
14	a	1113	CLA	MG-NA	7.21	2.23	2.06
16	B	2002	PQN	C3-C2	7.21	1.48	1.35
14	B	1224	CLA	MG-NA	7.21	2.23	2.06
14	B	1229	CLA	MG-NA	7.20	2.23	2.06
14	H	1217	CLA	MG-NA	7.20	2.23	2.06
18	B	4013	BCR	C16-C17	-7.20	1.20	1.43
16	A	2001	PQN	C3-C2	7.20	1.48	1.35
14	H	1229	CLA	MG-NA	7.20	2.23	2.06
14	H	1227	CLA	MG-NA	7.19	2.23	2.06
14	G	1110	CLA	MG-NA	7.19	2.23	2.06
14	H	1224	CLA	MG-NA	7.19	2.23	2.06
14	H	1022	CLA	MG-NA	7.19	2.23	2.06
14	b	1022	CLA	MG-NA	7.19	2.23	2.06
14	b	1224	CLA	MG-NA	7.18	2.23	2.06
14	A	1113	CLA	MG-NA	7.18	2.23	2.06
14	a	1118	CLA	MG-NA	7.18	2.23	2.06
14	b	1227	CLA	MG-NA	7.18	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1118	CLA	MG-NA	7.18	2.23	2.06
14	B	1022	CLA	MG-NA	7.17	2.23	2.06
14	B	1227	CLA	MG-NA	7.17	2.23	2.06
14	H	1212	CLA	MG-NA	7.17	2.23	2.06
14	G	1118	CLA	MG-NA	7.17	2.23	2.06
14	G	1131	CLA	MG-NA	7.16	2.23	2.06
14	a	1115	CLA	MG-NA	7.16	2.23	2.06
14	A	1131	CLA	MG-NA	7.16	2.23	2.06
16	G	2001	PQN	C3-C2	7.16	1.48	1.35
14	G	1115	CLA	MG-NA	7.16	2.23	2.06
14	a	1110	CLA	MG-NA	7.16	2.23	2.06
14	a	1131	CLA	MG-NA	7.16	2.23	2.06
14	a	1111	CLA	MG-NA	7.16	2.23	2.06
14	A	1110	CLA	MG-NA	7.16	2.23	2.06
14	b	1210	CLA	MG-NA	7.15	2.23	2.06
14	H	1210	CLA	MG-NA	7.15	2.23	2.06
14	a	1114	CLA	MG-NA	7.15	2.23	2.06
14	G	1012	CLA	MG-NA	7.15	2.23	2.06
14	A	1111	CLA	MG-NA	7.15	2.23	2.06
16	a	2001	PQN	C3-C2	7.15	1.48	1.35
14	A	1115	CLA	MG-NA	7.14	2.23	2.06
14	b	1231	CLA	MG-NA	7.14	2.23	2.06
14	A	1114	CLA	MG-NA	7.14	2.23	2.06
14	B	1235	CLA	MG-NA	7.14	2.23	2.06
14	G	1111	CLA	MG-NA	7.14	2.23	2.06
14	B	1210	CLA	MG-NA	7.14	2.23	2.06
14	G	1112	CLA	MG-NA	7.14	2.23	2.06
14	b	1212	CLA	MG-NA	7.14	2.23	2.06
14	G	1138	CLA	MG-NA	7.14	2.23	2.06
14	a	1112	CLA	MG-NA	7.14	2.23	2.06
14	B	1212	CLA	MG-NA	7.13	2.23	2.06
14	B	1234	CLA	MG-NA	7.13	2.23	2.06
14	B	1225	CLA	MG-NA	7.13	2.23	2.06
14	G	1137	CLA	MG-NA	7.13	2.23	2.06
14	H	1234	CLA	MG-NA	7.13	2.23	2.06
14	A	1105	CLA	MG-NA	7.13	2.23	2.06
14	B	1231	CLA	MG-NA	7.12	2.23	2.06
14	a	1105	CLA	MG-NA	7.12	2.23	2.06
14	A	1138	CLA	MG-NA	7.12	2.23	2.06
14	G	1120	CLA	MG-NA	7.12	2.23	2.06
14	A	1129	CLA	MG-NA	7.12	2.23	2.06
14	a	1120	CLA	MG-NA	7.11	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1138	CLA	MG-NA	7.11	2.23	2.06
14	b	1234	CLA	MG-NA	7.11	2.23	2.06
14	G	1105	CLA	MG-NA	7.11	2.23	2.06
14	A	1116	CLA	MG-NA	7.11	2.23	2.06
14	a	1129	CLA	MG-NA	7.11	2.23	2.06
14	a	1012	CLA	MG-NA	7.11	2.23	2.06
14	A	1137	CLA	MG-NA	7.11	2.23	2.06
14	A	1120	CLA	MG-NA	7.11	2.23	2.06
14	A	1107	CLA	MG-NA	7.11	2.23	2.06
14	G	1129	CLA	MG-NA	7.10	2.23	2.06
14	a	1137	CLA	MG-NA	7.10	2.23	2.06
14	b	1225	CLA	MG-NA	7.10	2.23	2.06
14	H	1231	CLA	MG-NA	7.10	2.23	2.06
14	A	1130	CLA	MG-NA	7.10	2.23	2.06
14	a	1107	CLA	MG-NA	7.10	2.23	2.06
14	a	1122	CLA	MG-NA	7.10	2.23	2.06
14	G	1107	CLA	MG-NA	7.09	2.23	2.06
14	G	1133	CLA	MG-NA	7.09	2.23	2.06
14	A	1112	CLA	MG-NA	7.09	2.23	2.06
14	H	1225	CLA	MG-NA	7.09	2.23	2.06
14	b	1235	CLA	MG-NA	7.09	2.23	2.06
14	H	1235	CLA	MG-NA	7.09	2.23	2.06
14	A	1122	CLA	MG-NA	7.09	2.23	2.06
14	L	1501	CLA	MG-NA	7.09	2.23	2.06
14	l	1501	CLA	MG-NA	7.09	2.23	2.06
14	B	1228	CLA	MG-NA	7.09	2.23	2.06
14	A	1101	CLA	MG-NA	7.09	2.23	2.06
14	U	1501	CLA	MG-NA	7.08	2.23	2.06
14	b	1228	CLA	MG-NA	7.08	2.23	2.06
14	G	1130	CLA	MG-NA	7.08	2.23	2.06
14	A	1012	CLA	MG-NA	7.08	2.23	2.06
15	H	1230	F6C	C2A-C3A	7.08	1.52	1.36
14	G	1122	CLA	MG-NA	7.08	2.23	2.06
14	A	1133	CLA	MG-NA	7.08	2.23	2.06
14	a	1116	CLA	MG-NA	7.07	2.23	2.06
14	a	1130	CLA	MG-NA	7.07	2.23	2.06
14	G	1101	CLA	MG-NA	7.06	2.23	2.06
14	G	1116	CLA	MG-NA	7.06	2.23	2.06
15	H	1207	F6C	C2A-C3A	7.06	1.52	1.36
15	B	1207	F6C	C2A-C3A	7.06	1.52	1.36
14	H	1228	CLA	MG-NA	7.06	2.23	2.06
14	a	1133	CLA	MG-NA	7.06	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1101	CLA	MG-NA	7.06	2.23	2.06
14	a	1102	CLA	MG-NA	7.05	2.23	2.06
14	H	1204	CLA	MG-NA	7.05	2.23	2.06
14	G	1102	CLA	MG-NA	7.04	2.23	2.06
15	b	1207	F6C	C2A-C3A	7.04	1.51	1.36
15	B	1230	F6C	C2A-C3A	7.03	1.51	1.36
14	A	1102	CLA	MG-NA	7.03	2.23	2.06
14	G	1109	CLA	MG-NA	7.03	2.23	2.06
15	b	1230	F6C	C2A-C3A	7.03	1.51	1.36
14	a	1132	CLA	MG-NA	7.02	2.23	2.06
14	B	1204	CLA	MG-NA	7.02	2.22	2.06
14	G	1132	CLA	MG-NA	7.02	2.22	2.06
14	A	1109	CLA	MG-NA	7.01	2.22	2.06
14	b	1215	CLA	MG-NA	7.01	2.22	2.06
14	b	1204	CLA	MG-NA	7.01	2.22	2.06
14	a	1109	CLA	MG-NA	7.01	2.22	2.06
14	B	1215	CLA	MG-NA	7.00	2.22	2.06
14	b	1220	CLA	MG-NA	7.00	2.22	2.06
14	B	1208	CLA	MG-NA	7.00	2.22	2.06
14	H	1215	CLA	MG-NA	7.00	2.22	2.06
14	H	1208	CLA	MG-NA	7.00	2.22	2.06
14	b	1236	CLA	MG-NA	7.00	2.22	2.06
14	A	1132	CLA	MG-NA	7.00	2.22	2.06
14	H	1236	CLA	MG-NA	6.99	2.22	2.06
14	b	1208	CLA	MG-NA	6.99	2.22	2.06
14	G	1108	CLA	MG-NA	6.99	2.22	2.06
14	B	1216	CLA	MG-NA	6.99	2.22	2.06
14	B	1236	CLA	MG-NA	6.99	2.22	2.06
14	B	1220	CLA	MG-NA	6.99	2.22	2.06
14	H	1216	CLA	MG-NA	6.98	2.22	2.06
13	a	1011	CL0	C1B-C2B	6.98	1.47	1.39
14	b	1216	CLA	MG-NA	6.98	2.22	2.06
14	B	1211	CLA	MG-NA	6.97	2.22	2.06
14	A	1128	CLA	MG-NA	6.97	2.22	2.06
14	B	1222	CLA	MG-NA	6.97	2.22	2.06
14	a	1136	CLA	MG-NA	6.97	2.22	2.06
14	b	1211	CLA	MG-NA	6.97	2.22	2.06
14	H	1220	CLA	MG-NA	6.97	2.22	2.06
14	A	1108	CLA	MG-NA	6.96	2.22	2.06
13	A	1011	CL0	C1B-C2B	6.96	1.47	1.39
14	H	1203	CLA	MG-NA	6.96	2.22	2.06
14	a	1128	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	1136	CLA	MG-NA	6.95	2.22	2.06
14	G	1136	CLA	MG-NA	6.95	2.22	2.06
14	a	1108	CLA	MG-NA	6.95	2.22	2.06
14	B	1203	CLA	MG-NA	6.95	2.22	2.06
14	H	1211	CLA	MG-NA	6.95	2.22	2.06
14	B	1221	CLA	MG-NA	6.95	2.22	2.06
14	H	1221	CLA	MG-NA	6.94	2.22	2.06
14	H	1222	CLA	MG-NA	6.94	2.22	2.06
15	A	1121	F6C	C2A-C3A	6.93	1.51	1.36
14	b	1221	CLA	MG-NA	6.93	2.22	2.06
14	b	1222	CLA	MG-NA	6.93	2.22	2.06
14	G	1128	CLA	MG-NA	6.93	2.22	2.06
14	b	1203	CLA	MG-NA	6.93	2.22	2.06
13	G	1011	CL0	C1B-C2B	6.93	1.47	1.39
15	G	1121	F6C	C2A-C3A	6.93	1.51	1.36
14	G	1117	CLA	MG-NA	6.92	2.22	2.06
14	A	1106	CLA	MG-NA	6.92	2.22	2.06
14	A	1117	CLA	MG-NA	6.91	2.22	2.06
14	a	1106	CLA	MG-NA	6.90	2.22	2.06
14	a	1117	CLA	MG-NA	6.90	2.22	2.06
14	b	1226	CLA	MG-NA	6.90	2.22	2.06
14	H	1226	CLA	MG-NA	6.90	2.22	2.06
15	a	1121	F6C	C2A-C3A	6.90	1.51	1.36
14	G	1106	CLA	MG-NA	6.90	2.22	2.06
14	l	1503	CLA	MG-NA	6.89	2.22	2.06
14	A	1125	CLA	MG-NA	6.88	2.22	2.06
14	a	1125	CLA	MG-NA	6.88	2.22	2.06
14	A	1126	CLA	MG-NA	6.87	2.22	2.06
14	G	1126	CLA	MG-NA	6.87	2.22	2.06
14	U	1503	CLA	MG-NA	6.87	2.22	2.06
14	B	1226	CLA	MG-NA	6.87	2.22	2.06
14	G	1125	CLA	MG-NA	6.86	2.22	2.06
14	a	1124	CLA	MG-NA	6.86	2.22	2.06
14	A	1124	CLA	MG-NA	6.86	2.22	2.06
14	L	1503	CLA	MG-NA	6.86	2.22	2.06
14	a	1126	CLA	MG-NA	6.86	2.22	2.06
14	H	1201	CLA	MG-NA	6.85	2.22	2.06
14	H	1202	CLA	MG-NA	6.83	2.22	2.06
14	B	1201	CLA	MG-NA	6.83	2.22	2.06
14	b	1201	CLA	MG-NA	6.83	2.22	2.06
14	B	1202	CLA	MG-NA	6.83	2.22	2.06
14	H	1206	CLA	MG-NA	6.83	2.22	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1124	CLA	MG-NA	6.82	2.22	2.06
14	b	1206	CLA	MG-NA	6.82	2.22	2.06
14	H	1205	CLA	MG-NA	6.82	2.22	2.06
14	B	1206	CLA	MG-NA	6.82	2.22	2.06
14	B	1205	CLA	MG-NA	6.81	2.22	2.06
14	b	1205	CLA	MG-NA	6.81	2.22	2.06
14	l	1502	CLA	MG-NA	6.81	2.22	2.06
14	L	1502	CLA	MG-NA	6.81	2.22	2.06
14	b	1202	CLA	MG-NA	6.80	2.22	2.06
14	U	1502	CLA	MG-NA	6.79	2.22	2.06
14	G	1104	CLA	MG-NA	6.75	2.22	2.06
14	a	1104	CLA	MG-NA	6.73	2.22	2.06
15	b	1238	F6C	C2A-C3A	6.72	1.51	1.36
14	A	1104	CLA	MG-NA	6.70	2.22	2.06
15	H	1238	F6C	C2A-C3A	6.69	1.51	1.36
15	B	1238	F6C	C2A-C3A	6.69	1.51	1.36
15	B	1237	F6C	C2A-C3A	6.68	1.51	1.36
15	H	1237	F6C	C2A-C3A	6.68	1.51	1.36
15	b	1237	F6C	C2A-C3A	6.67	1.51	1.36
14	A	1013	CLA	MG-NA	6.63	2.22	2.06
14	a	1013	CLA	MG-NA	6.63	2.22	2.06
14	b	1021	CLA	MG-NA	6.63	2.22	2.06
14	G	1013	CLA	MG-NA	6.62	2.22	2.06
14	H	1021	CLA	MG-NA	6.62	2.22	2.06
14	a	1119	CLA	MG-NA	6.62	2.22	2.06
14	G	1119	CLA	MG-NA	6.62	2.22	2.06
14	A	1119	CLA	MG-NA	6.62	2.22	2.06
14	B	1023	CLA	MG-NA	6.62	2.22	2.06
14	G	1103	CLA	MG-NA	6.61	2.22	2.06
14	B	1021	CLA	MG-NA	6.61	2.22	2.06
14	a	1103	CLA	MG-NA	6.60	2.22	2.06
14	A	1103	CLA	MG-NA	6.60	2.21	2.06
14	H	1023	CLA	MG-NA	6.58	2.21	2.06
14	b	1023	CLA	MG-NA	6.57	2.21	2.06
18	A	4002	BCR	C10-C9	-5.69	1.22	1.35
18	G	4002	BCR	C10-C9	-5.68	1.22	1.35
18	a	4002	BCR	C10-C9	-5.65	1.22	1.35
14	H	1215	CLA	O2A-C1	5.55	1.61	1.46
14	B	1215	CLA	O2A-C1	5.54	1.61	1.46
14	b	1215	CLA	O2A-C1	5.51	1.61	1.46
14	b	1225	CLA	O2A-C1	5.51	1.60	1.46
14	H	1225	CLA	O2A-C1	5.50	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1225	CLA	O2A-C1	5.46	1.60	1.46
14	G	1116	CLA	O2A-C1	5.46	1.60	1.46
14	G	1123	CLA	O2A-C1	5.46	1.60	1.46
14	a	1123	CLA	O2A-C1	5.45	1.60	1.46
14	a	1116	CLA	O2A-C1	5.45	1.60	1.46
14	A	1123	CLA	O2A-C1	5.44	1.60	1.46
14	A	1118	CLA	O2A-C1	5.44	1.60	1.46
14	A	1116	CLA	O2A-C1	5.43	1.60	1.46
14	H	1213	CLA	O2A-C1	5.43	1.60	1.46
14	B	1213	CLA	O2A-C1	5.42	1.60	1.46
14	a	1118	CLA	O2A-C1	5.42	1.60	1.46
14	b	1213	CLA	O2A-C1	5.42	1.60	1.46
15	B	1238	F6C	O2A-C1	5.40	1.60	1.46
14	G	1118	CLA	O2A-C1	5.40	1.60	1.46
14	G	1133	CLA	O2A-C1	5.40	1.60	1.46
14	a	1133	CLA	O2A-C1	5.40	1.60	1.46
14	a	1109	CLA	O2A-C1	5.40	1.60	1.46
15	H	1238	F6C	O2A-C1	5.40	1.60	1.46
14	A	1133	CLA	O2A-C1	5.39	1.60	1.46
15	b	1238	F6C	O2A-C1	5.39	1.60	1.46
14	A	1109	CLA	O2A-C1	5.39	1.60	1.46
14	A	1130	CLA	O2A-C1	5.39	1.60	1.46
14	H	1208	CLA	O2A-C1	5.39	1.60	1.46
14	G	1109	CLA	O2A-C1	5.38	1.60	1.46
14	a	1130	CLA	O2A-C1	5.38	1.60	1.46
14	G	1130	CLA	O2A-C1	5.38	1.60	1.46
14	H	1217	CLA	O2A-C1	5.36	1.60	1.46
14	A	1140	CLA	O2A-C1	5.36	1.60	1.46
14	B	1208	CLA	O2A-C1	5.36	1.60	1.46
14	b	1217	CLA	O2A-C1	5.36	1.60	1.46
14	x	1701	CLA	O2A-C1	5.36	1.60	1.46
14	b	1228	CLA	O2A-C1	5.35	1.60	1.46
14	b	1208	CLA	O2A-C1	5.35	1.60	1.46
13	G	1011	CL0	C3D-C4D	-5.35	1.33	1.41
14	B	1211	CLA	O2A-C1	5.34	1.60	1.46
14	b	1211	CLA	O2A-C1	5.34	1.60	1.46
14	X	1701	CLA	O2A-C1	5.34	1.60	1.46
14	H	1228	CLA	O2A-C1	5.34	1.60	1.46
14	U	1503	CLA	O2A-C1	5.33	1.60	1.46
15	H	1207	F6C	O2A-C1	5.33	1.60	1.46
14	B	1228	CLA	O2A-C1	5.33	1.60	1.46
14	B	1217	CLA	O2A-C1	5.32	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1211	CLA	O2A-C1	5.32	1.60	1.46
14	l	1503	CLA	O2A-C1	5.32	1.60	1.46
15	b	1207	F6C	O2A-C1	5.32	1.60	1.46
15	B	1207	F6C	O2A-C1	5.32	1.60	1.46
14	L	1503	CLA	O2A-C1	5.31	1.60	1.46
14	G	1140	CLA	O2A-C1	5.31	1.60	1.46
14	a	1140	CLA	O2A-C1	5.31	1.60	1.46
14	a	1125	CLA	O2A-C1	5.30	1.60	1.46
14	G	1119	CLA	O2A-C1	5.30	1.60	1.46
14	W	1701	CLA	O2A-C1	5.30	1.60	1.46
14	A	1125	CLA	O2A-C1	5.30	1.60	1.46
14	G	1122	CLA	O2A-C1	5.29	1.60	1.46
14	a	1119	CLA	O2A-C1	5.29	1.60	1.46
14	B	1221	CLA	O2A-C1	5.28	1.60	1.46
14	A	1137	CLA	O2A-C1	5.28	1.60	1.46
14	b	1221	CLA	O2A-C1	5.28	1.60	1.46
14	G	1125	CLA	O2A-C1	5.28	1.60	1.46
13	a	1011	CL0	C3D-C4D	-5.27	1.33	1.41
14	A	1119	CLA	O2A-C1	5.27	1.60	1.46
14	a	1129	CLA	O2A-C1	5.27	1.60	1.46
13	A	1011	CL0	C3D-C4D	-5.27	1.33	1.41
14	G	1112	CLA	O2A-C1	5.27	1.60	1.46
14	G	1115	CLA	O2A-C1	5.27	1.60	1.46
14	H	1221	CLA	O2A-C1	5.27	1.60	1.46
14	A	1122	CLA	O2A-C1	5.26	1.60	1.46
14	b	1231	CLA	O2A-C1	5.26	1.60	1.46
14	A	1129	CLA	O2A-C1	5.26	1.60	1.46
14	H	1229	CLA	O2A-C1	5.25	1.60	1.46
14	B	1231	CLA	O2A-C1	5.25	1.60	1.46
14	H	1201	CLA	O2A-C1	5.25	1.60	1.46
14	A	1112	CLA	O2A-C1	5.25	1.60	1.46
14	a	1137	CLA	O2A-C1	5.25	1.60	1.46
14	A	1138	CLA	O2A-C1	5.25	1.60	1.46
14	a	1112	CLA	O2A-C1	5.25	1.60	1.46
14	a	1122	CLA	O2A-C1	5.25	1.60	1.46
14	B	1201	CLA	O2A-C1	5.25	1.60	1.46
14	b	1201	CLA	O2A-C1	5.25	1.60	1.46
14	G	1138	CLA	O2A-C1	5.24	1.60	1.46
14	a	1102	CLA	O2A-C1	5.24	1.60	1.46
14	G	1129	CLA	O2A-C1	5.24	1.60	1.46
14	H	1231	CLA	O2A-C1	5.24	1.60	1.46
14	B	1234	CLA	O2A-C1	5.24	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1137	CLA	O2A-C1	5.24	1.60	1.46
14	G	1102	CLA	O2A-C1	5.24	1.60	1.46
14	a	1115	CLA	O2A-C1	5.23	1.60	1.46
14	b	1234	CLA	O2A-C1	5.23	1.60	1.46
14	b	1229	CLA	O2A-C1	5.23	1.60	1.46
14	a	1138	CLA	O2A-C1	5.23	1.60	1.46
14	A	1115	CLA	O2A-C1	5.23	1.60	1.46
14	A	1102	CLA	O2A-C1	5.22	1.60	1.46
14	H	1234	CLA	O2A-C1	5.22	1.60	1.46
18	A	4007	BCR	C10-C9	-5.22	1.23	1.35
14	A	1128	CLA	O2A-C1	5.21	1.60	1.46
14	B	1022	CLA	O2A-C1	5.21	1.60	1.46
18	G	4008	BCR	C10-C9	-5.21	1.23	1.35
14	G	1104	CLA	O2A-C1	5.21	1.60	1.46
18	a	4008	BCR	C10-C9	-5.21	1.23	1.35
14	A	1132	CLA	O2A-C1	5.21	1.60	1.46
18	A	4008	BCR	C10-C9	-5.21	1.23	1.35
14	b	1022	CLA	O2A-C1	5.21	1.60	1.46
14	A	1013	CLA	O2A-C1	5.20	1.60	1.46
14	H	1022	CLA	O2A-C1	5.20	1.60	1.46
18	a	4007	BCR	C10-C9	-5.20	1.23	1.35
14	a	1013	CLA	O2A-C1	5.20	1.60	1.46
14	B	1229	CLA	O2A-C1	5.20	1.60	1.46
14	b	1202	CLA	O2A-C1	5.20	1.60	1.46
14	b	1214	CLA	O2A-C1	5.19	1.60	1.46
14	H	1202	CLA	O2A-C1	5.19	1.60	1.46
14	G	1013	CLA	O2A-C1	5.19	1.60	1.46
14	A	1104	CLA	O2A-C1	5.18	1.60	1.46
14	G	1103	CLA	O2A-C1	5.18	1.60	1.46
15	H	1207	F6C	C4A-NA	-5.18	1.31	1.37
14	G	1132	CLA	O2A-C1	5.18	1.60	1.46
14	B	1214	CLA	O2A-C1	5.18	1.60	1.46
14	A	1103	CLA	O2A-C1	5.18	1.60	1.46
15	b	1207	F6C	C4A-NA	-5.18	1.31	1.37
14	G	1131	CLA	O2A-C1	5.18	1.60	1.46
14	L	1502	CLA	O2A-C1	5.17	1.60	1.46
14	G	1128	CLA	O2A-C1	5.17	1.60	1.46
14	H	1214	CLA	O2A-C1	5.17	1.60	1.46
14	a	1128	CLA	O2A-C1	5.17	1.60	1.46
14	B	1220	CLA	O2A-C1	5.17	1.60	1.46
14	a	1104	CLA	O2A-C1	5.17	1.60	1.46
14	a	1132	CLA	O2A-C1	5.17	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	U	1502	CLA	O2A-C1	5.17	1.60	1.46
14	A	1130	CLA	C3D-C4D	-5.17	1.32	1.44
14	B	1202	CLA	O2A-C1	5.16	1.60	1.46
14	H	1226	CLA	O2A-C1	5.16	1.60	1.46
14	a	1103	CLA	O2A-C1	5.16	1.60	1.46
15	B	1207	F6C	C4A-NA	-5.16	1.31	1.37
14	B	1226	CLA	O2A-C1	5.16	1.60	1.46
14	b	1220	CLA	O2A-C1	5.16	1.60	1.46
14	A	1126	CLA	O2A-C1	5.16	1.60	1.46
14	G	1126	CLA	O2A-C1	5.16	1.60	1.46
14	G	1130	CLA	C3D-C4D	-5.16	1.32	1.44
14	H	1220	CLA	O2A-C1	5.16	1.60	1.46
14	b	1226	CLA	O2A-C1	5.16	1.60	1.46
14	l	1502	CLA	O2A-C1	5.16	1.60	1.46
18	G	4007	BCR	C10-C9	-5.15	1.23	1.35
14	A	1012	CLA	O2A-C1	5.15	1.60	1.46
14	A	1131	CLA	O2A-C1	5.15	1.60	1.46
14	a	1126	CLA	O2A-C1	5.15	1.60	1.46
14	b	1216	CLA	O2A-C1	5.15	1.60	1.46
14	a	1012	CLA	O2A-C1	5.14	1.60	1.46
14	a	1131	CLA	O2A-C1	5.14	1.60	1.46
14	H	1216	CLA	O2A-C1	5.14	1.60	1.46
14	B	1216	CLA	O2A-C1	5.14	1.60	1.46
14	a	1130	CLA	C3D-C4D	-5.13	1.32	1.44
14	A	1111	CLA	O2A-C1	5.13	1.59	1.46
18	R	4020	BCR	C10-C9	-5.13	1.23	1.35
14	G	1012	CLA	O2A-C1	5.13	1.59	1.46
14	G	1111	CLA	O2A-C1	5.12	1.59	1.46
14	a	1111	CLA	O2A-C1	5.12	1.59	1.46
15	B	1238	F6C	C4A-NA	-5.12	1.31	1.37
18	I	4020	BCR	C10-C9	-5.12	1.24	1.35
13	A	1011	CL0	O2A-C1	5.12	1.59	1.46
14	B	1235	CLA	O2A-C1	5.12	1.59	1.46
14	B	1224	CLA	O2A-C1	5.11	1.59	1.46
18	i	4020	BCR	C10-C9	-5.11	1.24	1.35
14	b	1235	CLA	O2A-C1	5.11	1.59	1.46
13	G	1011	CL0	O2A-C1	5.11	1.59	1.46
13	a	1011	CL0	O2A-C1	5.10	1.59	1.46
14	H	1224	CLA	O2A-C1	5.10	1.59	1.46
14	B	1204	CLA	O2A-C1	5.09	1.59	1.46
14	a	1117	CLA	O2A-C1	5.09	1.59	1.46
14	A	1117	CLA	O2A-C1	5.09	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1136	CLA	O2A-C1	5.09	1.59	1.46
14	G	1117	CLA	O2A-C1	5.09	1.59	1.46
14	H	1204	CLA	O2A-C1	5.09	1.59	1.46
14	b	1204	CLA	O2A-C1	5.09	1.59	1.46
14	H	1235	CLA	O2A-C1	5.09	1.59	1.46
14	a	1136	CLA	O2A-C1	5.09	1.59	1.46
14	G	1136	CLA	O2A-C1	5.08	1.59	1.46
15	H	1237	F6C	O2A-C1	5.08	1.59	1.46
14	B	1203	CLA	O2A-C1	5.08	1.59	1.46
14	b	1224	CLA	O2A-C1	5.08	1.59	1.46
15	B	1237	F6C	O2A-C1	5.08	1.59	1.46
14	b	1210	CLA	O2A-C1	5.07	1.59	1.46
14	H	1223	CLA	O2A-C1	5.07	1.59	1.46
14	G	1135	CLA	O2A-C1	5.07	1.59	1.46
15	b	1238	F6C	C4A-NA	-5.07	1.31	1.37
14	G	1124	CLA	O2A-C1	5.07	1.59	1.46
14	b	1203	CLA	O2A-C1	5.07	1.59	1.46
14	b	1223	CLA	O2A-C1	5.07	1.59	1.46
14	k	1401	CLA	O2D-CGD	5.07	1.45	1.33
15	B	1237	F6C	C4A-NA	-5.07	1.31	1.37
15	A	1121	F6C	C4A-NA	-5.07	1.31	1.37
14	B	1222	CLA	O2A-C1	5.07	1.59	1.46
14	H	1210	CLA	O2A-C1	5.07	1.59	1.46
14	a	1135	CLA	O2A-C1	5.06	1.59	1.46
14	A	1124	CLA	O2A-C1	5.06	1.59	1.46
14	K	1401	CLA	O2D-CGD	5.06	1.45	1.33
14	T	1401	CLA	O2D-CGD	5.06	1.45	1.33
14	B	1223	CLA	O2A-C1	5.06	1.59	1.46
14	H	1203	CLA	O2A-C1	5.06	1.59	1.46
14	G	1012	CLA	C3D-C4D	-5.06	1.32	1.44
14	a	1124	CLA	O2A-C1	5.06	1.59	1.46
14	G	1125	CLA	C3D-C4D	-5.05	1.32	1.44
15	a	1121	F6C	C4A-NA	-5.05	1.31	1.37
15	H	1237	F6C	C4A-NA	-5.05	1.31	1.37
15	b	1237	F6C	O2A-C1	5.05	1.59	1.46
14	L	1501	CLA	O2A-C1	5.05	1.59	1.46
14	a	1012	CLA	C3D-C4D	-5.04	1.32	1.44
18	B	4010	BCR	C10-C9	-5.04	1.24	1.35
14	a	1125	CLA	C3D-C4D	-5.04	1.32	1.44
14	B	1210	CLA	O2A-C1	5.04	1.59	1.46
14	A	1135	CLA	O2A-C1	5.03	1.59	1.46
18	b	4010	BCR	C10-C9	-5.03	1.24	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1238	F6C	C4A-NA	-5.03	1.31	1.37
14	A	1012	CLA	C3D-C4D	-5.03	1.32	1.44
14	l	1501	CLA	O2A-C1	5.03	1.59	1.46
14	B	1205	CLA	O2A-C1	5.03	1.59	1.46
18	H	4010	BCR	C10-C9	-5.02	1.24	1.35
14	H	1222	CLA	O2A-C1	5.02	1.59	1.46
14	b	1233	CLA	O2D-CGD	5.02	1.45	1.33
14	B	1220	CLA	O2D-CGD	5.02	1.45	1.33
14	H	1239	CLA	O2A-C1	5.01	1.59	1.46
14	b	1239	CLA	O2A-C1	5.01	1.59	1.46
14	H	1220	CLA	O2D-CGD	5.01	1.45	1.33
14	H	1233	CLA	O2D-CGD	5.01	1.45	1.33
14	B	1239	CLA	O2A-C1	5.01	1.59	1.46
14	U	1501	CLA	O2A-C1	5.01	1.59	1.46
14	A	1138	CLA	O2D-CGD	5.01	1.45	1.33
14	A	1125	CLA	C3D-C4D	-5.01	1.32	1.44
14	b	1205	CLA	O2A-C1	5.01	1.59	1.46
15	G	1121	F6C	C4A-NA	-5.01	1.31	1.37
14	H	1205	CLA	O2A-C1	5.00	1.59	1.46
14	b	1222	CLA	O2A-C1	5.00	1.59	1.46
15	b	1237	F6C	C4A-NA	-5.00	1.31	1.37
14	G	1138	CLA	O2D-CGD	5.00	1.45	1.33
14	B	1216	CLA	O2D-CGD	5.00	1.45	1.33
14	H	1218	CLA	O2D-CGD	4.99	1.45	1.33
14	b	1239	CLA	C3C-C2C	4.99	1.47	1.36
14	b	1220	CLA	O2D-CGD	4.99	1.45	1.33
14	B	1218	CLA	O2D-CGD	4.99	1.45	1.33
14	b	1216	CLA	O2D-CGD	4.99	1.45	1.33
14	a	1103	CLA	C3D-C4D	-4.99	1.33	1.44
14	H	1021	CLA	O2A-C1	4.98	1.59	1.46
14	B	1233	CLA	O2D-CGD	4.98	1.45	1.33
14	H	1239	CLA	C3C-C2C	4.98	1.47	1.36
14	a	1129	CLA	C3D-C4D	-4.98	1.33	1.44
14	G	1103	CLA	C3D-C4D	-4.97	1.33	1.44
14	b	1218	CLA	O2D-CGD	4.97	1.45	1.33
14	B	1203	CLA	C3D-C4D	-4.97	1.33	1.44
14	A	1126	CLA	C3D-C4D	-4.97	1.33	1.44
14	b	1021	CLA	O2A-C1	4.97	1.59	1.46
14	H	1203	CLA	C3D-C4D	-4.97	1.33	1.44
14	H	1023	CLA	O2A-C1	4.97	1.59	1.46
14	a	1138	CLA	O2D-CGD	4.96	1.45	1.33
14	H	1216	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1137	CLA	C3D-C4D	-4.96	1.33	1.44
14	B	1227	CLA	O2D-CGD	4.96	1.45	1.33
14	b	1203	CLA	C3D-C4D	-4.96	1.33	1.44
14	B	1021	CLA	O2A-C1	4.96	1.59	1.46
14	A	1137	CLA	C3D-C4D	-4.96	1.33	1.44
14	A	1103	CLA	C3D-C4D	-4.96	1.33	1.44
14	G	1126	CLA	C3D-C4D	-4.96	1.33	1.44
14	G	1137	CLA	C3D-C4D	-4.95	1.33	1.44
14	B	1239	CLA	C3C-C2C	4.95	1.47	1.36
14	G	1129	CLA	C3D-C4D	-4.95	1.33	1.44
14	b	1023	CLA	O2A-C1	4.94	1.59	1.46
14	H	1202	CLA	C3D-C4D	-4.94	1.33	1.44
14	a	1126	CLA	C3D-C4D	-4.94	1.33	1.44
14	B	1023	CLA	O2A-C1	4.94	1.59	1.46
14	G	1106	CLA	O2A-C1	4.93	1.59	1.46
14	H	1227	CLA	O2D-CGD	4.93	1.45	1.33
14	b	1202	CLA	C3D-C4D	-4.93	1.33	1.44
14	b	1227	CLA	O2D-CGD	4.93	1.45	1.33
14	A	1106	CLA	O2A-C1	4.93	1.59	1.46
14	a	1106	CLA	O2A-C1	4.92	1.59	1.46
14	b	1204	CLA	C3D-C4D	-4.91	1.33	1.44
14	G	1114	CLA	O2D-CGD	4.91	1.45	1.33
14	A	1114	CLA	O2D-CGD	4.91	1.45	1.33
14	H	1204	CLA	C3D-C4D	-4.91	1.33	1.44
18	B	4014	BCR	C10-C9	-4.91	1.24	1.35
14	a	1135	CLA	C3D-C4D	-4.91	1.33	1.44
14	a	1114	CLA	O2D-CGD	4.90	1.45	1.33
14	A	1135	CLA	C3D-C4D	-4.90	1.33	1.44
14	a	1127	CLA	O2A-C1	4.90	1.59	1.46
14	A	1129	CLA	C3D-C4D	-4.90	1.33	1.44
18	H	4014	BCR	C10-C9	-4.90	1.24	1.35
14	B	1202	CLA	C3D-C4D	-4.90	1.33	1.44
14	G	1127	CLA	O2A-C1	4.90	1.59	1.46
14	A	1127	CLA	O2A-C1	4.90	1.59	1.46
14	B	1204	CLA	C3D-C4D	-4.89	1.33	1.44
18	b	4014	BCR	C10-C9	-4.89	1.24	1.35
14	B	1206	CLA	C3D-C4D	-4.88	1.33	1.44
14	H	1214	CLA	C3D-C4D	-4.88	1.33	1.44
14	G	1135	CLA	C3D-C4D	-4.88	1.33	1.44
14	B	1214	CLA	C3D-C4D	-4.88	1.33	1.44
15	a	1121	F6C	O2D-CGD	4.87	1.45	1.33
14	a	1119	CLA	O2D-CGD	4.87	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1235	CLA	C3D-C4D	-4.87	1.33	1.44
14	b	1206	CLA	C3D-C4D	-4.87	1.33	1.44
14	a	1108	CLA	O2D-CGD	4.87	1.45	1.33
14	H	1206	CLA	C3D-C4D	-4.87	1.33	1.44
15	H	1230	F6C	O2D-CGD	4.87	1.45	1.33
14	A	1108	CLA	O2D-CGD	4.87	1.45	1.33
15	G	1121	F6C	O2D-CGD	4.87	1.45	1.33
14	B	1227	CLA	C3D-C4D	-4.87	1.33	1.44
14	L	1501	CLA	O2D-CGD	4.87	1.45	1.33
14	b	1234	CLA	C3D-C4D	-4.87	1.33	1.44
14	l	1501	CLA	O2D-CGD	4.87	1.45	1.33
14	b	1226	CLA	C3D-C4D	-4.86	1.33	1.44
14	b	1239	CLA	O2D-CGD	4.86	1.45	1.33
14	H	1226	CLA	C3D-C4D	-4.86	1.33	1.44
14	H	1022	CLA	C3D-C4D	-4.86	1.33	1.44
14	a	1138	CLA	C3D-C4D	-4.86	1.33	1.44
14	B	1226	CLA	C3D-C4D	-4.86	1.33	1.44
14	H	1219	CLA	O2D-CGD	4.86	1.45	1.33
14	b	1227	CLA	C3D-C4D	-4.86	1.33	1.44
15	b	1230	F6C	O2D-CGD	4.86	1.45	1.33
14	H	1239	CLA	O2D-CGD	4.86	1.45	1.33
14	B	1224	CLA	C3D-C4D	-4.86	1.33	1.44
14	U	1501	CLA	O2D-CGD	4.85	1.45	1.33
14	b	1235	CLA	C3D-C4D	-4.85	1.33	1.44
14	H	1214	CLA	O2D-CGD	4.85	1.45	1.33
15	B	1230	F6C	O2D-CGD	4.85	1.45	1.33
14	H	1224	CLA	C3D-C4D	-4.85	1.33	1.44
14	b	1219	CLA	O2D-CGD	4.85	1.45	1.33
14	a	1136	CLA	C3D-C4D	-4.85	1.33	1.44
14	G	1140	CLA	C3D-C4D	-4.85	1.33	1.44
14	b	1214	CLA	C3D-C4D	-4.85	1.33	1.44
14	B	1214	CLA	O2D-CGD	4.85	1.45	1.33
14	B	1235	CLA	C3D-C4D	-4.85	1.33	1.44
14	H	1234	CLA	C3D-C4D	-4.85	1.33	1.44
14	B	1021	CLA	C1D-ND	-4.85	1.31	1.37
14	G	1138	CLA	C3D-C4D	-4.85	1.33	1.44
14	B	1234	CLA	C3D-C4D	-4.84	1.33	1.44
14	b	1214	CLA	O2D-CGD	4.84	1.45	1.33
14	G	1108	CLA	O2D-CGD	4.84	1.45	1.33
14	B	1219	CLA	O2D-CGD	4.84	1.45	1.33
15	A	1121	F6C	O2D-CGD	4.84	1.45	1.33
14	a	1140	CLA	C3D-C4D	-4.84	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1136	CLA	C3D-C4D	-4.84	1.33	1.44
14	G	1131	CLA	C3D-C4D	-4.84	1.33	1.44
14	H	1227	CLA	C3D-C4D	-4.84	1.33	1.44
14	G	1119	CLA	O2D-CGD	4.84	1.45	1.33
14	b	1224	CLA	C3D-C4D	-4.83	1.33	1.44
14	A	1138	CLA	C3D-C4D	-4.83	1.33	1.44
14	b	1021	CLA	C1D-ND	-4.83	1.31	1.37
18	H	4016	BCR	C10-C9	-4.83	1.24	1.35
15	B	1237	F6C	O2D-CGD	4.83	1.45	1.33
14	A	1119	CLA	O2D-CGD	4.83	1.45	1.33
14	b	1236	CLA	C3D-C4D	-4.83	1.33	1.44
14	B	1223	CLA	C3D-C4D	-4.82	1.33	1.44
14	G	1120	CLA	O2D-CGD	4.82	1.45	1.33
14	a	1120	CLA	O2D-CGD	4.82	1.45	1.33
14	G	1136	CLA	C3D-C4D	-4.82	1.33	1.44
14	b	1022	CLA	C3D-C4D	-4.82	1.33	1.44
14	B	1236	CLA	C3D-C4D	-4.82	1.33	1.44
14	b	1201	CLA	C3D-C4D	-4.82	1.33	1.44
14	B	1022	CLA	C3D-C4D	-4.82	1.33	1.44
15	H	1237	F6C	O2D-CGD	4.82	1.45	1.33
14	B	1239	CLA	O2D-CGD	4.82	1.45	1.33
14	a	1124	CLA	C3D-C4D	-4.82	1.33	1.44
14	B	1225	CLA	C3D-C4D	-4.82	1.33	1.44
14	A	1131	CLA	C3D-C4D	-4.82	1.33	1.44
14	b	1223	CLA	C3D-C4D	-4.82	1.33	1.44
14	A	1104	CLA	O2D-CGD	4.81	1.45	1.33
14	H	1225	CLA	C3D-C4D	-4.81	1.33	1.44
15	b	1237	F6C	O2D-CGD	4.81	1.45	1.33
14	b	1225	CLA	C3D-C4D	-4.81	1.33	1.44
18	b	4016	BCR	C10-C9	-4.81	1.24	1.35
14	H	1021	CLA	C1D-ND	-4.81	1.31	1.37
14	H	1236	CLA	C3D-C4D	-4.81	1.33	1.44
14	H	1201	CLA	C3D-C4D	-4.81	1.33	1.44
14	H	1223	CLA	C3D-C4D	-4.81	1.33	1.44
14	B	1210	CLA	C3D-C4D	-4.81	1.33	1.44
14	a	1128	CLA	C3D-C4D	-4.81	1.33	1.44
14	A	1124	CLA	C3D-C4D	-4.80	1.33	1.44
14	B	1201	CLA	C3D-C4D	-4.80	1.33	1.44
14	G	1104	CLA	O2D-CGD	4.80	1.45	1.33
14	H	1211	CLA	C3D-C4D	-4.80	1.33	1.44
14	a	1131	CLA	C3D-C4D	-4.80	1.33	1.44
14	A	1140	CLA	C3D-C4D	-4.80	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1128	CLA	C3D-C4D	-4.80	1.33	1.44
18	B	4016	BCR	C10-C9	-4.79	1.24	1.35
14	B	1225	CLA	O2D-CGD	4.79	1.45	1.33
14	A	1120	CLA	O2D-CGD	4.79	1.45	1.33
14	a	1115	CLA	O2D-CGD	4.79	1.45	1.33
14	a	1134	CLA	O2D-CGD	4.79	1.45	1.33
14	G	1124	CLA	C3D-C4D	-4.79	1.33	1.44
14	b	1225	CLA	O2D-CGD	4.79	1.45	1.33
14	G	1102	CLA	C3D-C4D	-4.79	1.33	1.44
14	A	1128	CLA	C3D-C4D	-4.79	1.33	1.44
14	G	1134	CLA	O2D-CGD	4.78	1.45	1.33
14	A	1134	CLA	O2D-CGD	4.78	1.45	1.33
14	A	1102	CLA	C3D-C4D	-4.78	1.33	1.44
14	A	1123	CLA	O2D-CGD	4.78	1.45	1.33
14	a	1104	CLA	O2D-CGD	4.78	1.45	1.33
14	b	1210	CLA	C3D-C4D	-4.78	1.33	1.44
14	A	1125	CLA	O2D-CGD	4.77	1.45	1.33
14	H	1239	CLA	C3D-C4D	-4.77	1.33	1.44
14	b	1217	CLA	O2D-CGD	4.77	1.45	1.33
18	U	4022	BCR	C10-C9	-4.77	1.24	1.35
14	B	1239	CLA	C3D-C4D	-4.77	1.33	1.44
14	G	1123	CLA	O2D-CGD	4.77	1.44	1.33
18	m	4021	BCR	C10-C9	-4.77	1.24	1.35
14	G	1115	CLA	O2D-CGD	4.77	1.44	1.33
14	b	1239	CLA	C3D-C4D	-4.77	1.33	1.44
14	H	1210	CLA	C3D-C4D	-4.76	1.33	1.44
14	a	1139	CLA	C3D-C4D	-4.76	1.33	1.44
18	l	4022	BCR	C10-C9	-4.76	1.24	1.35
14	G	1125	CLA	O2D-CGD	4.76	1.44	1.33
14	a	1105	CLA	O2D-CGD	4.76	1.44	1.33
14	L	1501	CLA	C3D-C4D	-4.76	1.33	1.44
14	H	1021	CLA	C3D-C4D	-4.76	1.33	1.44
14	a	1102	CLA	C3D-C4D	-4.76	1.33	1.44
14	a	1123	CLA	O2D-CGD	4.76	1.44	1.33
14	A	1115	CLA	O2D-CGD	4.76	1.44	1.33
14	A	1013	CLA	C1D-ND	-4.76	1.31	1.37
14	b	1211	CLA	C3D-C4D	-4.76	1.33	1.44
14	A	1105	CLA	O2D-CGD	4.76	1.44	1.33
14	B	1217	CLA	O2D-CGD	4.76	1.44	1.33
14	B	1211	CLA	C3D-C4D	-4.76	1.33	1.44
18	L	4022	BCR	C10-C9	-4.76	1.24	1.35
14	G	1105	CLA	O2D-CGD	4.76	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1217	CLA	O2D-CGD	4.75	1.44	1.33
14	a	1125	CLA	O2D-CGD	4.75	1.44	1.33
14	l	1501	CLA	C3D-C4D	-4.75	1.33	1.44
14	H	1221	CLA	C3D-C4D	-4.75	1.33	1.44
14	b	1221	CLA	C3D-C4D	-4.75	1.33	1.44
18	M	4021	BCR	C10-C9	-4.75	1.24	1.35
14	U	1501	CLA	C3D-C4D	-4.75	1.33	1.44
14	B	1228	CLA	O2D-CGD	4.75	1.44	1.33
14	G	1107	CLA	O2D-CGD	4.75	1.44	1.33
18	V	4021	BCR	C10-C9	-4.74	1.24	1.35
14	a	1119	CLA	C3D-C4D	-4.74	1.33	1.44
14	b	1222	CLA	C3D-C4D	-4.74	1.33	1.44
14	b	1205	CLA	C3D-C4D	-4.74	1.33	1.44
14	H	1225	CLA	O2D-CGD	4.74	1.44	1.33
14	A	1013	CLA	CHC-C1C	4.74	1.48	1.38
14	G	1139	CLA	C3D-C4D	-4.74	1.33	1.44
14	G	1118	CLA	C3D-C4D	-4.73	1.33	1.44
18	a	4011	BCR	C10-C9	-4.73	1.24	1.35
14	a	1114	CLA	CHD-C1D	4.73	1.47	1.38
14	B	1021	CLA	C3D-C4D	-4.73	1.33	1.44
18	A	4001	BCR	C10-C9	-4.73	1.24	1.35
14	a	1130	CLA	O2D-CGD	4.73	1.44	1.33
14	B	1221	CLA	C3D-C4D	-4.73	1.33	1.44
14	b	1021	CLA	C3D-C4D	-4.73	1.33	1.44
14	G	1109	CLA	O2D-CGD	4.73	1.44	1.33
14	a	1118	CLA	C3D-C4D	-4.73	1.33	1.44
18	B	4017	BCR	C10-C9	-4.73	1.24	1.35
14	a	1132	CLA	C3D-C4D	-4.73	1.33	1.44
14	G	1113	CLA	O2D-CGD	4.73	1.44	1.33
14	A	1126	CLA	O2D-CGD	4.72	1.44	1.33
14	G	1013	CLA	CHC-C1C	4.72	1.47	1.38
14	H	1228	CLA	O2D-CGD	4.72	1.44	1.33
14	U	1503	CLA	O2D-CGD	4.72	1.44	1.33
14	A	1104	CLA	C3D-C4D	-4.72	1.33	1.44
14	G	1132	CLA	C3D-C4D	-4.72	1.33	1.44
14	a	1013	CLA	CHC-C1C	4.72	1.47	1.38
14	G	1127	CLA	O2D-CGD	4.72	1.44	1.33
14	A	1132	CLA	C3D-C4D	-4.72	1.33	1.44
14	A	1139	CLA	C3D-C4D	-4.72	1.33	1.44
14	A	1114	CLA	CHD-C1D	4.72	1.47	1.38
14	H	1228	CLA	C3D-C4D	-4.72	1.33	1.44
14	A	1130	CLA	O2D-CGD	4.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1107	CLA	O2D-CGD	4.72	1.44	1.33
14	l	1503	CLA	C3D-C4D	-4.71	1.33	1.44
18	H	4017	BCR	C10-C9	-4.71	1.24	1.35
14	B	1228	CLA	C3D-C4D	-4.71	1.33	1.44
14	a	1013	CLA	C1D-ND	-4.71	1.31	1.37
14	A	1136	CLA	O2D-CGD	4.71	1.44	1.33
14	B	1208	CLA	O2D-CGD	4.71	1.44	1.33
14	H	1205	CLA	C3D-C4D	-4.71	1.33	1.44
18	b	4017	BCR	C10-C9	-4.71	1.24	1.35
14	A	1119	CLA	C3D-C4D	-4.71	1.33	1.44
14	a	1113	CLA	O2D-CGD	4.71	1.44	1.33
14	B	1209	CLA	O2D-CGD	4.71	1.44	1.33
14	a	1116	CLA	O2D-CGD	4.71	1.44	1.33
14	b	1228	CLA	O2D-CGD	4.71	1.44	1.33
18	A	4011	BCR	C10-C9	-4.71	1.24	1.35
14	G	1111	CLA	C3D-C4D	-4.71	1.33	1.44
14	L	1503	CLA	O2D-CGD	4.71	1.44	1.33
18	a	4001	BCR	C10-C9	-4.70	1.24	1.35
14	a	1126	CLA	O2D-CGD	4.70	1.44	1.33
18	G	4001	BCR	C10-C9	-4.70	1.24	1.35
14	a	1127	CLA	O2D-CGD	4.70	1.44	1.33
14	b	1208	CLA	O2D-CGD	4.70	1.44	1.33
14	G	1116	CLA	C3D-C4D	-4.70	1.33	1.44
14	a	1117	CLA	O2D-CGD	4.70	1.44	1.33
14	A	1113	CLA	O2D-CGD	4.70	1.44	1.33
14	A	1116	CLA	O2D-CGD	4.70	1.44	1.33
14	A	1107	CLA	O2D-CGD	4.70	1.44	1.33
14	A	1109	CLA	O2D-CGD	4.70	1.44	1.33
14	X	1701	CLA	O2D-CGD	4.70	1.44	1.33
14	a	1109	CLA	O2D-CGD	4.70	1.44	1.33
14	G	1119	CLA	C3D-C4D	-4.70	1.33	1.44
14	B	1222	CLA	C3D-C4D	-4.70	1.33	1.44
14	G	1136	CLA	O2D-CGD	4.70	1.44	1.33
14	U	1503	CLA	C3D-C4D	-4.70	1.33	1.44
14	B	1232	CLA	O2D-CGD	4.70	1.44	1.33
18	H	4005	BCR	C10-C9	-4.70	1.24	1.35
14	G	1104	CLA	C3D-C4D	-4.70	1.33	1.44
14	L	1503	CLA	C3D-C4D	-4.70	1.33	1.44
18	G	4011	BCR	C10-C9	-4.69	1.24	1.35
14	A	1111	CLA	C3D-C4D	-4.69	1.33	1.44
18	l	4019	BCR	C10-C9	-4.69	1.24	1.35
14	B	1204	CLA	C1D-ND	-4.69	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1205	CLA	C3D-C4D	-4.69	1.33	1.44
14	H	1208	CLA	O2D-CGD	4.69	1.44	1.33
14	l	1503	CLA	O2D-CGD	4.69	1.44	1.33
14	b	1209	CLA	O2D-CGD	4.69	1.44	1.33
14	A	1106	CLA	C3D-C4D	-4.69	1.33	1.44
14	G	1116	CLA	O2D-CGD	4.69	1.44	1.33
14	G	1107	CLA	C3D-C4D	-4.69	1.33	1.44
14	A	1117	CLA	O2D-CGD	4.69	1.44	1.33
14	a	1113	CLA	C3D-C4D	-4.69	1.33	1.44
14	G	1130	CLA	O2D-CGD	4.69	1.44	1.33
14	b	1203	CLA	O2D-CGD	4.69	1.44	1.33
14	b	1229	CLA	C3D-C4D	-4.69	1.33	1.44
14	G	1126	CLA	O2D-CGD	4.68	1.44	1.33
14	B	1211	CLA	O2D-CGD	4.68	1.44	1.33
14	A	1118	CLA	C3D-C4D	-4.68	1.33	1.44
14	A	1133	CLA	O2D-CGD	4.68	1.44	1.33
14	a	1136	CLA	O2D-CGD	4.68	1.44	1.33
14	a	1107	CLA	C3D-C4D	-4.68	1.33	1.44
14	a	1111	CLA	C3D-C4D	-4.68	1.33	1.44
14	a	1127	CLA	C3D-C4D	-4.68	1.33	1.44
14	B	1203	CLA	O2D-CGD	4.68	1.44	1.33
14	H	1222	CLA	C3D-C4D	-4.68	1.33	1.44
14	G	1013	CLA	C1D-ND	-4.68	1.31	1.37
15	B	1230	F6C	C4A-NA	-4.68	1.31	1.37
14	a	1133	CLA	O2D-CGD	4.68	1.44	1.33
14	a	1123	CLA	C3D-C4D	-4.68	1.33	1.44
14	H	1215	CLA	C3D-C4D	-4.68	1.33	1.44
14	a	1104	CLA	C3D-C4D	-4.68	1.33	1.44
14	H	1221	CLA	O2D-CGD	4.68	1.44	1.33
14	b	1204	CLA	C1D-ND	-4.68	1.31	1.37
14	b	1228	CLA	C3D-C4D	-4.68	1.33	1.44
14	b	1211	CLA	O2D-CGD	4.68	1.44	1.33
18	B	4005	BCR	C10-C9	-4.68	1.25	1.35
14	H	1232	CLA	O2D-CGD	4.68	1.44	1.33
14	H	1204	CLA	C1D-ND	-4.68	1.31	1.37
14	W	1701	CLA	O2D-CGD	4.67	1.44	1.33
18	b	4005	BCR	C10-C9	-4.67	1.25	1.35
18	L	4019	BCR	C10-C9	-4.67	1.25	1.35
18	U	4019	BCR	C10-C9	-4.67	1.25	1.35
14	G	1106	CLA	C3D-C4D	-4.67	1.33	1.44
14	a	1139	CLA	O2D-CGD	4.67	1.44	1.33
14	H	1023	CLA	C3D-C4D	-4.67	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1203	CLA	O2D-CGD	4.67	1.44	1.33
14	b	1221	CLA	O2D-CGD	4.67	1.44	1.33
14	a	1109	CLA	C3D-C4D	-4.67	1.33	1.44
14	A	1123	CLA	C3D-C4D	-4.67	1.33	1.44
14	H	1204	CLA	O2D-CGD	4.67	1.44	1.33
14	b	1216	CLA	C3D-C4D	-4.67	1.33	1.44
14	A	1127	CLA	O2D-CGD	4.67	1.44	1.33
14	A	1113	CLA	C3D-C4D	-4.66	1.33	1.44
14	a	1106	CLA	C3D-C4D	-4.66	1.33	1.44
14	b	1208	CLA	C3D-C4D	-4.66	1.33	1.44
14	H	1229	CLA	C3D-C4D	-4.66	1.33	1.44
14	a	1105	CLA	C3D-C4D	-4.66	1.33	1.44
14	A	1107	CLA	C3D-C4D	-4.66	1.33	1.44
14	B	1221	CLA	O2D-CGD	4.66	1.44	1.33
14	x	1701	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1122	CLA	C3D-C4D	-4.66	1.33	1.44
14	H	1209	CLA	O2D-CGD	4.66	1.44	1.33
14	a	1116	CLA	C3D-C4D	-4.66	1.33	1.44
15	b	1230	F6C	C4A-NA	-4.66	1.31	1.37
14	G	1113	CLA	C3D-C4D	-4.66	1.33	1.44
14	G	1117	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1114	CLA	CHD-C1D	4.66	1.47	1.38
14	G	1139	CLA	O2D-CGD	4.66	1.44	1.33
14	l	1502	CLA	C3D-C4D	-4.66	1.33	1.44
14	B	1229	CLA	C3D-C4D	-4.66	1.33	1.44
14	H	1211	CLA	O2D-CGD	4.66	1.44	1.33
14	G	1117	CLA	C3D-C4D	-4.65	1.33	1.44
14	a	1122	CLA	C3D-C4D	-4.65	1.33	1.44
14	H	1213	CLA	O2D-CGD	4.65	1.44	1.33
14	B	1213	CLA	O2D-CGD	4.65	1.44	1.33
14	A	1116	CLA	C3D-C4D	-4.65	1.33	1.44
14	G	1123	CLA	C3D-C4D	-4.65	1.33	1.44
14	A	1134	CLA	CHD-C1D	4.65	1.47	1.38
14	G	1133	CLA	O2D-CGD	4.65	1.44	1.33
14	a	1117	CLA	C3D-C4D	-4.65	1.33	1.44
14	B	1215	CLA	C3D-C4D	-4.65	1.33	1.44
14	a	1122	CLA	O2D-CGD	4.65	1.44	1.33
14	A	1134	CLA	CHC-C1C	4.65	1.47	1.38
14	H	1208	CLA	C3D-C4D	-4.65	1.33	1.44
14	A	1105	CLA	C3D-C4D	-4.65	1.33	1.44
14	H	1236	CLA	O2D-CGD	4.65	1.44	1.33
14	B	1023	CLA	O2D-CGD	4.65	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1133	CLA	C3D-C4D	-4.65	1.33	1.44
15	H	1230	F6C	C4A-NA	-4.65	1.31	1.37
14	A	1112	CLA	O2D-CGD	4.65	1.44	1.33
15	H	1238	F6C	O2D-CGD	4.65	1.44	1.33
14	a	1134	CLA	CHC-C1C	4.64	1.47	1.38
14	G	1013	CLA	O2D-CGD	4.64	1.44	1.33
14	A	1106	CLA	O2D-CGD	4.64	1.44	1.33
14	H	1219	CLA	CHC-C1C	4.64	1.47	1.38
14	b	1215	CLA	C3D-C4D	-4.64	1.33	1.44
14	G	1112	CLA	O2D-CGD	4.64	1.44	1.33
14	b	1236	CLA	O2D-CGD	4.64	1.44	1.33
14	G	1127	CLA	C3D-C4D	-4.64	1.33	1.44
14	B	1208	CLA	C3D-C4D	-4.64	1.33	1.44
14	G	1110	CLA	C3D-C4D	-4.64	1.33	1.44
14	A	1127	CLA	C3D-C4D	-4.64	1.33	1.44
14	a	1110	CLA	O2D-CGD	4.64	1.44	1.33
14	b	1232	CLA	O2D-CGD	4.64	1.44	1.33
14	b	1234	CLA	CHC-C1C	4.64	1.47	1.38
14	H	1234	CLA	CHC-C1C	4.64	1.47	1.38
14	b	1204	CLA	O2D-CGD	4.64	1.44	1.33
14	b	1219	CLA	CHC-C1C	4.64	1.47	1.38
14	G	1114	CLA	C3D-C4D	-4.64	1.33	1.44
14	a	1108	CLA	C3D-C4D	-4.63	1.33	1.44
15	b	1238	F6C	O2D-CGD	4.63	1.44	1.33
14	A	1122	CLA	C3D-C4D	-4.63	1.33	1.44
14	A	1013	CLA	O2D-CGD	4.63	1.44	1.33
14	G	1109	CLA	C3D-C4D	-4.63	1.33	1.44
14	G	1112	CLA	C3D-C4D	-4.63	1.33	1.44
14	B	1219	CLA	CHC-C1C	4.63	1.47	1.38
14	B	1234	CLA	CHC-C1C	4.63	1.47	1.38
14	A	1108	CLA	C3D-C4D	-4.63	1.33	1.44
14	A	1110	CLA	C3D-C4D	-4.63	1.33	1.44
14	H	1023	CLA	O2D-CGD	4.63	1.44	1.33
14	a	1112	CLA	O2D-CGD	4.63	1.44	1.33
14	H	1216	CLA	C3D-C4D	-4.63	1.33	1.44
14	b	1023	CLA	O2D-CGD	4.63	1.44	1.33
14	A	1110	CLA	O2D-CGD	4.63	1.44	1.33
14	A	1139	CLA	O2D-CGD	4.63	1.44	1.33
14	G	1105	CLA	C3D-C4D	-4.62	1.33	1.44
14	B	1231	CLA	C3D-C4D	-4.62	1.33	1.44
14	B	1204	CLA	O2D-CGD	4.62	1.44	1.33
14	H	1226	CLA	O2D-CGD	4.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1122	CLA	O2D-CGD	4.62	1.44	1.33
14	A	1133	CLA	C3D-C4D	-4.62	1.33	1.44
14	B	1023	CLA	C3D-C4D	-4.62	1.33	1.44
14	A	1117	CLA	C3D-C4D	-4.62	1.33	1.44
14	B	1216	CLA	C3D-C4D	-4.62	1.33	1.44
14	G	1140	CLA	O2D-CGD	4.62	1.44	1.33
14	G	1102	CLA	O2D-CGD	4.62	1.44	1.33
14	a	1110	CLA	C3D-C4D	-4.62	1.33	1.44
14	A	1122	CLA	O2D-CGD	4.62	1.44	1.33
14	A	1140	CLA	O2D-CGD	4.62	1.44	1.33
15	B	1238	F6C	O2D-CGD	4.62	1.44	1.33
14	U	1502	CLA	C3D-C4D	-4.62	1.33	1.44
14	G	1106	CLA	O2D-CGD	4.62	1.44	1.33
14	B	1236	CLA	O2D-CGD	4.62	1.44	1.33
14	A	1109	CLA	C3D-C4D	-4.62	1.33	1.44
14	G	1110	CLA	O2D-CGD	4.62	1.44	1.33
14	b	1023	CLA	C3D-C4D	-4.61	1.33	1.44
14	a	1106	CLA	O2D-CGD	4.61	1.44	1.33
14	H	1231	CLA	C3D-C4D	-4.61	1.33	1.44
14	a	1134	CLA	C3C-C2C	4.61	1.46	1.36
14	a	1134	CLA	CHD-C1D	4.61	1.47	1.38
13	G	1011	CL0	CHC-C4B	4.61	1.47	1.39
14	a	1013	CLA	O2D-CGD	4.61	1.44	1.33
14	b	1231	CLA	C3D-C4D	-4.61	1.33	1.44
14	H	1229	CLA	CHC-C1C	4.61	1.47	1.38
14	b	1213	CLA	O2D-CGD	4.61	1.44	1.33
14	b	1231	CLA	O2D-CGD	4.61	1.44	1.33
14	b	1220	CLA	C3D-C4D	-4.61	1.33	1.44
14	B	1226	CLA	O2D-CGD	4.61	1.44	1.33
14	b	1229	CLA	CHC-C1C	4.61	1.47	1.38
14	a	1140	CLA	O2D-CGD	4.61	1.44	1.33
14	A	1114	CLA	C3D-C4D	-4.60	1.33	1.44
14	L	1502	CLA	C3D-C4D	-4.60	1.33	1.44
14	B	1217	CLA	C3D-C4D	-4.60	1.33	1.44
14	G	1134	CLA	CHD-C1D	4.60	1.47	1.38
14	G	1118	CLA	O2D-CGD	4.60	1.44	1.33
14	a	1114	CLA	C3D-C4D	-4.60	1.33	1.44
14	A	1118	CLA	O2D-CGD	4.60	1.44	1.33
14	B	1220	CLA	C3D-C4D	-4.60	1.33	1.44
14	B	1231	CLA	O2D-CGD	4.60	1.44	1.33
14	A	1112	CLA	C3D-C4D	-4.60	1.33	1.44
13	A	1011	CL0	CHC-C4B	4.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1134	CLA	CHC-C1C	4.60	1.47	1.38
14	G	1108	CLA	C3D-C4D	-4.60	1.33	1.44
14	b	1226	CLA	O2D-CGD	4.59	1.44	1.33
13	a	1011	CL0	CHC-C4B	4.59	1.47	1.39
14	a	1118	CLA	O2D-CGD	4.59	1.44	1.33
14	B	1213	CLA	C3D-C4D	-4.59	1.33	1.44
14	a	1102	CLA	O2D-CGD	4.59	1.44	1.33
14	a	1133	CLA	C3D-C4D	-4.59	1.33	1.44
14	H	1220	CLA	C3D-C4D	-4.59	1.33	1.44
14	a	1115	CLA	C3D-C4D	-4.59	1.33	1.44
14	b	1217	CLA	C3D-C4D	-4.59	1.33	1.44
14	B	1235	CLA	O2D-CGD	4.59	1.44	1.33
14	H	1217	CLA	C3D-C4D	-4.59	1.33	1.44
14	H	1231	CLA	O2D-CGD	4.58	1.44	1.33
14	G	1115	CLA	C3D-C4D	-4.58	1.33	1.44
14	H	1213	CLA	C3D-C4D	-4.58	1.33	1.44
14	B	1232	CLA	C3D-C4D	-4.58	1.33	1.44
14	b	1213	CLA	C3D-C4D	-4.58	1.33	1.44
14	b	1235	CLA	O2D-CGD	4.58	1.44	1.33
13	A	1011	CL0	O2D-CGD	4.58	1.44	1.33
18	i	4018	BCR	C10-C9	-4.58	1.25	1.35
14	A	1115	CLA	C3D-C4D	-4.58	1.33	1.44
14	G	1134	CLA	C3C-C2C	4.58	1.46	1.36
13	a	1011	CL0	O2D-CGD	4.58	1.44	1.33
14	b	1212	CLA	O2D-CGD	4.57	1.44	1.33
14	b	1224	CLA	O2D-CGD	4.57	1.44	1.33
14	B	1229	CLA	CHC-C1C	4.57	1.47	1.38
14	b	1232	CLA	C3D-C4D	-4.57	1.33	1.44
18	R	4018	BCR	C10-C9	-4.57	1.25	1.35
14	B	1222	CLA	O2D-CGD	4.57	1.44	1.33
14	B	1209	CLA	C3D-C4D	-4.57	1.33	1.44
14	H	1224	CLA	O2D-CGD	4.57	1.44	1.33
13	G	1011	CL0	O2D-CGD	4.57	1.44	1.33
14	H	1232	CLA	C3D-C4D	-4.56	1.33	1.44
14	b	1205	CLA	C1D-ND	-4.56	1.31	1.37
14	b	1201	CLA	O2D-CGD	4.56	1.44	1.33
14	H	1235	CLA	O2D-CGD	4.56	1.44	1.33
14	A	1102	CLA	O2D-CGD	4.56	1.44	1.33
14	b	1215	CLA	O2D-CGD	4.56	1.44	1.33
14	G	1120	CLA	C3D-C4D	-4.56	1.33	1.44
14	H	1222	CLA	O2D-CGD	4.55	1.44	1.33
14	B	1218	CLA	CHC-C1C	4.55	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1209	CLA	C3D-C4D	-4.55	1.33	1.44
14	B	1229	CLA	O2D-CGD	4.55	1.44	1.33
14	X	1701	CLA	CHC-C1C	4.55	1.47	1.38
14	H	1209	CLA	C3D-C4D	-4.55	1.33	1.44
14	b	1229	CLA	O2D-CGD	4.55	1.44	1.33
14	H	1022	CLA	CHC-C1C	4.55	1.47	1.38
14	B	1022	CLA	CHC-C1C	4.55	1.47	1.38
14	B	1201	CLA	O2D-CGD	4.55	1.44	1.33
14	B	1224	CLA	O2D-CGD	4.55	1.44	1.33
14	H	1229	CLA	O2D-CGD	4.55	1.44	1.33
14	B	1215	CLA	O2D-CGD	4.55	1.44	1.33
14	a	1112	CLA	C3D-C4D	-4.55	1.34	1.44
14	G	1110	CLA	CHC-C1C	4.54	1.47	1.38
14	A	1101	CLA	C3D-C4D	-4.54	1.34	1.44
14	b	1218	CLA	CHC-C1C	4.54	1.47	1.38
14	a	1101	CLA	C3D-C4D	-4.54	1.34	1.44
14	A	1134	CLA	C3C-C2C	4.54	1.46	1.36
14	H	1205	CLA	C1D-ND	-4.54	1.31	1.37
14	B	1212	CLA	O2D-CGD	4.53	1.44	1.33
14	B	1206	CLA	O2D-CGD	4.53	1.44	1.33
14	b	1222	CLA	O2D-CGD	4.53	1.44	1.33
14	H	1215	CLA	O2D-CGD	4.53	1.44	1.33
14	B	1205	CLA	C1D-ND	-4.53	1.31	1.37
14	H	1212	CLA	O2D-CGD	4.53	1.44	1.33
14	A	1013	CLA	C1B-NB	-4.53	1.31	1.37
14	x	1701	CLA	C3D-C4D	-4.53	1.34	1.44
14	H	1218	CLA	CHC-C1C	4.52	1.47	1.38
14	G	1101	CLA	O2D-CGD	4.52	1.44	1.33
14	a	1120	CLA	C3D-C4D	-4.52	1.34	1.44
14	x	1701	CLA	CHC-C1C	4.52	1.47	1.38
14	W	1701	CLA	CHC-C1C	4.52	1.47	1.38
14	A	1120	CLA	C3D-C4D	-4.52	1.34	1.44
14	G	1101	CLA	C3D-C4D	-4.52	1.34	1.44
18	I	4018	BCR	C10-C9	-4.52	1.25	1.35
14	H	1023	CLA	C1D-ND	-4.52	1.31	1.37
14	A	1101	CLA	O2D-CGD	4.51	1.44	1.33
20	a	5005	LMG	O8-C28	4.51	1.46	1.33
14	a	1110	CLA	CHC-C1C	4.51	1.47	1.38
14	a	1139	CLA	CHC-C1C	4.51	1.47	1.38
14	A	1013	CLA	C3D-C4D	-4.51	1.34	1.44
14	G	1116	CLA	CHC-C1C	4.51	1.47	1.38
14	W	1701	CLA	C3D-C4D	-4.50	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1022	CLA	CHC-C1C	4.50	1.47	1.38
14	H	1206	CLA	O2D-CGD	4.50	1.44	1.33
14	a	1101	CLA	O2D-CGD	4.50	1.44	1.33
14	b	1206	CLA	O2D-CGD	4.50	1.44	1.33
14	H	1201	CLA	O2D-CGD	4.50	1.44	1.33
14	U	1502	CLA	O2D-CGD	4.50	1.44	1.33
18	H	4009	BCR	C10-C9	-4.50	1.25	1.35
14	l	1502	CLA	O2D-CGD	4.50	1.44	1.33
20	G	5005	LMG	O8-C28	4.50	1.46	1.33
14	X	1701	CLA	C3D-C4D	-4.50	1.34	1.44
14	G	1129	CLA	O2D-CGD	4.49	1.44	1.33
14	T	1401	CLA	CHC-C1C	4.49	1.47	1.38
14	b	1223	CLA	O2D-CGD	4.49	1.44	1.33
14	K	1401	CLA	CHC-C1C	4.49	1.47	1.38
14	b	1227	CLA	CHD-C1D	4.49	1.47	1.38
14	H	1223	CLA	O2D-CGD	4.49	1.44	1.33
14	G	1103	CLA	O2D-CGD	4.48	1.44	1.33
14	B	1023	CLA	C1D-ND	-4.48	1.32	1.37
14	H	1205	CLA	O2D-CGD	4.48	1.44	1.33
14	G	1013	CLA	C3D-C4D	-4.48	1.34	1.44
20	A	5005	LMG	O8-C28	4.48	1.46	1.33
14	A	1103	CLA	O2D-CGD	4.48	1.44	1.33
14	A	1139	CLA	CHC-C1C	4.48	1.47	1.38
14	G	1114	CLA	C3C-C2C	4.48	1.46	1.36
14	b	1205	CLA	O2D-CGD	4.48	1.44	1.33
14	B	1223	CLA	O2D-CGD	4.48	1.44	1.33
14	A	1110	CLA	CHC-C1C	4.48	1.47	1.38
15	B	1238	F6C	CHC-C4B	4.48	1.47	1.38
18	b	4009	BCR	C10-C9	-4.47	1.25	1.35
14	A	1129	CLA	O2D-CGD	4.47	1.44	1.33
14	a	1013	CLA	C3D-C4D	-4.47	1.34	1.44
14	a	1103	CLA	O2D-CGD	4.47	1.44	1.33
14	H	1233	CLA	C3D-C4D	-4.47	1.34	1.44
14	L	1502	CLA	O2D-CGD	4.47	1.44	1.33
14	H	1233	CLA	CHD-C1D	4.47	1.47	1.38
14	A	1126	CLA	CHC-C1C	4.47	1.47	1.38
14	B	1212	CLA	CHC-C1C	4.47	1.47	1.38
18	B	4009	BCR	C10-C9	-4.47	1.25	1.35
14	k	1401	CLA	CHC-C1C	4.47	1.47	1.38
14	G	1131	CLA	O2D-CGD	4.47	1.44	1.33
14	A	1116	CLA	CHC-C1C	4.47	1.47	1.38
15	H	1238	F6C	CHC-C4B	4.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1131	CLA	O2D-CGD	4.47	1.44	1.33
14	G	1139	CLA	CHC-C1C	4.46	1.47	1.38
14	B	1213	CLA	CHC-C1C	4.46	1.47	1.38
14	a	1013	CLA	C1B-NB	-4.46	1.32	1.37
14	a	1129	CLA	O2D-CGD	4.46	1.44	1.33
18	G	4003	BCR	C10-C9	-4.46	1.25	1.35
14	b	1233	CLA	C3D-C4D	-4.46	1.34	1.44
14	a	1114	CLA	C3C-C2C	4.46	1.46	1.36
18	A	4003	BCR	C10-C9	-4.46	1.25	1.35
14	G	1126	CLA	CHC-C1C	4.46	1.47	1.38
14	b	1202	CLA	O2D-CGD	4.46	1.44	1.33
14	a	1116	CLA	CHC-C1C	4.46	1.47	1.38
14	B	1205	CLA	O2D-CGD	4.46	1.44	1.33
14	a	1126	CLA	CHC-C1C	4.46	1.47	1.38
14	A	1114	CLA	C3C-C2C	4.46	1.46	1.36
14	a	1124	CLA	CHC-C1C	4.46	1.47	1.38
14	B	1202	CLA	O2D-CGD	4.45	1.44	1.33
14	B	1219	CLA	C3D-C4D	-4.45	1.34	1.44
14	b	1233	CLA	CHD-C1D	4.45	1.47	1.38
14	a	1119	CLA	C3C-C2C	4.45	1.46	1.36
14	G	1124	CLA	CHC-C1C	4.45	1.47	1.38
14	H	1219	CLA	C3D-C4D	-4.45	1.34	1.44
14	H	1202	CLA	O2D-CGD	4.45	1.44	1.33
14	H	1227	CLA	CHD-C1D	4.45	1.47	1.38
14	B	1214	CLA	CHD-C1D	4.45	1.47	1.38
14	K	1401	CLA	CHD-C1D	4.45	1.47	1.38
14	b	1214	CLA	CHD-C1D	4.45	1.47	1.38
14	a	1131	CLA	O2D-CGD	4.45	1.44	1.33
14	A	1124	CLA	CHC-C1C	4.45	1.47	1.38
14	a	1119	CLA	CHD-C1D	4.45	1.47	1.38
14	A	1113	CLA	CHC-C1C	4.44	1.47	1.38
14	B	1222	CLA	CHC-C1C	4.44	1.47	1.38
14	b	1023	CLA	C1D-ND	-4.44	1.32	1.37
14	G	1102	CLA	CHC-C1C	4.44	1.47	1.38
14	B	1233	CLA	C3D-C4D	-4.44	1.34	1.44
14	H	1222	CLA	CHC-C1C	4.44	1.47	1.38
14	b	1213	CLA	CHC-C1C	4.44	1.47	1.38
15	b	1238	F6C	CHC-C4B	4.44	1.47	1.38
14	a	1135	CLA	O2D-CGD	4.44	1.44	1.33
14	G	1119	CLA	CHD-C1D	4.44	1.47	1.38
14	G	1128	CLA	C1D-ND	-4.44	1.32	1.37
14	b	1212	CLA	CHC-C1C	4.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	1011	CL0	CHB-C1B	4.44	1.46	1.39
14	G	1135	CLA	O2D-CGD	4.44	1.44	1.33
14	H	1212	CLA	CHC-C1C	4.44	1.47	1.38
14	A	1119	CLA	CHD-C1D	4.43	1.47	1.38
14	B	1227	CLA	CHD-C1D	4.43	1.47	1.38
14	b	1021	CLA	O2D-CGD	4.43	1.44	1.33
14	A	1135	CLA	O2D-CGD	4.43	1.44	1.33
14	a	1113	CLA	CHC-C1C	4.43	1.47	1.38
14	A	1119	CLA	C3C-C2C	4.43	1.46	1.36
14	H	1213	CLA	CHC-C1C	4.43	1.47	1.38
14	B	1218	CLA	C1D-ND	-4.43	1.32	1.37
14	b	1219	CLA	C3D-C4D	-4.43	1.34	1.44
14	A	1102	CLA	CHC-C1C	4.43	1.47	1.38
14	B	1233	CLA	CHD-C1D	4.43	1.47	1.38
14	B	1211	CLA	CHC-C1C	4.43	1.47	1.38
14	T	1401	CLA	CHD-C1D	4.42	1.47	1.38
14	H	1021	CLA	O2D-CGD	4.42	1.44	1.33
18	H	4006	BCR	C10-C9	-4.42	1.25	1.35
14	G	1113	CLA	CHC-C1C	4.42	1.47	1.38
14	b	1226	CLA	C1D-ND	-4.42	1.32	1.37
14	B	1227	CLA	CHC-C1C	4.42	1.47	1.38
18	a	4003	BCR	C10-C9	-4.42	1.25	1.35
14	A	1138	CLA	CHC-C1C	4.42	1.47	1.38
14	B	1021	CLA	O2D-CGD	4.42	1.44	1.33
14	H	1214	CLA	CHD-C1D	4.42	1.47	1.38
14	b	1222	CLA	CHC-C1C	4.42	1.47	1.38
14	G	1119	CLA	C3C-C2C	4.42	1.46	1.36
14	B	1232	CLA	CHC-C1C	4.42	1.47	1.38
14	G	1129	CLA	CHC-C1C	4.41	1.47	1.38
14	b	1211	CLA	CHC-C1C	4.41	1.47	1.38
14	H	1218	CLA	C1D-ND	-4.41	1.32	1.37
14	b	1218	CLA	C1D-ND	-4.41	1.32	1.37
14	b	1232	CLA	CHC-C1C	4.41	1.47	1.38
14	B	1218	CLA	C3D-C4D	-4.41	1.34	1.44
18	b	4006	BCR	C10-C9	-4.41	1.25	1.35
14	a	1120	CLA	CHC-C1C	4.40	1.47	1.38
14	A	1128	CLA	C1D-ND	-4.40	1.32	1.37
14	a	1102	CLA	CHC-C1C	4.40	1.47	1.38
14	a	1115	CLA	CHC-C1C	4.40	1.47	1.38
14	B	1216	CLA	CHD-C1D	4.40	1.47	1.38
14	b	1216	CLA	CHD-C1D	4.40	1.47	1.38
14	H	1211	CLA	CHC-C1C	4.40	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1216	CLA	CHD-C1D	4.40	1.47	1.38
14	H	1226	CLA	C1D-ND	-4.40	1.32	1.37
14	a	1128	CLA	C1D-ND	-4.39	1.32	1.37
14	A	1115	CLA	CHC-C1C	4.39	1.47	1.38
14	G	1013	CLA	C1B-NB	-4.39	1.32	1.37
13	A	1011	CL0	CHB-C1B	4.39	1.46	1.39
14	a	1122	CLA	CHD-C1D	4.39	1.47	1.38
14	b	1217	CLA	CHC-C1C	4.39	1.47	1.38
18	B	4006	BCR	C10-C9	-4.39	1.25	1.35
14	G	1117	CLA	CHD-C1D	4.39	1.47	1.38
14	B	1233	CLA	CHC-C1C	4.39	1.47	1.38
14	A	1128	CLA	O2D-CGD	4.38	1.44	1.33
14	k	1401	CLA	CHD-C1D	4.38	1.47	1.38
14	b	1227	CLA	CHC-C1C	4.38	1.47	1.38
14	G	1112	CLA	CHD-C1D	4.38	1.47	1.38
14	A	1122	CLA	CHD-C1D	4.38	1.47	1.38
14	G	1120	CLA	CHC-C1C	4.38	1.47	1.38
14	H	1233	CLA	CHC-C1C	4.38	1.47	1.38
14	B	1224	CLA	C1D-ND	-4.38	1.32	1.37
14	G	1115	CLA	CHC-C1C	4.38	1.47	1.38
14	H	1209	CLA	CHD-C1D	4.38	1.47	1.38
14	A	1106	CLA	CHC-C1C	4.38	1.47	1.38
14	G	1101	CLA	CHC-C1C	4.38	1.47	1.38
14	G	1138	CLA	CHC-C1C	4.38	1.47	1.38
14	a	1129	CLA	CHC-C1C	4.38	1.47	1.38
14	H	1232	CLA	CHC-C1C	4.38	1.47	1.38
14	H	1218	CLA	C3D-C4D	-4.38	1.34	1.44
14	a	1128	CLA	O2D-CGD	4.38	1.44	1.33
14	H	1227	CLA	CHC-C1C	4.38	1.47	1.38
14	A	1111	CLA	CHC-C1C	4.38	1.47	1.38
14	B	1209	CLA	CHC-C1C	4.38	1.47	1.38
14	b	1210	CLA	CHD-C1D	4.37	1.47	1.38
14	a	1138	CLA	CHC-C1C	4.37	1.47	1.38
14	G	1111	CLA	CHC-C1C	4.37	1.47	1.38
14	A	1120	CLA	CHC-C1C	4.37	1.47	1.38
14	B	1221	CLA	CHC-C1C	4.37	1.47	1.38
14	H	1217	CLA	CHC-C1C	4.37	1.47	1.38
13	G	1011	CL0	CHB-C1B	4.37	1.46	1.39
14	a	1112	CLA	CHD-C1D	4.37	1.46	1.38
14	H	1209	CLA	CHC-C1C	4.37	1.47	1.38
20	L	5007	LMG	O8-C28	4.37	1.46	1.33
14	b	1233	CLA	CHC-C1C	4.36	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1217	CLA	CHC-C1C	4.36	1.47	1.38
14	H	1223	CLA	CHC-C1C	4.36	1.47	1.38
14	G	1122	CLA	CHD-C1D	4.36	1.46	1.38
20	U	5007	LMG	O8-C28	4.36	1.46	1.33
14	A	1108	CLA	CHC-C1C	4.36	1.47	1.38
14	G	1106	CLA	CHC-C1C	4.36	1.47	1.38
14	H	1202	CLA	CHC-C1C	4.36	1.47	1.38
14	H	1210	CLA	CHD-C1D	4.36	1.46	1.38
14	A	1129	CLA	CHC-C1C	4.36	1.47	1.38
14	b	1227	CLA	C3C-C2C	4.36	1.46	1.36
14	B	1202	CLA	CHC-C1C	4.36	1.47	1.38
14	b	1218	CLA	C3D-C4D	-4.36	1.34	1.44
20	l	5007	LMG	O8-C28	4.36	1.46	1.33
14	a	1117	CLA	CHD-C1D	4.35	1.46	1.38
14	a	1111	CLA	CHC-C1C	4.35	1.47	1.38
14	H	1227	CLA	C3C-C2C	4.35	1.46	1.36
14	A	1131	CLA	CHD-C1D	4.35	1.46	1.38
14	B	1210	CLA	CHD-C1D	4.35	1.46	1.38
14	A	1132	CLA	C3C-C2C	4.35	1.46	1.36
14	B	1223	CLA	C3C-C2C	4.35	1.46	1.36
14	A	1134	CLA	C3D-C4D	-4.35	1.34	1.44
14	B	1233	CLA	C3C-C2C	4.35	1.46	1.36
14	H	1221	CLA	CHC-C1C	4.35	1.47	1.38
14	b	1209	CLA	CHC-C1C	4.35	1.47	1.38
14	b	1223	CLA	CHC-C1C	4.35	1.47	1.38
14	b	1202	CLA	CHC-C1C	4.35	1.47	1.38
14	G	1131	CLA	CHD-C1D	4.35	1.46	1.38
14	a	1131	CLA	CHD-C1D	4.35	1.46	1.38
14	B	1234	CLA	O2D-CGD	4.35	1.43	1.33
14	a	1101	CLA	CHC-C1C	4.35	1.47	1.38
14	A	1101	CLA	CHC-C1C	4.35	1.47	1.38
14	A	1112	CLA	CHD-C1D	4.34	1.46	1.38
14	A	1127	CLA	C1D-ND	-4.34	1.32	1.37
14	H	1233	CLA	C3C-C2C	4.34	1.46	1.36
14	a	1132	CLA	C3C-C2C	4.34	1.46	1.36
14	a	1127	CLA	C1D-ND	-4.34	1.32	1.37
14	b	1221	CLA	CHC-C1C	4.34	1.47	1.38
19	G	5001	LHG	O8-C23	4.34	1.46	1.33
14	a	1108	CLA	CHC-C1C	4.34	1.47	1.38
14	H	1224	CLA	C1D-ND	-4.34	1.32	1.37
14	a	1130	CLA	CHC-C1C	4.34	1.47	1.38
14	G	1137	CLA	O2D-CGD	4.34	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1108	CLA	CHC-C1C	4.34	1.47	1.38
14	A	1132	CLA	CHC-C1C	4.34	1.47	1.38
14	B	1209	CLA	CHD-C1D	4.34	1.46	1.38
14	a	1106	CLA	CHC-C1C	4.34	1.47	1.38
14	H	1212	CLA	C3D-C4D	-4.34	1.34	1.44
14	B	1223	CLA	CHC-C1C	4.33	1.47	1.38
14	G	1132	CLA	C3C-C2C	4.33	1.46	1.36
14	T	1401	CLA	C3C-C2C	4.33	1.46	1.36
14	H	1208	CLA	CHC-C1C	4.33	1.47	1.38
14	B	1212	CLA	C3D-C4D	-4.33	1.34	1.44
14	b	1224	CLA	C1D-ND	-4.33	1.32	1.37
14	G	1128	CLA	O2D-CGD	4.33	1.43	1.33
14	B	1235	CLA	CHC-C1C	4.33	1.47	1.38
14	G	1124	CLA	O2D-CGD	4.33	1.43	1.33
14	a	1137	CLA	O2D-CGD	4.33	1.43	1.33
14	H	1210	CLA	CHC-C1C	4.33	1.47	1.38
14	b	1235	CLA	CHD-C1D	4.33	1.46	1.38
14	G	1136	CLA	CHC-C1C	4.33	1.47	1.38
14	b	1235	CLA	CHC-C1C	4.33	1.47	1.38
14	b	1212	CLA	C3D-C4D	-4.33	1.34	1.44
14	G	1105	CLA	CHD-C1D	4.33	1.46	1.38
14	H	1229	CLA	C3C-C2C	4.33	1.46	1.36
14	a	1112	CLA	CHC-C1C	4.33	1.47	1.38
14	H	1216	CLA	CHC-C1C	4.32	1.47	1.38
14	b	1234	CLA	O2D-CGD	4.32	1.43	1.33
14	A	1117	CLA	CHD-C1D	4.32	1.46	1.38
14	B	1216	CLA	CHC-C1C	4.32	1.47	1.38
14	H	1223	CLA	C3C-C2C	4.32	1.46	1.36
14	B	1216	CLA	C3C-C2C	4.32	1.46	1.36
14	a	1109	CLA	CHC-C1C	4.32	1.47	1.38
14	G	1130	CLA	CHC-C1C	4.32	1.47	1.38
14	H	1235	CLA	CHC-C1C	4.32	1.47	1.38
14	b	1214	CLA	CHC-C1C	4.32	1.47	1.38
14	a	1124	CLA	O2D-CGD	4.32	1.43	1.33
14	B	1235	CLA	CHD-C1D	4.32	1.46	1.38
14	b	1216	CLA	CHC-C1C	4.32	1.47	1.38
14	b	1223	CLA	C3C-C2C	4.32	1.46	1.36
14	A	1128	CLA	C1B-NB	-4.32	1.32	1.37
14	U	1503	CLA	C3C-C2C	4.32	1.46	1.36
14	G	1134	CLA	C3D-C4D	-4.32	1.34	1.44
14	G	1127	CLA	C1D-ND	-4.32	1.32	1.37
14	A	1105	CLA	CHD-C1D	4.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1109	CLA	CHC-C1C	4.32	1.47	1.38
14	H	1219	CLA	CHD-C1D	4.32	1.46	1.38
14	b	1209	CLA	CHD-C1D	4.32	1.46	1.38
14	b	1233	CLA	C3C-C2C	4.31	1.46	1.36
14	B	1227	CLA	C3C-C2C	4.31	1.46	1.36
14	G	1105	CLA	CHC-C1C	4.31	1.47	1.38
14	H	1234	CLA	O2D-CGD	4.31	1.43	1.33
14	G	1132	CLA	O2D-CGD	4.31	1.43	1.33
14	l	1503	CLA	C3C-C2C	4.31	1.46	1.36
14	B	1219	CLA	CHD-C1D	4.31	1.46	1.38
19	A	5001	LHG	O8-C23	4.31	1.45	1.33
14	H	1235	CLA	CHD-C1D	4.31	1.46	1.38
14	a	1132	CLA	CHC-C1C	4.31	1.47	1.38
14	A	1137	CLA	O2D-CGD	4.31	1.43	1.33
14	B	1222	CLA	C3C-C2C	4.31	1.46	1.36
14	b	1225	CLA	CHC-C1C	4.31	1.47	1.38
14	a	1128	CLA	C1B-NB	-4.31	1.32	1.37
14	A	1140	CLA	CHC-C1C	4.31	1.47	1.38
14	H	1225	CLA	CHC-C1C	4.31	1.47	1.38
18	b	4013	BCR	C10-C9	-4.31	1.25	1.35
14	H	1222	CLA	C3C-C2C	4.31	1.46	1.36
14	a	1134	CLA	C3D-C4D	-4.30	1.34	1.44
14	A	1130	CLA	CHC-C1C	4.30	1.47	1.38
15	a	1121	F6C	CHC-C4B	4.30	1.47	1.38
14	G	1124	CLA	C3C-C2C	4.30	1.46	1.36
14	b	1216	CLA	C3C-C2C	4.30	1.46	1.36
15	H	1238	F6C	C3D-C4D	-4.30	1.32	1.44
14	b	1219	CLA	CHD-C1D	4.30	1.46	1.38
15	G	1121	F6C	CHC-C4B	4.30	1.47	1.38
14	b	1226	CLA	C3C-C2C	4.30	1.46	1.36
14	a	1140	CLA	CHC-C1C	4.30	1.47	1.38
14	A	1132	CLA	O2D-CGD	4.30	1.43	1.33
14	a	1132	CLA	O2D-CGD	4.30	1.43	1.33
14	A	1109	CLA	CHC-C1C	4.29	1.47	1.38
14	B	1209	CLA	C3C-C2C	4.29	1.46	1.36
18	H	4013	BCR	C10-C9	-4.29	1.25	1.35
14	H	1214	CLA	CHC-C1C	4.29	1.47	1.38
15	A	1121	F6C	CHC-C4B	4.29	1.47	1.38
14	A	1124	CLA	O2D-CGD	4.29	1.43	1.33
15	B	1238	F6C	C3D-C4D	-4.29	1.32	1.44
14	a	1136	CLA	CHC-C1C	4.29	1.47	1.38
14	a	1116	CLA	C3C-C2C	4.29	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1226	CLA	C3C-C2C	4.29	1.46	1.36
14	b	1229	CLA	C3C-C2C	4.29	1.46	1.36
14	a	1105	CLA	CHD-C1D	4.29	1.46	1.38
14	K	1401	CLA	C3C-C2C	4.29	1.46	1.36
18	b	4004	BCR	C10-C9	-4.29	1.25	1.35
14	H	1201	CLA	CHC-C1C	4.29	1.47	1.38
14	B	1232	CLA	CHD-C1D	4.29	1.46	1.38
19	a	5001	LHG	O8-C23	4.29	1.45	1.33
14	B	1229	CLA	C3C-C2C	4.29	1.46	1.36
14	B	1226	CLA	C1D-ND	-4.29	1.32	1.37
14	a	1138	CLA	CHD-C1D	4.29	1.46	1.38
14	k	1401	CLA	C3C-C2C	4.29	1.46	1.36
14	b	1222	CLA	C3C-C2C	4.28	1.46	1.36
14	G	1112	CLA	C3C-C2C	4.28	1.46	1.36
18	B	4004	BCR	C10-C9	-4.28	1.25	1.35
14	B	1225	CLA	C1D-ND	-4.28	1.32	1.37
14	H	1232	CLA	CHD-C1D	4.28	1.46	1.38
14	b	1209	CLA	C3C-C2C	4.28	1.46	1.36
14	b	1232	CLA	CHD-C1D	4.28	1.46	1.38
14	G	1112	CLA	CHC-C1C	4.28	1.47	1.38
15	b	1238	F6C	C3D-C4D	-4.28	1.32	1.44
14	A	1128	CLA	C3C-C2C	4.28	1.46	1.36
14	b	1201	CLA	CHC-C1C	4.28	1.47	1.38
14	H	1216	CLA	C3C-C2C	4.28	1.46	1.36
14	L	1502	CLA	CHC-C1C	4.28	1.47	1.38
14	b	1201	CLA	CHD-C1D	4.28	1.46	1.38
14	b	1208	CLA	CHC-C1C	4.28	1.47	1.38
14	b	1210	CLA	CHC-C1C	4.28	1.47	1.38
14	H	1225	CLA	C1D-ND	-4.27	1.32	1.37
14	G	1138	CLA	CHD-C1D	4.27	1.46	1.38
18	B	4013	BCR	C10-C9	-4.27	1.25	1.35
14	b	1203	CLA	CHC-C1C	4.27	1.47	1.38
14	A	1136	CLA	CHC-C1C	4.27	1.47	1.38
14	a	1105	CLA	CHC-C1C	4.27	1.47	1.38
14	A	1107	CLA	CHC-C1C	4.27	1.47	1.38
14	G	1140	CLA	CHC-C1C	4.27	1.47	1.38
14	A	1124	CLA	C3C-C2C	4.27	1.46	1.36
14	L	1503	CLA	C3C-C2C	4.27	1.46	1.36
15	b	1207	F6C	C1C-NC	-4.27	1.32	1.37
14	A	1123	CLA	CHC-C1C	4.27	1.47	1.38
14	a	1124	CLA	C3C-C2C	4.27	1.46	1.36
14	B	1225	CLA	CHC-C1C	4.26	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4004	BCR	C10-C9	-4.26	1.25	1.35
14	a	1112	CLA	C3C-C2C	4.26	1.46	1.36
14	H	1210	CLA	O2D-CGD	4.26	1.43	1.33
14	B	1208	CLA	CHC-C1C	4.26	1.47	1.38
14	b	1210	CLA	O2D-CGD	4.26	1.43	1.33
14	H	1209	CLA	C3C-C2C	4.26	1.46	1.36
14	A	1112	CLA	CHC-C1C	4.26	1.47	1.38
14	A	1138	CLA	CHD-C1D	4.26	1.46	1.38
14	A	1112	CLA	C3C-C2C	4.26	1.46	1.36
14	B	1210	CLA	CHC-C1C	4.26	1.47	1.38
14	A	1116	CLA	C3C-C2C	4.26	1.46	1.36
14	A	1105	CLA	CHC-C1C	4.26	1.47	1.38
14	G	1128	CLA	C1B-NB	-4.26	1.32	1.37
14	G	1132	CLA	CHC-C1C	4.26	1.47	1.38
14	b	1023	CLA	C1C-NC	-4.25	1.31	1.37
14	U	1503	CLA	CHC-C1C	4.25	1.47	1.38
14	H	1201	CLA	CHD-C1D	4.25	1.46	1.38
14	B	1228	CLA	C3C-C2C	4.25	1.45	1.36
14	H	1203	CLA	CHC-C1C	4.25	1.47	1.38
14	a	1128	CLA	C3C-C2C	4.25	1.45	1.36
14	a	1133	CLA	CHD-C1D	4.25	1.46	1.38
15	b	1230	F6C	C1C-NC	-4.25	1.32	1.37
14	a	1108	CLA	CHD-C1D	4.25	1.46	1.38
14	G	1116	CLA	C3C-C2C	4.25	1.45	1.36
14	b	1225	CLA	C1D-ND	-4.25	1.32	1.37
14	H	1236	CLA	CHC-C1C	4.25	1.47	1.38
14	B	1201	CLA	CHC-C1C	4.25	1.47	1.38
14	A	1108	CLA	CHD-C1D	4.25	1.46	1.38
14	B	1214	CLA	CHC-C1C	4.25	1.47	1.38
14	b	1228	CLA	C3C-C2C	4.24	1.45	1.36
14	K	1401	CLA	C3D-C4D	-4.24	1.34	1.44
14	G	1108	CLA	CHD-C1D	4.24	1.46	1.38
14	H	1215	CLA	CHD-C1D	4.24	1.46	1.38
14	G	1107	CLA	CHC-C1C	4.24	1.47	1.38
14	T	1401	CLA	C3D-C4D	-4.24	1.34	1.44
14	U	1502	CLA	CHC-C1C	4.24	1.47	1.38
14	A	1133	CLA	CHD-C1D	4.24	1.46	1.38
14	B	1201	CLA	CHD-C1D	4.24	1.46	1.38
14	H	1231	CLA	CHC-C1C	4.24	1.47	1.38
14	G	1128	CLA	C3C-C2C	4.24	1.45	1.36
14	B	1203	CLA	CHC-C1C	4.24	1.47	1.38
14	B	1226	CLA	C3C-C2C	4.24	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1110	CLA	C3C-C2C	4.24	1.45	1.36
14	A	1136	CLA	CHD-C1D	4.24	1.46	1.38
15	B	1230	F6C	C1C-NC	-4.24	1.32	1.37
20	H	5002	LMG	O8-C28	4.23	1.45	1.33
14	H	1228	CLA	C3C-C2C	4.23	1.45	1.36
14	k	1401	CLA	C3D-C4D	-4.23	1.34	1.44
14	B	1231	CLA	CHC-C1C	4.23	1.47	1.38
14	l	1502	CLA	CHC-C1C	4.23	1.47	1.38
14	l	1503	CLA	CHC-C1C	4.23	1.47	1.38
14	G	1123	CLA	CHC-C1C	4.23	1.47	1.38
15	H	1207	F6C	O2D-CGD	4.23	1.43	1.33
14	G	1133	CLA	CHD-C1D	4.23	1.46	1.38
14	G	1104	CLA	CHC-C1C	4.23	1.47	1.38
14	H	1204	CLA	CHC-C1C	4.23	1.47	1.38
14	b	1236	CLA	CHC-C1C	4.23	1.47	1.38
14	A	1102	CLA	CHD-C1D	4.23	1.46	1.38
14	b	1231	CLA	CHC-C1C	4.23	1.47	1.38
14	L	1503	CLA	CHC-C1C	4.23	1.47	1.38
14	a	1102	CLA	C3C-C2C	4.23	1.45	1.36
14	B	1210	CLA	O2D-CGD	4.23	1.43	1.33
14	H	1226	CLA	CHD-C1D	4.22	1.46	1.38
14	b	1219	CLA	C3C-C2C	4.22	1.45	1.36
15	H	1230	F6C	C1C-NC	-4.22	1.32	1.37
14	G	1136	CLA	CHD-C1D	4.22	1.46	1.38
15	b	1207	F6C	O2D-CGD	4.22	1.43	1.33
15	B	1207	F6C	C1C-NC	-4.22	1.32	1.37
14	A	1111	CLA	O2D-CGD	4.22	1.43	1.33
14	H	1232	CLA	C3C-C2C	4.22	1.45	1.36
14	G	1132	CLA	CHD-C1D	4.22	1.46	1.38
14	a	1123	CLA	CHC-C1C	4.22	1.46	1.38
14	B	1219	CLA	C3C-C2C	4.22	1.45	1.36
14	a	1104	CLA	CHC-C1C	4.22	1.46	1.38
14	A	1102	CLA	C3C-C2C	4.22	1.45	1.36
15	H	1207	F6C	C1C-NC	-4.21	1.32	1.37
14	a	1136	CLA	CHD-C1D	4.21	1.46	1.38
14	B	1226	CLA	CHD-C1D	4.21	1.46	1.38
14	a	1110	CLA	C3C-C2C	4.21	1.45	1.36
14	H	1211	CLA	CHD-C1D	4.21	1.46	1.38
14	G	1111	CLA	O2D-CGD	4.21	1.43	1.33
14	B	1235	CLA	C3C-C2C	4.21	1.45	1.36
20	i	5006	LMG	O8-C28	4.21	1.45	1.33
20	R	5006	LMG	O8-C28	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1215	CLA	CHD-C1D	4.21	1.46	1.38
14	b	1212	CLA	C3C-C2C	4.21	1.45	1.36
14	H	1229	CLA	CHD-C1D	4.21	1.46	1.38
14	G	1102	CLA	CHD-C1D	4.21	1.46	1.38
14	H	1219	CLA	C3C-C2C	4.21	1.45	1.36
14	A	1104	CLA	CHC-C1C	4.21	1.46	1.38
14	b	1217	CLA	C3C-C2C	4.21	1.45	1.36
14	B	1224	CLA	CHC-C1C	4.20	1.46	1.38
14	a	1107	CLA	CHC-C1C	4.20	1.46	1.38
14	b	1211	CLA	CHD-C1D	4.20	1.46	1.38
14	b	1224	CLA	CHC-C1C	4.20	1.46	1.38
14	a	1132	CLA	CHD-C1D	4.20	1.46	1.38
19	b	5004	LHG	O8-C23	4.20	1.45	1.33
14	a	1111	CLA	O2D-CGD	4.20	1.43	1.33
14	H	1224	CLA	CHC-C1C	4.20	1.46	1.38
14	a	1118	CLA	CHD-C1D	4.20	1.46	1.38
14	b	1235	CLA	C3C-C2C	4.20	1.45	1.36
15	B	1207	F6C	O2D-CGD	4.20	1.43	1.33
20	B	5002	LMG	O8-C28	4.20	1.45	1.33
14	A	1126	CLA	C1D-ND	-4.20	1.32	1.37
14	A	1110	CLA	C3C-C2C	4.20	1.45	1.36
14	G	1126	CLA	C1D-ND	-4.20	1.32	1.37
14	b	1204	CLA	CHC-C1C	4.20	1.46	1.38
14	H	1023	CLA	C1C-NC	-4.20	1.31	1.37
14	B	1236	CLA	CHC-C1C	4.19	1.46	1.38
13	A	1011	CL0	CHB-C4A	-4.19	1.33	1.38
14	B	1232	CLA	C3C-C2C	4.19	1.45	1.36
14	G	1129	CLA	C3C-C2C	4.19	1.45	1.36
14	H	1228	CLA	CHC-C1C	4.19	1.46	1.38
14	A	1118	CLA	CHD-C1D	4.19	1.46	1.38
15	b	1207	F6C	CHC-C4B	4.19	1.46	1.38
14	B	1229	CLA	CHD-C1D	4.19	1.46	1.38
14	B	1205	CLA	CHC-C1C	4.19	1.46	1.38
14	B	1204	CLA	CHC-C1C	4.19	1.46	1.38
14	B	1023	CLA	C1C-NC	-4.19	1.31	1.37
14	H	1205	CLA	CHC-C1C	4.19	1.46	1.38
20	b	5002	LMG	O8-C28	4.19	1.45	1.33
14	a	1102	CLA	CHD-C1D	4.19	1.46	1.38
14	G	1102	CLA	C3C-C2C	4.19	1.45	1.36
14	H	1225	CLA	C1B-NB	-4.19	1.32	1.37
14	A	1133	CLA	C3C-C2C	4.18	1.45	1.36
14	a	1109	CLA	CHD-C1D	4.18	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1108	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1229	CLA	CHD-C1D	4.18	1.46	1.38
15	b	1230	F6C	CHC-C4B	4.18	1.46	1.38
19	B	5004	LHG	O8-C23	4.18	1.45	1.33
14	H	1212	CLA	C3C-C2C	4.18	1.45	1.36
14	B	1225	CLA	C1B-NB	-4.18	1.32	1.37
14	G	1133	CLA	C3C-C2C	4.18	1.45	1.36
14	a	1133	CLA	C3C-C2C	4.18	1.45	1.36
14	B	1236	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1228	CLA	CHC-C1C	4.18	1.46	1.38
14	a	1114	CLA	CHC-C1C	4.18	1.46	1.38
14	H	1235	CLA	C3C-C2C	4.18	1.45	1.36
14	A	1136	CLA	C3C-C2C	4.18	1.45	1.36
20	U	5007	LMG	O7-C10	4.18	1.46	1.34
14	B	1228	CLA	CHC-C1C	4.18	1.46	1.38
15	G	1121	F6C	CHD-C1D	4.18	1.46	1.38
20	I	5006	LMG	O8-C28	4.18	1.45	1.33
14	A	1109	CLA	CHD-C1D	4.18	1.46	1.38
14	a	1108	CLA	C3C-C2C	4.18	1.45	1.36
14	b	1208	CLA	CHD-C1D	4.18	1.46	1.38
14	B	1217	CLA	C3C-C2C	4.17	1.45	1.36
14	a	1118	CLA	CHC-C1C	4.17	1.46	1.38
14	A	1132	CLA	CHD-C1D	4.17	1.46	1.38
14	b	1236	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1118	CLA	C3C-C2C	4.17	1.45	1.36
14	H	1208	CLA	CHD-C1D	4.17	1.46	1.38
14	b	1205	CLA	CHC-C1C	4.17	1.46	1.38
14	G	1118	CLA	CHD-C1D	4.17	1.46	1.38
14	B	1211	CLA	CHD-C1D	4.17	1.46	1.38
14	b	1214	CLA	C3C-C2C	4.17	1.45	1.36
13	a	1011	CL0	CHB-C4A	-4.17	1.33	1.38
14	b	1232	CLA	C3C-C2C	4.17	1.45	1.36
14	A	1114	CLA	CHC-C1C	4.17	1.46	1.38
14	A	1130	CLA	C3C-C2C	4.17	1.45	1.36
14	B	1215	CLA	CHD-C1D	4.16	1.46	1.38
20	l	5007	LMG	O7-C10	4.16	1.46	1.34
19	H	5004	LHG	O8-C23	4.16	1.45	1.33
15	H	1230	F6C	CHC-C4B	4.16	1.46	1.38
14	G	1127	CLA	CHC-C1C	4.16	1.46	1.38
14	A	1129	CLA	C3C-C2C	4.16	1.45	1.36
15	A	1121	F6C	CHD-C1D	4.16	1.46	1.38
20	a	5005	LMG	O7-C10	4.16	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1214	CLA	C3C-C2C	4.16	1.45	1.36
14	H	1217	CLA	C3C-C2C	4.16	1.45	1.36
14	B	1208	CLA	CHD-C1D	4.16	1.46	1.38
14	A	1127	CLA	CHC-C1C	4.16	1.46	1.38
14	a	1126	CLA	C1D-ND	-4.16	1.32	1.37
14	a	1127	CLA	CHC-C1C	4.16	1.46	1.38
20	A	5005	LMG	O7-C10	4.16	1.46	1.34
14	A	1118	CLA	CHC-C1C	4.16	1.46	1.38
14	b	1226	CLA	CHD-C1D	4.16	1.46	1.38
20	L	5007	LMG	O7-C10	4.16	1.46	1.34
14	G	1118	CLA	C3C-C2C	4.15	1.45	1.36
14	a	1130	CLA	C3C-C2C	4.15	1.45	1.36
14	A	1108	CLA	C3C-C2C	4.15	1.45	1.36
14	B	1226	CLA	C1B-NB	-4.15	1.32	1.37
20	G	5005	LMG	O7-C10	4.15	1.46	1.34
14	B	1218	CLA	C3C-C2C	4.15	1.45	1.36
14	a	1103	CLA	CHD-C1D	4.15	1.46	1.38
14	b	1225	CLA	C1B-NB	-4.15	1.32	1.37
14	B	1208	CLA	C3C-C2C	4.15	1.45	1.36
14	G	1114	CLA	CHC-C1C	4.15	1.46	1.38
14	B	1212	CLA	C3C-C2C	4.15	1.45	1.36
14	a	1125	CLA	C1C-NC	-4.15	1.31	1.37
14	G	1136	CLA	C3C-C2C	4.15	1.45	1.36
14	H	1236	CLA	C3C-C2C	4.15	1.45	1.36
15	B	1230	F6C	CHC-C4B	4.15	1.46	1.38
14	l	1502	CLA	C1D-ND	-4.15	1.32	1.37
14	G	1109	CLA	CHD-C1D	4.15	1.46	1.38
14	a	1129	CLA	C3C-C2C	4.15	1.45	1.36
14	G	1118	CLA	CHC-C1C	4.15	1.46	1.38
14	G	1138	CLA	C3C-C2C	4.14	1.45	1.36
16	G	2001	PQN	C10-C5	4.14	1.47	1.40
14	G	1109	CLA	C3C-C2C	4.14	1.45	1.36
14	b	1226	CLA	C1B-NB	-4.14	1.32	1.37
15	B	1207	F6C	CHC-C4B	4.14	1.46	1.38
14	B	1214	CLA	C3C-C2C	4.14	1.45	1.36
15	H	1207	F6C	CHC-C4B	4.14	1.46	1.38
14	A	1105	CLA	C3C-C2C	4.14	1.45	1.36
14	l	1501	CLA	C3C-C2C	4.14	1.45	1.36
14	U	1501	CLA	C3C-C2C	4.14	1.45	1.36
14	H	1211	CLA	C3C-C2C	4.14	1.45	1.36
14	G	1130	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1109	CLA	C3C-C2C	4.13	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1215	CLA	CHC-C1C	4.13	1.46	1.38
14	G	1131	CLA	CHC-C1C	4.13	1.46	1.38
14	a	1136	CLA	C3C-C2C	4.13	1.45	1.36
14	b	1208	CLA	C3C-C2C	4.13	1.45	1.36
14	G	1103	CLA	CHD-C1D	4.13	1.46	1.38
14	H	1213	CLA	CHD-C1D	4.13	1.46	1.38
14	G	1113	CLA	CHD-C1D	4.13	1.46	1.38
14	G	1106	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1103	CLA	CHD-C1D	4.13	1.46	1.38
14	G	1125	CLA	C1C-NC	-4.13	1.31	1.37
14	a	1109	CLA	C3C-C2C	4.13	1.45	1.36
14	a	1107	CLA	C3C-C2C	4.13	1.45	1.36
14	A	1125	CLA	C1C-NC	-4.13	1.31	1.37
14	G	1105	CLA	C3C-C2C	4.13	1.45	1.36
14	L	1501	CLA	C3C-C2C	4.13	1.45	1.36
14	b	1218	CLA	C3C-C2C	4.13	1.45	1.36
14	U	1502	CLA	C1D-ND	-4.13	1.32	1.37
14	H	1228	CLA	CHD-C1D	4.13	1.46	1.38
14	A	1103	CLA	CHC-C1C	4.13	1.46	1.38
14	G	1122	CLA	CHC-C1C	4.13	1.46	1.38
14	H	1215	CLA	CHC-C1C	4.13	1.46	1.38
14	L	1502	CLA	C1D-ND	-4.13	1.32	1.37
15	H	1237	F6C	CHC-C4B	4.12	1.46	1.38
14	H	1226	CLA	C1B-NB	-4.12	1.32	1.37
15	a	1121	F6C	CHD-C1D	4.12	1.46	1.38
14	H	1208	CLA	C3C-C2C	4.12	1.45	1.36
14	H	1201	CLA	C3C-C2C	4.12	1.45	1.36
14	b	1022	CLA	O2D-CGD	4.12	1.43	1.33
14	a	1118	CLA	C3C-C2C	4.12	1.45	1.36
14	H	1218	CLA	C3C-C2C	4.12	1.45	1.36
14	a	1137	CLA	CHC-C1C	4.12	1.46	1.38
14	B	1213	CLA	CHD-C1D	4.12	1.46	1.38
14	b	1213	CLA	CHD-C1D	4.12	1.46	1.38
14	G	1103	CLA	CHC-C1C	4.12	1.46	1.38
15	b	1237	F6C	CHC-C4B	4.12	1.46	1.38
14	G	1126	CLA	C3C-C2C	4.11	1.45	1.36
14	H	1022	CLA	O2D-CGD	4.11	1.43	1.33
14	a	1105	CLA	C3C-C2C	4.11	1.45	1.36
14	A	1107	CLA	C3C-C2C	4.11	1.45	1.36
14	a	1103	CLA	CHC-C1C	4.11	1.46	1.38
14	b	1211	CLA	C3C-C2C	4.11	1.45	1.36
14	G	1107	CLA	C3C-C2C	4.11	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1131	CLA	CHC-C1C	4.11	1.46	1.38
14	A	1131	CLA	CHC-C1C	4.11	1.46	1.38
14	B	1228	CLA	CHD-C1D	4.11	1.46	1.38
13	G	1011	CL0	CHB-C4A	-4.11	1.33	1.38
14	a	1138	CLA	C3C-C2C	4.11	1.45	1.36
14	A	1138	CLA	C3C-C2C	4.11	1.45	1.36
14	a	1113	CLA	CHD-C1D	4.11	1.46	1.38
14	B	1201	CLA	C3C-C2C	4.11	1.45	1.36
14	G	1137	CLA	CHC-C1C	4.11	1.46	1.38
14	B	1215	CLA	CHC-C1C	4.11	1.46	1.38
14	A	1115	CLA	C3C-C2C	4.11	1.45	1.36
14	B	1022	CLA	O2D-CGD	4.10	1.43	1.33
14	a	1133	CLA	CHC-C1C	4.10	1.46	1.38
14	B	1206	CLA	CHD-C1D	4.10	1.46	1.38
14	B	1206	CLA	C1D-ND	-4.10	1.32	1.37
14	b	1206	CLA	C1D-ND	-4.10	1.32	1.37
14	G	1107	CLA	CHD-C1D	4.10	1.46	1.38
14	G	1111	CLA	CHD-C1D	4.10	1.46	1.38
14	H	1231	CLA	CHD-C1D	4.10	1.46	1.38
14	A	1107	CLA	CHD-C1D	4.10	1.46	1.38
14	A	1111	CLA	CHD-C1D	4.10	1.46	1.38
15	B	1237	F6C	CHC-C4B	4.10	1.46	1.38
14	A	1127	CLA	C3C-C2C	4.10	1.45	1.36
16	A	2001	PQN	C10-C5	4.10	1.47	1.40
14	H	1206	CLA	C1D-ND	-4.10	1.32	1.37
14	b	1228	CLA	CHD-C1D	4.10	1.46	1.38
14	A	1126	CLA	C3C-C2C	4.10	1.45	1.36
14	b	1231	CLA	CHD-C1D	4.09	1.46	1.38
14	G	1115	CLA	C3C-C2C	4.09	1.45	1.36
14	a	1115	CLA	C3C-C2C	4.09	1.45	1.36
14	a	1135	CLA	C3C-C2C	4.09	1.45	1.36
14	a	1126	CLA	C3C-C2C	4.09	1.45	1.36
14	G	1135	CLA	C3C-C2C	4.09	1.45	1.36
14	A	1113	CLA	C3C-C2C	4.09	1.45	1.36
14	A	1137	CLA	CHC-C1C	4.09	1.46	1.38
14	G	1101	CLA	CHD-C1D	4.09	1.46	1.38
14	H	1213	CLA	C3C-C2C	4.09	1.45	1.36
14	a	1106	CLA	C3C-C2C	4.09	1.45	1.36
14	A	1113	CLA	CHD-C1D	4.09	1.46	1.38
14	U	1502	CLA	C3C-C2C	4.08	1.45	1.36
14	B	1234	CLA	C3C-C2C	4.08	1.45	1.36
14	b	1201	CLA	C3C-C2C	4.08	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1207	F6C	C3D-C4D	-4.08	1.33	1.44
14	A	1106	CLA	C3C-C2C	4.08	1.45	1.36
14	G	1012	CLA	O2D-CGD	4.08	1.43	1.33
14	G	1127	CLA	C3C-C2C	4.08	1.45	1.36
14	H	1206	CLA	CHD-C1D	4.08	1.46	1.38
14	a	1111	CLA	CHD-C1D	4.08	1.46	1.38
14	A	1123	CLA	CHD-C1D	4.08	1.46	1.38
14	G	1117	CLA	C3C-C2C	4.08	1.45	1.36
14	A	1122	CLA	CHC-C1C	4.08	1.46	1.38
14	a	1107	CLA	CHD-C1D	4.08	1.46	1.38
14	B	1222	CLA	C1D-ND	-4.08	1.32	1.37
14	b	1239	CLA	CHD-C1D	4.08	1.46	1.38
14	A	1104	CLA	C3C-C2C	4.08	1.45	1.36
14	L	1502	CLA	C3C-C2C	4.08	1.45	1.36
18	a	4008	BCR	C11-C12	-4.08	1.24	1.34
14	b	1206	CLA	CHD-C1D	4.08	1.46	1.38
14	l	1502	CLA	C3C-C2C	4.07	1.45	1.36
14	a	1101	CLA	C3C-C2C	4.07	1.45	1.36
14	A	1012	CLA	CHD-C1D	4.07	1.46	1.38
14	A	1117	CLA	C3C-C2C	4.07	1.45	1.36
14	B	1211	CLA	C3C-C2C	4.07	1.45	1.36
14	a	1101	CLA	CHD-C1D	4.07	1.46	1.38
14	a	1122	CLA	CHC-C1C	4.07	1.46	1.38
14	G	1113	CLA	C3C-C2C	4.07	1.45	1.36
14	a	1117	CLA	C3C-C2C	4.07	1.45	1.36
14	l	1501	CLA	CHC-C1C	4.07	1.46	1.38
14	L	1502	CLA	CHD-C1D	4.07	1.46	1.38
14	a	1120	CLA	C3C-C2C	4.07	1.45	1.36
14	b	1204	CLA	C3C-C2C	4.07	1.45	1.36
16	a	2001	PQN	C10-C5	4.07	1.47	1.40
14	A	1135	CLA	C3C-C2C	4.07	1.45	1.36
14	G	1130	CLA	CHD-C1D	4.07	1.46	1.38
14	B	1220	CLA	C3C-C2C	4.06	1.45	1.36
14	A	1012	CLA	O2D-CGD	4.06	1.43	1.33
14	a	1012	CLA	CHD-C1D	4.06	1.46	1.38
15	b	1207	F6C	C3D-C4D	-4.06	1.33	1.44
18	G	4008	BCR	C11-C12	-4.06	1.24	1.34
14	b	1234	CLA	C3C-C2C	4.06	1.45	1.36
14	a	1104	CLA	C3C-C2C	4.06	1.45	1.36
14	G	1135	CLA	CHD-C1D	4.06	1.46	1.38
14	a	1113	CLA	C3C-C2C	4.06	1.45	1.36
14	a	1127	CLA	C3C-C2C	4.06	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1239	CLA	CHD-C1D	4.06	1.46	1.38
14	A	1133	CLA	CHC-C1C	4.06	1.46	1.38
14	A	1131	CLA	C3C-C2C	4.06	1.45	1.36
14	A	1101	CLA	CHD-C1D	4.06	1.46	1.38
14	G	1135	CLA	CHC-C1C	4.06	1.46	1.38
14	L	1501	CLA	CHC-C1C	4.05	1.46	1.38
14	a	1116	CLA	CHD-C1D	4.05	1.46	1.38
14	A	1101	CLA	C3C-C2C	4.05	1.45	1.36
14	B	1213	CLA	C3C-C2C	4.05	1.45	1.36
14	b	1213	CLA	C3C-C2C	4.05	1.45	1.36
14	H	1220	CLA	C3C-C2C	4.05	1.45	1.36
14	H	1022	CLA	C1D-ND	-4.05	1.32	1.37
14	U	1502	CLA	CHD-C1D	4.05	1.46	1.38
14	B	1231	CLA	CHD-C1D	4.05	1.46	1.38
14	b	1220	CLA	C3C-C2C	4.05	1.45	1.36
14	H	1234	CLA	C3C-C2C	4.05	1.45	1.36
14	b	1220	CLA	CHC-C1C	4.05	1.46	1.38
14	a	1012	CLA	O2D-CGD	4.05	1.43	1.33
14	G	1131	CLA	C3C-C2C	4.05	1.45	1.36
14	A	1120	CLA	C3C-C2C	4.05	1.45	1.36
14	A	1115	CLA	CHD-C1D	4.05	1.46	1.38
14	H	1224	CLA	C3C-C2C	4.05	1.45	1.36
14	G	1012	CLA	CHD-C1D	4.05	1.46	1.38
15	B	1207	F6C	C3D-C4D	-4.05	1.33	1.44
14	a	1130	CLA	CHD-C1D	4.05	1.46	1.38
14	G	1104	CLA	C3C-C2C	4.05	1.45	1.36
14	a	1137	CLA	CHD-C1D	4.04	1.46	1.38
14	G	1133	CLA	CHC-C1C	4.04	1.46	1.38
14	B	1021	CLA	CHC-C1C	4.04	1.46	1.38
14	U	1501	CLA	CHC-C1C	4.04	1.46	1.38
14	G	1101	CLA	C3C-C2C	4.04	1.45	1.36
14	A	1114	CLA	CHD-C4C	4.04	1.48	1.39
14	b	1021	CLA	CHC-C1C	4.04	1.46	1.38
14	W	1701	CLA	C3C-C2C	4.04	1.45	1.36
14	G	1123	CLA	CHD-C1D	4.04	1.46	1.38
14	L	1503	CLA	CHD-C1D	4.04	1.46	1.38
14	A	1012	CLA	C3C-C2C	4.04	1.45	1.36
15	H	1237	F6C	C3D-C4D	-4.04	1.33	1.44
14	B	1224	CLA	C3C-C2C	4.04	1.45	1.36
14	A	1129	CLA	C1D-ND	-4.04	1.32	1.37
14	G	1110	CLA	CHD-C1D	4.04	1.46	1.38
14	U	1503	CLA	CHD-C1D	4.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1140	CLA	C3C-C2C	4.03	1.45	1.36
14	a	1128	CLA	CHD-C1D	4.03	1.46	1.38
20	R	5006	LMG	O7-C10	4.03	1.45	1.34
14	a	1012	CLA	C3C-C2C	4.03	1.45	1.36
14	B	1204	CLA	C3C-C2C	4.03	1.45	1.36
14	A	1130	CLA	CHD-C1D	4.03	1.46	1.38
14	a	1129	CLA	CHD-C1D	4.03	1.46	1.38
14	a	1135	CLA	CHD-C1D	4.03	1.46	1.38
14	G	1114	CLA	CHD-C4C	4.03	1.48	1.39
18	b	4010	BCR	C11-C12	-4.03	1.24	1.34
14	x	1701	CLA	C3C-C2C	4.03	1.45	1.36
14	l	1502	CLA	CHD-C1D	4.03	1.46	1.38
14	A	1110	CLA	CHD-C1D	4.03	1.46	1.38
14	G	1012	CLA	C3C-C2C	4.03	1.45	1.36
14	a	1115	CLA	CHD-C1D	4.03	1.46	1.38
14	b	1222	CLA	C1D-ND	-4.03	1.32	1.37
14	H	1204	CLA	C3C-C2C	4.03	1.45	1.36
14	H	1021	CLA	CHC-C1C	4.03	1.46	1.38
14	b	1220	CLA	CHD-C1D	4.03	1.46	1.38
14	G	1139	CLA	C3C-C2C	4.03	1.45	1.36
14	G	1140	CLA	C3C-C2C	4.03	1.45	1.36
14	A	1135	CLA	CHC-C1C	4.03	1.46	1.38
14	G	1128	CLA	CHD-C1D	4.03	1.46	1.38
14	a	1114	CLA	CHD-C4C	4.03	1.48	1.39
14	a	1135	CLA	CHC-C1C	4.03	1.46	1.38
14	X	1701	CLA	C3C-C2C	4.03	1.45	1.36
18	A	4008	BCR	C11-C12	-4.02	1.24	1.34
14	G	1115	CLA	CHD-C1D	4.02	1.46	1.38
14	G	1126	CLA	CHD-C1D	4.02	1.46	1.38
14	A	1135	CLA	CHD-C1D	4.02	1.46	1.38
14	a	1129	CLA	C1D-ND	-4.02	1.32	1.37
14	A	1116	CLA	CHD-C1D	4.02	1.46	1.38
14	H	1220	CLA	CHC-C1C	4.02	1.46	1.38
14	G	1116	CLA	CHD-C1D	4.02	1.46	1.38
15	b	1237	F6C	C3D-C4D	-4.02	1.33	1.44
14	B	1239	CLA	CHD-C1D	4.02	1.46	1.38
14	a	1123	CLA	CHD-C1D	4.02	1.46	1.38
14	A	1128	CLA	CHD-C1D	4.02	1.46	1.38
14	B	1225	CLA	C3C-C2C	4.02	1.45	1.36
14	A	1012	CLA	C1D-ND	-4.01	1.32	1.37
14	B	1231	CLA	C3C-C2C	4.01	1.45	1.36
18	H	4010	BCR	C11-C12	-4.01	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1131	CLA	C3C-C2C	4.01	1.45	1.36
14	A	1139	CLA	C3C-C2C	4.01	1.45	1.36
14	a	1139	CLA	C3C-C2C	4.01	1.45	1.36
14	B	1206	CLA	C1B-NB	-4.01	1.32	1.37
14	A	1125	CLA	CHC-C1C	4.00	1.46	1.38
14	b	1202	CLA	C1D-ND	-4.00	1.32	1.37
14	a	1110	CLA	CHD-C1D	4.00	1.46	1.38
14	G	1012	CLA	CHC-C1C	4.00	1.46	1.38
18	B	4010	BCR	C11-C12	-4.00	1.24	1.34
14	A	1126	CLA	CHD-C1D	4.00	1.46	1.38
20	I	5006	LMG	O7-C10	4.00	1.45	1.34
16	H	2002	PQN	C10-C5	4.00	1.47	1.40
14	b	1206	CLA	C1B-NB	-4.00	1.32	1.37
14	B	1202	CLA	C1D-ND	-4.00	1.32	1.37
14	b	1231	CLA	C3C-C2C	4.00	1.45	1.36
14	b	1224	CLA	C3C-C2C	4.00	1.45	1.36
14	l	1503	CLA	CHD-C1D	3.99	1.46	1.38
15	B	1237	F6C	C3D-C4D	-3.99	1.33	1.44
14	a	1137	CLA	C1D-ND	-3.99	1.32	1.37
14	b	1239	CLA	C1D-ND	-3.99	1.32	1.37
14	G	1129	CLA	C1D-ND	-3.99	1.32	1.37
14	a	1140	CLA	CHD-C1D	3.99	1.46	1.38
14	G	1123	CLA	C3C-C2C	3.99	1.45	1.36
14	H	1206	CLA	C1B-NB	-3.99	1.32	1.37
14	B	1022	CLA	C1D-ND	-3.99	1.32	1.37
14	H	1220	CLA	CHD-C1D	3.99	1.46	1.38
14	A	1123	CLA	C3C-C2C	3.99	1.45	1.36
14	B	1220	CLA	CHC-C1C	3.99	1.46	1.38
14	b	1022	CLA	C1D-ND	-3.99	1.32	1.37
14	a	1012	CLA	CHC-C1C	3.99	1.46	1.38
20	i	5006	LMG	O7-C10	3.99	1.45	1.34
14	B	1220	CLA	CHD-C1D	3.99	1.46	1.38
14	G	1120	CLA	C3C-C2C	3.99	1.45	1.36
14	b	1225	CLA	C3C-C2C	3.98	1.45	1.36
14	b	1236	CLA	C1D-ND	-3.98	1.32	1.37
14	B	1217	CLA	CHD-C1D	3.98	1.46	1.38
14	B	1221	CLA	CHD-C1D	3.98	1.46	1.38
14	a	1125	CLA	CHC-C1C	3.98	1.46	1.38
14	A	1012	CLA	CHC-C1C	3.98	1.46	1.38
14	G	1140	CLA	CHD-C1D	3.98	1.46	1.38
14	A	1137	CLA	CHD-C1D	3.98	1.46	1.38
18	R	4020	BCR	C11-C12	-3.98	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1205	CLA	C3C-C2C	3.98	1.45	1.36
14	a	1126	CLA	CHD-C1D	3.98	1.46	1.38
14	A	1124	CLA	C1D-ND	-3.98	1.32	1.37
14	a	1123	CLA	C3C-C2C	3.97	1.45	1.36
14	A	1140	CLA	C3C-C2C	3.97	1.45	1.36
14	G	1125	CLA	CHC-C1C	3.97	1.46	1.38
14	B	1205	CLA	C3C-C2C	3.97	1.45	1.36
14	G	1129	CLA	CHD-C1D	3.97	1.46	1.38
14	H	1205	CLA	C3C-C2C	3.97	1.45	1.36
14	A	1129	CLA	CHD-C1D	3.97	1.46	1.38
14	a	1134	CLA	CHD-C4C	3.97	1.48	1.39
14	H	1225	CLA	C3C-C2C	3.96	1.45	1.36
14	A	1140	CLA	CHD-C1D	3.96	1.46	1.38
14	A	1130	CLA	C1D-ND	-3.96	1.32	1.37
18	I	4020	BCR	C11-C12	-3.96	1.24	1.34
14	B	1225	CLA	CHD-C1D	3.96	1.46	1.38
14	A	1137	CLA	C3C-C2C	3.96	1.45	1.36
14	H	1222	CLA	C1D-ND	-3.96	1.32	1.37
14	H	1204	CLA	CHD-C4C	3.96	1.48	1.39
14	H	1231	CLA	C3C-C2C	3.96	1.45	1.36
14	a	1131	CLA	C1D-ND	-3.96	1.32	1.37
14	G	1124	CLA	CHD-C1D	3.95	1.46	1.38
14	G	1124	CLA	C1D-ND	-3.95	1.32	1.37
14	b	1234	CLA	C1D-ND	-3.95	1.32	1.37
15	H	1207	F6C	CHD-C1D	3.95	1.46	1.38
14	A	1131	CLA	C1D-ND	-3.95	1.32	1.37
14	L	1501	CLA	C1D-ND	-3.95	1.32	1.37
19	B	5004	LHG	O7-C7	3.95	1.45	1.34
14	U	1501	CLA	C1D-ND	-3.95	1.32	1.37
14	b	1225	CLA	CHD-C1D	3.95	1.46	1.38
19	b	5004	LHG	O7-C7	3.95	1.45	1.34
14	B	1236	CLA	C1D-ND	-3.95	1.32	1.37
14	b	1023	CLA	CHC-C1C	3.95	1.46	1.38
14	G	1134	CLA	CHD-C4C	3.95	1.48	1.39
14	H	1217	CLA	CHD-C1D	3.95	1.46	1.38
13	a	1011	CL0	CHD-C4C	3.95	1.46	1.39
14	G	1137	CLA	CHD-C1D	3.95	1.46	1.38
14	B	1023	CLA	CHC-C1C	3.95	1.46	1.38
16	b	2002	PQN	C10-C5	3.95	1.47	1.40
14	A	1124	CLA	CHD-C1D	3.95	1.46	1.38
14	H	1225	CLA	CHD-C1D	3.94	1.46	1.38
14	G	1137	CLA	C3C-C2C	3.94	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1102	CLA	C1D-ND	-3.94	1.32	1.37
14	G	1131	CLA	C1D-ND	-3.94	1.32	1.37
14	G	1137	CLA	C1D-ND	-3.94	1.32	1.37
14	a	1111	CLA	C3C-C2C	3.94	1.45	1.36
15	a	1121	F6C	C3D-C4D	-3.94	1.33	1.44
14	b	1217	CLA	CHD-C1D	3.94	1.46	1.38
16	B	2002	PQN	C10-C5	3.94	1.47	1.40
14	G	1130	CLA	C1D-ND	-3.94	1.32	1.37
14	H	1202	CLA	C1D-ND	-3.93	1.32	1.37
14	B	1239	CLA	C1D-ND	-3.93	1.32	1.37
14	H	1206	CLA	C3C-C2C	3.93	1.45	1.36
14	A	1134	CLA	CHD-C4C	3.93	1.48	1.39
14	a	1013	CLA	C3C-C2C	3.93	1.45	1.36
15	B	1237	F6C	C1C-NC	-3.93	1.32	1.37
13	A	1011	CL0	CHD-C4C	3.93	1.46	1.39
14	H	1236	CLA	C1D-ND	-3.93	1.32	1.37
14	l	1501	CLA	C1D-ND	-3.93	1.32	1.37
18	i	4020	BCR	C11-C12	-3.93	1.24	1.34
15	G	1121	F6C	C3D-C4D	-3.93	1.33	1.44
14	a	1130	CLA	C1D-ND	-3.92	1.32	1.37
14	H	1022	CLA	C3C-C2C	3.92	1.45	1.36
14	H	1239	CLA	C1D-ND	-3.92	1.32	1.37
14	a	1137	CLA	C3C-C2C	3.92	1.45	1.36
14	b	1227	CLA	CHD-C4C	3.92	1.48	1.39
14	b	1022	CLA	C3C-C2C	3.92	1.45	1.36
14	B	1221	CLA	C1D-ND	-3.92	1.32	1.37
14	b	1206	CLA	C3C-C2C	3.92	1.45	1.36
19	H	5004	LHG	O7-C7	3.92	1.45	1.34
14	H	1234	CLA	C1D-ND	-3.92	1.32	1.37
15	A	1121	F6C	C3D-C4D	-3.92	1.33	1.44
14	G	1012	CLA	C1D-ND	-3.92	1.32	1.37
13	G	1011	CL0	CHD-C4C	3.92	1.46	1.39
14	H	1226	CLA	CHC-C1C	3.92	1.46	1.38
14	G	1139	CLA	CHD-C1D	3.92	1.46	1.38
14	H	1023	CLA	CHC-C1C	3.92	1.46	1.38
14	G	1013	CLA	C3C-C2C	3.92	1.45	1.36
14	b	1221	CLA	CHD-C1D	3.92	1.46	1.38
14	A	1139	CLA	CHD-C1D	3.92	1.46	1.38
14	a	1012	CLA	C1D-ND	-3.92	1.32	1.37
14	a	1124	CLA	C1D-ND	-3.92	1.32	1.37
14	A	1117	CLA	CHC-C1C	3.92	1.46	1.38
14	b	1226	CLA	CHC-C1C	3.91	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1013	CLA	C3C-C2C	3.91	1.45	1.36
14	B	1227	CLA	CHD-C4C	3.91	1.48	1.39
14	A	1111	CLA	C3C-C2C	3.91	1.45	1.36
14	H	1227	CLA	CHD-C4C	3.91	1.48	1.39
18	A	4007	BCR	C11-C12	-3.91	1.24	1.34
14	B	1226	CLA	CHC-C1C	3.91	1.46	1.38
14	A	1102	CLA	C1D-ND	-3.91	1.32	1.37
14	a	1124	CLA	CHD-C1D	3.91	1.46	1.38
14	a	1102	CLA	C1D-ND	-3.90	1.32	1.37
14	b	1204	CLA	CHD-C4C	3.90	1.48	1.39
15	b	1237	F6C	C1C-NC	-3.90	1.32	1.37
14	H	1215	CLA	C3C-C2C	3.90	1.45	1.36
14	H	1221	CLA	CHD-C1D	3.90	1.46	1.38
15	B	1230	F6C	C3D-C4D	-3.90	1.33	1.44
15	H	1237	F6C	C1C-NC	-3.90	1.32	1.37
15	b	1207	F6C	CHD-C1D	3.90	1.46	1.38
14	B	1206	CLA	C3C-C2C	3.90	1.45	1.36
13	G	1011	CL0	C3D-C2D	3.90	1.46	1.39
14	x	1701	CLA	CHD-C1D	3.89	1.46	1.38
14	b	1221	CLA	C1D-ND	-3.89	1.32	1.37
14	B	1234	CLA	C1D-ND	-3.89	1.32	1.37
14	H	1221	CLA	C3C-C2C	3.89	1.45	1.36
14	B	1204	CLA	CHD-C4C	3.89	1.48	1.39
13	a	1011	CL0	C3D-C2D	3.89	1.46	1.39
14	X	1701	CLA	CHD-C1D	3.89	1.46	1.38
18	G	4007	BCR	C11-C12	-3.89	1.24	1.34
14	G	1111	CLA	C3C-C2C	3.89	1.45	1.36
14	B	1219	CLA	CHD-C4C	3.89	1.48	1.39
14	b	1215	CLA	C3C-C2C	3.89	1.45	1.36
14	B	1022	CLA	C3C-C2C	3.89	1.45	1.36
18	a	4007	BCR	C11-C12	-3.89	1.24	1.34
14	b	1203	CLA	C1B-NB	-3.88	1.32	1.37
14	a	1128	CLA	MG-ND	-3.88	1.98	2.05
14	B	1214	CLA	CHD-C4C	3.88	1.48	1.39
14	b	1204	CLA	CHD-C1D	3.88	1.46	1.38
14	G	1117	CLA	CHC-C1C	3.88	1.46	1.38
14	b	1236	CLA	CHD-C1D	3.88	1.46	1.38
15	B	1207	F6C	CHD-C1D	3.88	1.46	1.38
14	G	1106	CLA	CHD-C1D	3.88	1.46	1.38
14	A	1128	CLA	MG-ND	-3.88	1.98	2.05
14	a	1116	CLA	C1D-ND	-3.88	1.32	1.37
14	b	1214	CLA	CHD-C4C	3.87	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1117	CLA	CHC-C1C	3.87	1.46	1.38
14	a	1131	CLA	CHD-C4C	3.87	1.48	1.39
14	a	1135	CLA	C1D-ND	-3.87	1.32	1.37
14	G	1123	CLA	C1D-ND	-3.87	1.32	1.37
14	A	1119	CLA	CHD-C4C	3.87	1.48	1.39
14	A	1137	CLA	C1D-ND	-3.87	1.32	1.37
14	H	1233	CLA	CHD-C4C	3.87	1.48	1.39
14	H	1228	CLA	CHD-C4C	3.87	1.48	1.39
14	H	1203	CLA	C1B-NB	-3.87	1.32	1.37
14	b	1203	CLA	C1D-ND	-3.87	1.32	1.37
14	A	1123	CLA	C1D-ND	-3.87	1.32	1.37
14	B	1236	CLA	CHD-C1D	3.87	1.46	1.38
14	H	1221	CLA	C1D-ND	-3.87	1.32	1.37
14	G	1131	CLA	CHD-C4C	3.87	1.48	1.39
14	b	1221	CLA	C3C-C2C	3.87	1.45	1.36
14	W	1701	CLA	CHD-C1D	3.87	1.46	1.38
14	A	1106	CLA	CHD-C1D	3.87	1.46	1.38
14	B	1215	CLA	C3C-C2C	3.87	1.45	1.36
14	B	1221	CLA	C3C-C2C	3.86	1.45	1.36
15	b	1230	F6C	C3D-C4D	-3.86	1.33	1.44
14	b	1219	CLA	CHD-C4C	3.86	1.48	1.39
14	B	1203	CLA	C1B-NB	-3.86	1.32	1.37
14	H	1203	CLA	C1D-ND	-3.86	1.32	1.37
14	H	1236	CLA	CHD-C1D	3.86	1.45	1.38
13	A	1011	CL0	C3D-C2D	3.86	1.46	1.39
14	a	1139	CLA	CHD-C1D	3.86	1.45	1.38
14	a	1119	CLA	CHD-C4C	3.86	1.48	1.39
14	H	1219	CLA	CHD-C4C	3.85	1.48	1.39
14	B	1203	CLA	C1D-ND	-3.85	1.32	1.37
14	H	1214	CLA	CHD-C4C	3.85	1.48	1.39
14	G	1134	CLA	OBD-CAD	3.85	1.29	1.22
14	G	1128	CLA	MG-ND	-3.85	1.98	2.05
14	T	1401	CLA	CHD-C4C	3.85	1.48	1.39
14	G	1119	CLA	CHD-C4C	3.85	1.48	1.39
18	R	4018	BCR	C11-C12	-3.85	1.24	1.34
14	H	1203	CLA	C3C-C2C	3.84	1.45	1.36
14	G	1135	CLA	C1D-ND	-3.84	1.32	1.37
14	G	1140	CLA	C1D-ND	-3.84	1.32	1.37
14	a	1128	CLA	CHC-C1C	3.84	1.46	1.38
14	A	1128	CLA	CHC-C1C	3.84	1.46	1.38
14	b	1203	CLA	C3C-C2C	3.84	1.45	1.36
15	H	1230	F6C	C3D-C4D	-3.84	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1228	CLA	CHD-C4C	3.84	1.47	1.39
14	A	1136	CLA	C1D-ND	-3.84	1.32	1.37
14	k	1401	CLA	CHD-C4C	3.84	1.47	1.39
14	K	1401	CLA	CHD-C4C	3.84	1.47	1.39
14	a	1130	CLA	C1B-NB	-3.84	1.32	1.37
18	I	4018	BCR	C11-C12	-3.84	1.24	1.34
14	a	1106	CLA	CHD-C1D	3.84	1.45	1.38
18	i	4018	BCR	C11-C12	-3.84	1.24	1.34
14	A	1131	CLA	CHD-C4C	3.84	1.47	1.39
14	G	1128	CLA	CHC-C1C	3.84	1.46	1.38
14	A	1130	CLA	C1B-NB	-3.84	1.32	1.37
14	b	1228	CLA	CHD-C4C	3.84	1.47	1.39
14	A	1139	CLA	CHC-C4B	3.83	1.48	1.39
14	H	1239	CLA	CHC-C1C	3.83	1.46	1.38
14	B	1204	CLA	CHD-C1D	3.83	1.45	1.38
14	B	1203	CLA	C3C-C2C	3.83	1.45	1.36
14	b	1023	CLA	C1B-NB	-3.83	1.32	1.37
14	B	1233	CLA	CHD-C4C	3.83	1.47	1.39
14	b	1239	CLA	CHC-C1C	3.83	1.46	1.38
14	H	1215	CLA	C1D-ND	-3.83	1.32	1.37
14	a	1123	CLA	C1D-ND	-3.83	1.32	1.37
14	G	1130	CLA	C1B-NB	-3.83	1.32	1.37
14	b	1233	CLA	CHD-C4C	3.83	1.47	1.39
14	a	1104	CLA	C1D-ND	-3.82	1.32	1.37
14	A	1140	CLA	C1D-ND	-3.82	1.32	1.37
14	b	1209	CLA	CHD-C4C	3.82	1.47	1.39
14	b	1215	CLA	C1D-ND	-3.82	1.32	1.37
14	a	1139	CLA	CHC-C4B	3.82	1.48	1.39
14	a	1119	CLA	CHC-C1C	3.82	1.46	1.38
14	H	1204	CLA	CHD-C1D	3.82	1.45	1.38
14	L	1503	CLA	C1D-ND	-3.82	1.32	1.37
14	A	1119	CLA	CHC-C1C	3.82	1.46	1.38
14	B	1021	CLA	C3C-C2C	3.82	1.45	1.36
13	a	1011	CL0	OBD-CAD	3.82	1.27	1.22
14	B	1239	CLA	CHC-C1C	3.82	1.46	1.38
14	a	1125	CLA	C1D-ND	-3.82	1.32	1.37
14	G	1135	CLA	C1B-NB	-3.81	1.32	1.37
14	B	1202	CLA	C3C-C2C	3.81	1.45	1.36
14	H	1021	CLA	C3C-C2C	3.81	1.45	1.36
14	A	1104	CLA	C1D-ND	-3.81	1.32	1.37
14	H	1212	CLA	C1D-ND	-3.81	1.32	1.37
14	H	1206	CLA	CHC-C1C	3.81	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1116	CLA	C1D-ND	-3.81	1.32	1.37
14	H	1209	CLA	CHD-C4C	3.81	1.47	1.39
14	H	1023	CLA	C4B-NB	-3.81	1.32	1.37
14	G	1140	CLA	CHC-C4B	3.81	1.48	1.39
14	B	1201	CLA	CHD-C4C	3.81	1.47	1.39
13	A	1011	CL0	OBD-CAD	3.81	1.27	1.22
13	G	1011	CL0	OBD-CAD	3.81	1.27	1.22
14	b	1201	CLA	CHD-C4C	3.81	1.47	1.39
14	H	1223	CLA	CHD-C1D	3.80	1.45	1.38
14	H	1201	CLA	CHD-C4C	3.80	1.47	1.39
14	B	1209	CLA	CHD-C4C	3.80	1.47	1.39
14	A	1138	CLA	CHD-C4C	3.80	1.47	1.39
14	U	1501	CLA	CHD-C1D	3.80	1.45	1.38
14	b	1235	CLA	C1D-ND	-3.80	1.32	1.37
14	H	1218	CLA	CHC-C4B	3.80	1.47	1.39
14	b	1202	CLA	C3C-C2C	3.80	1.45	1.36
14	H	1023	CLA	C3C-C2C	3.80	1.45	1.36
14	K	1401	CLA	CHC-C4B	3.80	1.47	1.39
20	U	5007	LMG	C19-C18	-3.80	1.32	1.51
14	G	1103	CLA	C3C-C2C	3.80	1.45	1.36
14	a	1103	CLA	C3C-C2C	3.80	1.45	1.36
14	B	1023	CLA	C3C-C2C	3.80	1.45	1.36
14	G	1108	CLA	CHD-C4C	3.80	1.47	1.39
14	b	1210	CLA	C3C-C2C	3.80	1.45	1.36
14	b	1204	CLA	C1B-NB	-3.80	1.32	1.37
14	l	1501	CLA	CHD-C1D	3.79	1.45	1.38
14	B	1205	CLA	CHD-C1D	3.79	1.45	1.38
14	G	1122	CLA	C3C-C2C	3.79	1.44	1.36
14	B	1206	CLA	CHC-C1C	3.79	1.46	1.38
14	A	1125	CLA	C1D-ND	-3.79	1.32	1.37
14	b	1021	CLA	C3C-C2C	3.79	1.44	1.36
14	A	1103	CLA	C3C-C2C	3.79	1.44	1.36
14	a	1140	CLA	C1D-ND	-3.79	1.32	1.37
14	b	1208	CLA	C1D-ND	-3.79	1.32	1.37
14	A	1120	CLA	C1D-ND	-3.79	1.32	1.37
14	B	1210	CLA	C3C-C2C	3.79	1.44	1.36
20	A	5005	LMG	C40-C39	-3.79	1.32	1.51
14	L	1501	CLA	CHD-C1D	3.79	1.45	1.38
14	B	1023	CLA	C1B-NB	-3.79	1.32	1.37
14	B	1218	CLA	CHC-C4B	3.79	1.47	1.39
14	a	1135	CLA	C1B-NB	-3.79	1.32	1.37
14	G	1120	CLA	C1D-ND	-3.78	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1125	CLA	C1D-ND	-3.78	1.32	1.37
14	a	1136	CLA	C1D-ND	-3.78	1.32	1.37
14	T	1401	CLA	CHC-C4B	3.78	1.47	1.39
20	U	5007	LMG	C40-C39	-3.78	1.33	1.51
14	G	1116	CLA	C1D-ND	-3.78	1.32	1.37
14	l	1503	CLA	C1D-ND	-3.78	1.32	1.37
14	U	1503	CLA	C1D-ND	-3.78	1.32	1.37
20	l	5007	LMG	C40-C39	-3.78	1.33	1.51
14	B	1235	CLA	C1D-ND	-3.78	1.32	1.37
14	H	1204	CLA	C1B-NB	-3.78	1.32	1.37
14	b	1023	CLA	C4B-NB	-3.78	1.32	1.37
14	B	1212	CLA	C1D-ND	-3.78	1.32	1.37
20	L	5007	LMG	C19-C18	-3.78	1.33	1.51
20	a	5005	LMG	C40-C39	-3.78	1.33	1.51
14	A	1135	CLA	C1D-ND	-3.78	1.32	1.37
14	a	1140	CLA	CHC-C4B	3.78	1.47	1.39
20	L	5007	LMG	C40-C39	-3.78	1.33	1.51
14	H	1023	CLA	C1B-NB	-3.78	1.32	1.37
14	b	1023	CLA	C3C-C2C	3.78	1.44	1.36
14	b	1206	CLA	CHC-C1C	3.78	1.46	1.38
14	A	1134	CLA	OBD-CAD	3.78	1.29	1.22
20	b	5002	LMG	C22-C21	-3.78	1.33	1.51
14	G	1136	CLA	C1D-ND	-3.77	1.32	1.37
14	H	1222	CLA	CHD-C1D	3.77	1.45	1.38
14	H	1202	CLA	C3C-C2C	3.77	1.44	1.36
14	A	1108	CLA	CHD-C4C	3.77	1.47	1.39
14	A	1135	CLA	C1B-NB	-3.77	1.32	1.37
14	k	1401	CLA	CHC-C4B	3.77	1.47	1.39
14	b	1212	CLA	C1D-ND	-3.77	1.32	1.37
14	a	1134	CLA	OBD-CAD	3.77	1.29	1.22
14	H	1210	CLA	C3C-C2C	3.77	1.44	1.36
14	H	1220	CLA	C1D-ND	-3.77	1.32	1.37
14	G	1138	CLA	CHD-C4C	3.77	1.47	1.39
14	H	1205	CLA	CHD-C1D	3.77	1.45	1.38
14	a	1138	CLA	CHD-C4C	3.77	1.47	1.39
14	A	1105	CLA	CHD-C4C	3.77	1.47	1.39
14	b	1205	CLA	CHD-C1D	3.77	1.45	1.38
14	B	1212	CLA	CHD-C1D	3.77	1.45	1.38
20	G	5005	LMG	C40-C39	-3.77	1.33	1.51
20	l	5007	LMG	C19-C18	-3.77	1.33	1.51
14	l	1502	CLA	CHD-C4C	3.77	1.47	1.39
14	H	1235	CLA	C1D-ND	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1115	CLA	CHD-C4C	3.77	1.47	1.39
20	B	5002	LMG	C22-C21	-3.77	1.33	1.51
14	G	1139	CLA	CHC-C4B	3.77	1.47	1.39
14	a	1105	CLA	CHD-C4C	3.77	1.47	1.39
14	B	1023	CLA	C4B-NB	-3.77	1.32	1.37
19	G	5001	LHG	O7-C7	3.77	1.44	1.34
14	a	1120	CLA	C1D-ND	-3.77	1.32	1.37
15	b	1230	F6C	CHD-C1D	3.77	1.46	1.38
14	a	1133	CLA	C1D-ND	-3.77	1.32	1.37
14	G	1119	CLA	CHC-C1C	3.77	1.46	1.38
14	B	1223	CLA	CHD-C1D	3.76	1.45	1.38
13	G	1011	CL0	CHD-C1D	3.76	1.45	1.39
14	b	1222	CLA	CHD-C1D	3.76	1.45	1.38
14	A	1140	CLA	CHC-C4B	3.76	1.47	1.39
15	H	1230	F6C	CHD-C1D	3.76	1.46	1.38
14	b	1218	CLA	CHC-C4B	3.76	1.47	1.39
14	G	1104	CLA	C1D-ND	-3.76	1.32	1.37
14	B	1204	CLA	C1B-NB	-3.76	1.32	1.37
18	H	4014	BCR	C11-C12	-3.76	1.24	1.34
14	G	1118	CLA	CHD-C4C	3.76	1.47	1.39
14	G	1112	CLA	CHD-C4C	3.76	1.47	1.39
14	A	1119	CLA	C1B-NB	-3.76	1.32	1.37
14	B	1220	CLA	C1D-ND	-3.76	1.32	1.37
14	a	1108	CLA	CHD-C4C	3.76	1.47	1.39
14	B	1235	CLA	CHD-C4C	3.76	1.47	1.39
20	H	5002	LMG	C22-C21	-3.76	1.33	1.51
14	A	1113	CLA	CHC-C4B	3.75	1.47	1.39
14	b	1226	CLA	CHD-C4C	3.75	1.47	1.39
14	b	1235	CLA	CHD-C4C	3.75	1.47	1.39
14	A	1127	CLA	CHD-C1D	3.75	1.45	1.38
14	a	1138	CLA	C1D-ND	-3.75	1.32	1.37
14	B	1215	CLA	C1D-ND	-3.75	1.32	1.37
14	H	1022	CLA	CHD-C1D	3.75	1.45	1.38
14	b	1216	CLA	CHD-C4C	3.75	1.47	1.39
14	b	1223	CLA	CHD-C1D	3.75	1.45	1.38
19	a	5001	LHG	O7-C7	3.75	1.44	1.34
14	a	1118	CLA	CHD-C4C	3.75	1.47	1.39
14	B	1022	CLA	CHD-C1D	3.75	1.45	1.38
15	B	1230	F6C	CHD-C1D	3.75	1.46	1.38
14	B	1220	CLA	CHB-C1B	3.75	1.47	1.39
14	a	1134	CLA	CHC-C4B	3.75	1.47	1.39
14	A	1134	CLA	CHC-C4B	3.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1224	CLA	CHD-C1D	3.75	1.45	1.38
14	b	1220	CLA	CHB-C1B	3.74	1.47	1.39
20	B	5002	LMG	C37-C36	-3.74	1.33	1.51
14	H	1216	CLA	CHD-C4C	3.74	1.47	1.39
14	L	1502	CLA	CHD-C4C	3.74	1.47	1.39
14	B	1229	CLA	CHC-C4B	3.74	1.47	1.39
14	b	1220	CLA	C1D-ND	-3.74	1.32	1.37
14	B	1232	CLA	CHD-C4C	3.74	1.47	1.39
14	H	1235	CLA	CHD-C4C	3.74	1.47	1.39
14	G	1109	CLA	CHD-C4C	3.74	1.47	1.39
14	b	1212	CLA	CHD-C1D	3.74	1.45	1.38
14	A	1112	CLA	CHD-C4C	3.74	1.47	1.39
14	G	1134	CLA	CHC-C4B	3.74	1.47	1.39
14	H	1208	CLA	C1D-ND	-3.74	1.33	1.37
14	G	1110	CLA	CHC-C4B	3.74	1.47	1.39
14	B	1222	CLA	CHD-C1D	3.74	1.45	1.38
15	a	1121	F6C	CHD-C4C	3.74	1.47	1.39
14	A	1109	CLA	CHD-C4C	3.74	1.47	1.39
14	a	1127	CLA	CHD-C1D	3.73	1.45	1.38
20	l	5007	LMG	C37-C36	-3.73	1.33	1.51
20	U	5007	LMG	C37-C36	-3.73	1.33	1.51
14	b	1210	CLA	C1D-ND	-3.73	1.33	1.37
14	B	1208	CLA	C1D-ND	-3.73	1.33	1.37
14	x	1701	CLA	CHC-C4B	3.73	1.47	1.39
15	A	1121	F6C	CHD-C4C	3.73	1.47	1.39
14	B	1234	CLA	CHC-C4B	3.73	1.47	1.39
14	H	1232	CLA	CHD-C4C	3.73	1.47	1.39
14	A	1122	CLA	CHD-C4C	3.73	1.47	1.39
14	G	1106	CLA	C1D-ND	-3.73	1.33	1.37
18	L	4022	BCR	C11-C12	-3.73	1.24	1.34
18	b	4017	BCR	C11-C12	-3.73	1.24	1.34
14	b	1224	CLA	CHD-C1D	3.73	1.45	1.38
14	H	1229	CLA	CHC-C4B	3.73	1.47	1.39
14	a	1109	CLA	CHD-C4C	3.73	1.47	1.39
14	B	1216	CLA	CHD-C4C	3.73	1.47	1.39
14	a	1103	CLA	C1D-ND	-3.73	1.33	1.37
20	b	5002	LMG	C37-C36	-3.73	1.33	1.51
14	H	1220	CLA	CHB-C1B	3.73	1.47	1.39
14	a	1110	CLA	CHC-C4B	3.73	1.47	1.39
14	A	1110	CLA	CHC-C4B	3.73	1.47	1.39
14	G	1122	CLA	CHD-C4C	3.73	1.47	1.39
14	H	1215	CLA	CHD-C4C	3.73	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	5001	LHG	O7-C7	3.73	1.44	1.34
18	B	4014	BCR	C11-C12	-3.73	1.24	1.34
14	a	1112	CLA	CHD-C4C	3.73	1.47	1.39
14	G	1119	CLA	C1B-NB	-3.73	1.33	1.37
18	H	4017	BCR	C11-C12	-3.73	1.24	1.34
14	B	1210	CLA	CHD-C4C	3.73	1.47	1.39
14	H	1234	CLA	CHC-C4B	3.73	1.47	1.39
20	L	5007	LMG	C37-C36	-3.73	1.33	1.51
14	U	1502	CLA	CHD-C4C	3.73	1.47	1.39
14	a	1122	CLA	CHD-C4C	3.73	1.47	1.39
14	a	1119	CLA	C1B-NB	-3.73	1.33	1.37
14	H	1212	CLA	CHD-C1D	3.72	1.45	1.38
20	G	5005	LMG	C43-C42	-3.72	1.33	1.51
14	G	1105	CLA	CHD-C4C	3.72	1.47	1.39
14	a	1115	CLA	CHD-C4C	3.72	1.47	1.39
14	b	1234	CLA	CHC-C4B	3.72	1.47	1.39
14	G	1124	CLA	C1B-NB	-3.72	1.33	1.37
14	H	1226	CLA	CHD-C4C	3.72	1.47	1.39
20	A	5005	LMG	C43-C42	-3.72	1.33	1.51
14	A	1136	CLA	CHD-C4C	3.72	1.47	1.39
14	G	1113	CLA	CHC-C4B	3.72	1.47	1.39
14	a	1113	CLA	CHC-C4B	3.72	1.47	1.39
14	b	1229	CLA	CHC-C4B	3.72	1.47	1.39
20	H	5002	LMG	C37-C36	-3.72	1.33	1.51
14	W	1701	CLA	CHC-C4B	3.72	1.47	1.39
14	a	1012	CLA	MG-ND	-3.72	1.98	2.05
14	X	1701	CLA	CHC-C4B	3.72	1.47	1.39
14	a	1124	CLA	CHD-C4C	3.72	1.47	1.39
14	A	1122	CLA	C3C-C2C	3.72	1.44	1.36
14	A	1115	CLA	CHD-C4C	3.71	1.47	1.39
18	l	4022	BCR	C11-C12	-3.71	1.25	1.34
15	H	1237	F6C	CHD-C1D	3.71	1.45	1.38
14	b	1215	CLA	CHD-C4C	3.71	1.47	1.39
14	A	1118	CLA	CHD-C4C	3.71	1.47	1.39
14	A	1110	CLA	C1D-ND	-3.71	1.33	1.37
14	a	1136	CLA	CHD-C4C	3.71	1.47	1.39
14	b	1210	CLA	CHD-C4C	3.71	1.47	1.39
14	H	1231	CLA	C1D-ND	-3.71	1.33	1.37
14	b	1232	CLA	CHD-C4C	3.71	1.47	1.39
14	B	1215	CLA	CHD-C4C	3.71	1.47	1.39
14	b	1222	CLA	C1B-NB	-3.71	1.33	1.37
18	b	4014	BCR	C11-C12	-3.71	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1124	CLA	CHD-C4C	3.71	1.47	1.39
20	a	5005	LMG	C43-C42	-3.71	1.33	1.51
14	G	1127	CLA	CHD-C1D	3.71	1.45	1.38
13	a	1011	CL0	CHD-C1D	3.71	1.45	1.39
14	b	1022	CLA	CHD-C1D	3.71	1.45	1.38
14	G	1110	CLA	C1D-ND	-3.71	1.33	1.37
14	a	1122	CLA	C3C-C2C	3.71	1.44	1.36
14	B	1226	CLA	CHD-C4C	3.71	1.47	1.39
14	H	1236	CLA	CHC-C4B	3.71	1.47	1.39
14	H	1216	CLA	CHC-C4B	3.71	1.47	1.39
15	G	1121	F6C	CHD-C4C	3.71	1.47	1.39
14	H	1210	CLA	C1D-ND	-3.71	1.33	1.37
14	G	1103	CLA	C1D-ND	-3.70	1.33	1.37
18	B	4017	BCR	C11-C12	-3.70	1.25	1.34
14	G	1138	CLA	C1D-ND	-3.70	1.33	1.37
14	B	1231	CLA	C1D-ND	-3.70	1.33	1.37
15	b	1237	F6C	CHD-C1D	3.70	1.45	1.38
18	U	4022	BCR	C11-C12	-3.70	1.25	1.34
14	a	1110	CLA	C1D-ND	-3.70	1.33	1.37
14	a	1117	CLA	CHD-C4C	3.70	1.47	1.39
14	A	1124	CLA	CHD-C4C	3.70	1.47	1.39
14	A	1106	CLA	C1D-ND	-3.70	1.33	1.37
14	A	1133	CLA	C1D-ND	-3.69	1.33	1.37
14	H	1210	CLA	CHD-C4C	3.69	1.47	1.39
14	A	1117	CLA	CHD-C4C	3.69	1.47	1.39
20	b	5002	LMG	C19-C18	-3.69	1.33	1.51
14	A	1116	CLA	CHD-C4C	3.69	1.47	1.39
14	H	1214	CLA	C1B-NB	-3.69	1.33	1.37
14	a	1106	CLA	C1D-ND	-3.69	1.33	1.37
13	A	1011	CL0	CHD-C1D	3.69	1.45	1.39
14	G	1132	CLA	C1D-ND	-3.69	1.33	1.37
15	B	1237	F6C	CHD-C1D	3.69	1.45	1.38
14	B	1229	CLA	CHD-C4C	3.69	1.47	1.39
20	B	5002	LMG	C19-C18	-3.69	1.33	1.51
14	H	1224	CLA	CHD-C1D	3.69	1.45	1.38
14	G	1136	CLA	CHD-C4C	3.69	1.47	1.39
14	A	1124	CLA	C1B-NB	-3.69	1.33	1.37
14	a	1119	CLA	C1C-NC	-3.69	1.32	1.37
14	A	1118	CLA	C1D-ND	-3.69	1.33	1.37
14	H	1222	CLA	C1B-NB	-3.69	1.33	1.37
14	b	1229	CLA	CHD-C4C	3.69	1.47	1.39
14	B	1216	CLA	CHC-C4B	3.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1138	CLA	C1D-ND	-3.68	1.33	1.37
14	B	1236	CLA	CHC-C4B	3.68	1.47	1.39
20	H	5002	LMG	C19-C18	-3.68	1.33	1.51
18	b	4005	BCR	C11-C12	-3.68	1.25	1.34
14	G	1125	CLA	C4B-NB	-3.68	1.33	1.37
14	b	1216	CLA	CHC-C4B	3.68	1.47	1.39
14	G	1133	CLA	CHD-C4C	3.68	1.47	1.39
14	b	1215	CLA	C1B-NB	-3.68	1.33	1.37
14	b	1236	CLA	CHC-C4B	3.68	1.47	1.39
14	B	1021	CLA	MG-ND	-3.68	1.98	2.05
14	b	1231	CLA	C1D-ND	-3.68	1.33	1.37
14	a	1126	CLA	CHD-C4C	3.68	1.47	1.39
14	a	1125	CLA	C4B-NB	-3.68	1.33	1.37
14	b	1233	CLA	CHC-C4B	3.68	1.47	1.39
14	b	1214	CLA	C1B-NB	-3.68	1.33	1.37
14	H	1229	CLA	CHD-C4C	3.68	1.47	1.39
14	H	1224	CLA	MG-ND	-3.68	1.98	2.05
14	A	1119	CLA	C1C-NC	-3.68	1.32	1.37
14	b	1021	CLA	C1B-NB	-3.68	1.33	1.37
14	B	1213	CLA	CHD-C4C	3.68	1.47	1.39
14	G	1117	CLA	CHD-C4C	3.68	1.47	1.39
14	G	1012	CLA	MG-ND	-3.68	1.98	2.05
14	B	1233	CLA	CHC-C4B	3.67	1.47	1.39
14	b	1227	CLA	C1D-ND	-3.67	1.33	1.37
14	B	1214	CLA	C1D-ND	-3.67	1.33	1.37
14	a	1132	CLA	CHD-C4C	3.67	1.47	1.39
14	a	1129	CLA	C1B-NB	-3.67	1.33	1.37
14	A	1115	CLA	C1D-ND	-3.67	1.33	1.37
14	b	1224	CLA	MG-ND	-3.67	1.98	2.05
14	G	1118	CLA	C1D-ND	-3.67	1.33	1.37
14	G	1115	CLA	C1D-ND	-3.67	1.33	1.37
14	A	1132	CLA	C1D-ND	-3.67	1.33	1.37
18	B	4005	BCR	C11-C12	-3.67	1.25	1.34
14	a	1133	CLA	CHD-C4C	3.67	1.47	1.39
14	b	1209	CLA	CHC-C4B	3.67	1.47	1.39
14	A	1012	CLA	MG-ND	-3.67	1.98	2.05
14	A	1132	CLA	CHD-C4C	3.67	1.47	1.39
14	B	1208	CLA	CHD-C4C	3.67	1.47	1.39
14	a	1124	CLA	C1B-NB	-3.67	1.33	1.37
14	H	1021	CLA	MG-ND	-3.67	1.98	2.05
14	G	1102	CLA	CHD-C4C	3.67	1.47	1.39
14	b	1226	CLA	MG-ND	-3.67	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	M	4021	BCR	C11-C12	-3.67	1.25	1.34
14	G	1120	CLA	CHD-C1D	3.67	1.45	1.38
14	B	1218	CLA	CHD-C1D	3.67	1.45	1.38
14	G	1125	CLA	MG-ND	-3.67	1.98	2.05
14	B	1219	CLA	CHC-C4B	3.67	1.47	1.39
14	b	1021	CLA	MG-ND	-3.67	1.98	2.05
15	H	1238	F6C	C1D-ND	-3.67	1.32	1.37
14	A	1102	CLA	CHD-C4C	3.67	1.47	1.39
20	H	5002	LMG	O7-C10	3.67	1.44	1.34
14	B	1222	CLA	C1B-NB	-3.66	1.33	1.37
14	B	1227	CLA	C1D-ND	-3.66	1.33	1.37
14	a	1101	CLA	CHD-C4C	3.66	1.47	1.39
14	b	1201	CLA	C1D-ND	-3.66	1.33	1.37
14	H	1201	CLA	C1D-ND	-3.66	1.33	1.37
14	H	1208	CLA	CHD-C4C	3.66	1.47	1.39
14	H	1217	CLA	CHC-C4B	3.66	1.47	1.39
14	G	1136	CLA	C1B-NB	-3.66	1.33	1.37
14	H	1227	CLA	C1D-ND	-3.66	1.33	1.37
14	a	1132	CLA	C1D-ND	-3.66	1.33	1.37
14	a	1120	CLA	CHD-C1D	3.66	1.45	1.38
14	a	1102	CLA	CHD-C4C	3.66	1.47	1.39
14	G	1139	CLA	C1D-ND	-3.66	1.33	1.37
14	G	1116	CLA	CHD-C4C	3.66	1.47	1.39
14	H	1239	CLA	CHD-C4C	3.66	1.47	1.39
14	A	1120	CLA	CHD-C1D	3.66	1.45	1.38
14	A	1103	CLA	C1D-ND	-3.66	1.33	1.37
14	B	1226	CLA	MG-ND	-3.66	1.98	2.05
14	A	1101	CLA	CHC-C4B	3.66	1.47	1.39
18	A	4011	BCR	C11-C12	-3.66	1.25	1.34
14	G	1101	CLA	CHD-C4C	3.66	1.47	1.39
18	H	4005	BCR	C11-C12	-3.66	1.25	1.34
14	a	1107	CLA	C1D-ND	-3.66	1.33	1.37
14	H	1209	CLA	CHC-C4B	3.66	1.47	1.39
14	G	1132	CLA	CHD-C4C	3.65	1.47	1.39
18	a	4001	BCR	C11-C12	-3.65	1.25	1.34
15	B	1238	F6C	C1D-ND	-3.65	1.32	1.37
14	H	1218	CLA	CHD-C1D	3.65	1.45	1.38
15	b	1238	F6C	C1D-ND	-3.65	1.32	1.37
14	G	1013	CLA	CHC-C4B	3.65	1.47	1.39
14	A	1133	CLA	CHD-C4C	3.65	1.47	1.39
14	G	1133	CLA	C1D-ND	-3.65	1.33	1.37
13	a	1011	CL0	CHC-C1C	3.65	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1127	CLA	C1B-NB	-3.65	1.33	1.37
14	b	1206	CLA	MG-ND	-3.65	1.98	2.05
14	b	1213	CLA	CHD-C4C	3.65	1.47	1.39
20	B	5002	LMG	O7-C10	3.65	1.44	1.34
14	b	1204	CLA	MG-ND	-3.65	1.98	2.05
14	A	1101	CLA	CHD-C4C	3.65	1.47	1.39
14	B	1201	CLA	C1D-ND	-3.65	1.33	1.37
14	H	1233	CLA	CHC-C4B	3.65	1.47	1.39
14	a	1118	CLA	C1D-ND	-3.65	1.33	1.37
14	H	1023	CLA	CHD-C1D	3.65	1.45	1.38
14	B	1210	CLA	C1D-ND	-3.65	1.33	1.37
14	b	1228	CLA	C1D-ND	-3.65	1.33	1.37
14	A	1125	CLA	MG-ND	-3.65	1.98	2.05
14	B	1224	CLA	MG-ND	-3.65	1.98	2.05
14	a	1122	CLA	C1D-ND	-3.65	1.33	1.37
14	a	1116	CLA	CHD-C4C	3.65	1.47	1.39
14	a	1125	CLA	MG-ND	-3.65	1.98	2.05
14	b	1218	CLA	CHD-C1D	3.64	1.45	1.38
14	A	1111	CLA	CHD-C4C	3.64	1.47	1.39
14	G	1111	CLA	CHD-C4C	3.64	1.47	1.39
14	A	1116	CLA	CHC-C4B	3.64	1.47	1.39
14	b	1208	CLA	CHD-C4C	3.64	1.47	1.39
14	A	1013	CLA	CHC-C4B	3.64	1.47	1.39
14	b	1239	CLA	CHD-C4C	3.64	1.47	1.39
14	B	1217	CLA	CHC-C4B	3.64	1.47	1.39
18	m	4021	BCR	C11-C12	-3.64	1.25	1.34
14	b	1211	CLA	CHD-C4C	3.64	1.47	1.39
14	B	1209	CLA	CHC-C4B	3.64	1.47	1.39
18	G	4001	BCR	C11-C12	-3.64	1.25	1.34
14	a	1115	CLA	C1D-ND	-3.64	1.33	1.37
14	a	1139	CLA	C1D-ND	-3.64	1.33	1.37
14	B	1211	CLA	CHD-C4C	3.64	1.47	1.39
20	b	5002	LMG	O7-C10	3.64	1.44	1.34
14	H	1217	CLA	CHB-C1B	3.64	1.47	1.39
18	a	4011	BCR	C11-C12	-3.64	1.25	1.34
14	b	1213	CLA	CHC-C4B	3.64	1.47	1.39
14	H	1213	CLA	CHC-C4B	3.64	1.47	1.39
14	H	1219	CLA	CHC-C4B	3.64	1.47	1.39
14	b	1023	CLA	CHD-C1D	3.64	1.45	1.38
14	a	1111	CLA	CHD-C4C	3.64	1.47	1.39
14	B	1239	CLA	CHD-C4C	3.64	1.47	1.39
14	a	1116	CLA	CHC-C4B	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1109	CLA	C1D-ND	-3.63	1.33	1.37
14	H	1203	CLA	CHD-C1D	3.63	1.45	1.38
14	H	1202	CLA	CHD-C1D	3.63	1.45	1.38
14	H	1204	CLA	MG-ND	-3.63	1.98	2.05
14	B	1218	CLA	CHB-C1B	3.63	1.47	1.39
18	A	4001	BCR	C11-C12	-3.63	1.25	1.34
14	B	1221	CLA	C1B-NB	-3.63	1.33	1.37
14	A	1129	CLA	C1B-NB	-3.63	1.33	1.37
14	b	1219	CLA	CHC-C4B	3.63	1.47	1.39
14	H	1228	CLA	C1D-ND	-3.63	1.33	1.37
13	A	1011	CL0	CHC-C1C	3.63	1.46	1.39
14	a	1013	CLA	CHC-C4B	3.63	1.47	1.39
14	A	1107	CLA	C1D-ND	-3.63	1.33	1.37
14	k	1401	CLA	CHB-C1B	3.63	1.47	1.39
14	G	1116	CLA	CHC-C4B	3.63	1.47	1.39
14	H	1206	CLA	CHD-C4C	3.63	1.47	1.39
14	G	1107	CLA	C1D-ND	-3.63	1.33	1.37
14	B	1023	CLA	CHD-C1D	3.63	1.45	1.38
14	B	1217	CLA	CHB-C1B	3.63	1.47	1.39
14	W	1701	CLA	CHD-C4C	3.63	1.47	1.39
14	B	1228	CLA	C1D-ND	-3.63	1.33	1.37
14	b	1217	CLA	CHB-C1B	3.63	1.47	1.39
14	A	1126	CLA	CHD-C4C	3.62	1.47	1.39
14	G	1105	CLA	C1D-ND	-3.62	1.33	1.37
14	B	1202	CLA	CHD-C1D	3.62	1.45	1.38
14	b	1223	CLA	CHC-C4B	3.62	1.47	1.39
14	B	1204	CLA	MG-ND	-3.62	1.98	2.05
14	A	1122	CLA	C1D-ND	-3.62	1.33	1.37
20	G	5005	LMG	C37-C36	-3.62	1.33	1.51
15	B	1238	F6C	CHC-C1C	3.62	1.47	1.39
14	G	1104	CLA	CHD-C1D	3.62	1.45	1.38
14	b	1023	CLA	MG-ND	-3.62	1.98	2.05
14	B	1231	CLA	CHC-C4B	3.62	1.47	1.39
14	H	1226	CLA	MG-ND	-3.62	1.98	2.05
14	B	1214	CLA	C1B-NB	-3.62	1.33	1.37
18	L	4019	BCR	C11-C12	-3.62	1.25	1.34
14	G	1127	CLA	C1B-NB	-3.62	1.33	1.37
14	a	1123	CLA	C1B-NB	-3.62	1.33	1.37
14	G	1108	CLA	OBD-CAD	3.62	1.28	1.22
14	a	1136	CLA	C1B-NB	-3.62	1.33	1.37
14	G	1126	CLA	CHD-C4C	3.62	1.47	1.39
20	A	5005	LMG	C37-C36	-3.62	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1231	CLA	CHD-C4C	3.62	1.47	1.39
14	b	1206	CLA	CHD-C4C	3.62	1.47	1.39
14	H	1213	CLA	CHD-C4C	3.62	1.47	1.39
14	A	1109	CLA	C1D-ND	-3.62	1.33	1.37
14	G	1101	CLA	CHC-C4B	3.61	1.47	1.39
14	b	1217	CLA	CHC-C4B	3.61	1.47	1.39
18	V	4021	BCR	C11-C12	-3.61	1.25	1.34
14	H	1221	CLA	C1B-NB	-3.61	1.33	1.37
18	G	4011	BCR	C11-C12	-3.61	1.25	1.34
14	H	1231	CLA	CHC-C4B	3.61	1.47	1.39
14	b	1202	CLA	CHD-C1D	3.61	1.45	1.38
14	b	1214	CLA	C1D-ND	-3.61	1.33	1.37
14	K	1401	CLA	CHB-C1B	3.61	1.47	1.39
14	A	1125	CLA	C4B-NB	-3.61	1.33	1.37
14	B	1021	CLA	C1B-NB	-3.61	1.33	1.37
20	a	5005	LMG	C37-C36	-3.61	1.33	1.51
14	A	1104	CLA	CHD-C1D	3.61	1.45	1.38
14	H	1211	CLA	CHD-C4C	3.61	1.47	1.39
14	H	1223	CLA	CHC-C4B	3.61	1.47	1.39
14	B	1223	CLA	CHC-C4B	3.61	1.47	1.39
14	X	1701	CLA	CHD-C4C	3.61	1.47	1.39
14	a	1101	CLA	CHC-C4B	3.61	1.47	1.39
14	A	1105	CLA	C1D-ND	-3.60	1.33	1.37
14	G	1119	CLA	C1C-NC	-3.60	1.32	1.37
14	B	1213	CLA	CHC-C4B	3.60	1.47	1.39
13	G	1011	CL0	CHC-C1C	3.60	1.46	1.39
14	A	1139	CLA	C1D-ND	-3.60	1.33	1.37
18	l	4019	BCR	C11-C12	-3.60	1.25	1.34
18	U	4019	BCR	C11-C12	-3.60	1.25	1.34
14	b	1231	CLA	CHC-C4B	3.60	1.47	1.39
14	H	1021	CLA	C1B-NB	-3.60	1.33	1.37
14	H	1214	CLA	C1D-ND	-3.60	1.33	1.37
14	a	1117	CLA	C1B-NB	-3.60	1.33	1.37
14	a	1126	CLA	C4B-NB	-3.60	1.33	1.37
14	A	1127	CLA	C1B-NB	-3.60	1.33	1.37
14	b	1231	CLA	CHD-C4C	3.60	1.47	1.39
15	B	1230	F6C	CHB-C1B	3.60	1.47	1.39
14	H	1205	CLA	C1B-NB	-3.60	1.33	1.37
14	T	1401	CLA	CHB-C1B	3.60	1.47	1.39
14	A	1110	CLA	CHD-C4C	3.60	1.47	1.39
14	A	1118	CLA	CHC-C4B	3.59	1.47	1.39
15	b	1230	F6C	CHB-C1B	3.59	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1203	CLA	CHD-C1D	3.59	1.45	1.38
14	a	1105	CLA	C1D-ND	-3.59	1.33	1.37
14	H	1220	CLA	CHD-C4C	3.59	1.47	1.39
14	b	1218	CLA	CHB-C1B	3.59	1.47	1.39
14	a	1104	CLA	CHD-C1D	3.59	1.45	1.38
14	b	1210	CLA	OBD-CAD	3.59	1.28	1.22
14	G	1123	CLA	C1B-NB	-3.59	1.33	1.37
14	H	1206	CLA	MG-ND	-3.59	1.98	2.05
14	G	1122	CLA	C1D-ND	-3.59	1.33	1.37
14	B	1022	CLA	CHC-C4B	3.59	1.47	1.39
15	b	1238	F6C	CHC-C1C	3.59	1.47	1.39
14	H	1023	CLA	MG-ND	-3.59	1.98	2.05
14	A	1136	CLA	C1B-NB	-3.59	1.33	1.37
14	x	1701	CLA	CHD-C4C	3.59	1.47	1.39
14	x	1701	CLA	CHB-C1B	3.59	1.47	1.39
14	B	1023	CLA	MG-ND	-3.59	1.98	2.05
14	B	1206	CLA	CHD-C4C	3.59	1.47	1.39
14	A	1125	CLA	C3C-C2C	3.59	1.44	1.36
14	U	1503	CLA	CHD-C4C	3.59	1.47	1.39
14	H	1215	CLA	C1B-NB	-3.58	1.33	1.37
14	A	1123	CLA	C1B-NB	-3.58	1.33	1.37
14	a	1108	CLA	OBD-CAD	3.58	1.28	1.22
14	G	1109	CLA	C1D-ND	-3.58	1.33	1.37
15	B	1238	F6C	C1C-NC	-3.58	1.33	1.37
14	b	1239	CLA	CHB-C1B	3.58	1.47	1.39
14	H	1217	CLA	CHD-C4C	3.58	1.47	1.39
14	b	1222	CLA	CHC-C4B	3.58	1.47	1.39
14	b	1217	CLA	CHD-C4C	3.58	1.47	1.39
14	H	1222	CLA	CHC-C4B	3.58	1.47	1.39
14	A	1139	CLA	CHB-C1B	3.58	1.47	1.39
14	K	1401	CLA	OBD-CAD	3.58	1.28	1.22
14	X	1701	CLA	CHB-C1B	3.58	1.47	1.39
14	B	1217	CLA	CHD-C4C	3.58	1.47	1.39
14	H	1022	CLA	CHC-C4B	3.58	1.47	1.39
14	a	1139	CLA	CHB-C1B	3.58	1.47	1.39
14	B	1218	CLA	MG-ND	-3.58	1.98	2.05
14	a	1125	CLA	C3C-C2C	3.58	1.44	1.36
14	B	1210	CLA	OBD-CAD	3.58	1.28	1.22
14	B	1215	CLA	C1B-NB	-3.58	1.33	1.37
15	H	1238	F6C	CHC-C1C	3.58	1.47	1.39
14	b	1220	CLA	CHD-C4C	3.58	1.47	1.39
14	b	1224	CLA	C1B-NB	-3.58	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	OBD-CAD	3.58	1.28	1.22
14	G	1114	CLA	OBD-CAD	3.58	1.28	1.22
14	b	1218	CLA	MG-ND	-3.58	1.98	2.05
14	B	1231	CLA	CHD-C4C	3.57	1.47	1.39
14	A	1124	CLA	CHC-C4B	3.57	1.47	1.39
14	G	1103	CLA	CHD-C4C	3.57	1.47	1.39
15	H	1230	F6C	CHB-C1B	3.57	1.47	1.39
14	B	1236	CLA	CHD-C4C	3.57	1.47	1.39
14	A	1114	CLA	OBD-CAD	3.57	1.28	1.22
14	b	1022	CLA	CHC-C4B	3.57	1.47	1.39
14	B	1239	CLA	CHB-C1B	3.57	1.47	1.39
14	G	1117	CLA	C1D-ND	-3.57	1.33	1.37
14	B	1203	CLA	CHD-C1D	3.57	1.45	1.38
14	a	1135	CLA	CHD-C4C	3.57	1.47	1.39
14	A	1113	CLA	CHD-C4C	3.57	1.47	1.39
14	b	1231	CLA	OBD-CAD	3.57	1.28	1.22
14	B	1022	CLA	MG-ND	-3.57	1.98	2.05
14	H	1231	CLA	OBD-CAD	3.57	1.28	1.22
14	B	1206	CLA	MG-ND	-3.57	1.98	2.05
14	H	1218	CLA	CHB-C1B	3.57	1.47	1.39
14	L	1503	CLA	CHD-C4C	3.57	1.47	1.39
14	l	1503	CLA	CHD-C4C	3.57	1.47	1.39
14	H	1225	CLA	MG-ND	-3.57	1.98	2.05
14	G	1134	CLA	CHB-C1B	3.57	1.47	1.39
14	W	1701	CLA	CHB-C1B	3.57	1.47	1.39
14	H	1218	CLA	MG-ND	-3.57	1.98	2.05
14	B	1220	CLA	CHD-C4C	3.57	1.47	1.39
14	T	1401	CLA	OBD-CAD	3.56	1.28	1.22
14	G	1115	CLA	CHC-C4B	3.56	1.47	1.39
14	H	1239	CLA	CHB-C1B	3.56	1.47	1.39
14	G	1129	CLA	CHD-C4C	3.56	1.47	1.39
14	G	1135	CLA	CHD-C4C	3.56	1.47	1.39
14	G	1120	CLA	CHB-C1B	3.56	1.47	1.39
15	B	1238	F6C	CHD-C1D	3.56	1.45	1.38
14	G	1129	CLA	C1B-NB	-3.56	1.33	1.37
15	H	1238	F6C	C1C-NC	-3.56	1.33	1.37
14	a	1120	CLA	CHB-C1B	3.56	1.47	1.39
14	H	1223	CLA	C1D-ND	-3.56	1.33	1.37
14	a	1118	CLA	CHC-C4B	3.56	1.47	1.39
14	a	1110	CLA	CHD-C4C	3.56	1.47	1.39
14	a	1106	CLA	CHC-C4B	3.56	1.47	1.39
14	a	1104	CLA	C1B-NB	-3.56	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1222	CLA	CHC-C4B	3.56	1.47	1.39
15	H	1238	F6C	CHD-C1D	3.56	1.45	1.38
14	G	1124	CLA	CHC-C4B	3.56	1.47	1.39
14	G	1113	CLA	CHD-C4C	3.56	1.47	1.39
14	A	1134	CLA	CHB-C1B	3.56	1.47	1.39
14	G	1110	CLA	CHD-C4C	3.56	1.47	1.39
14	H	1022	CLA	MG-ND	-3.56	1.98	2.05
14	U	1501	CLA	C1B-NB	-3.56	1.33	1.37
14	b	1208	CLA	CHC-C4B	3.56	1.47	1.39
14	G	1139	CLA	CHB-C1B	3.55	1.47	1.39
14	G	1137	CLA	C4B-NB	-3.55	1.33	1.37
14	G	1118	CLA	CHC-C4B	3.55	1.47	1.39
14	G	1125	CLA	C3C-C2C	3.55	1.44	1.36
14	b	1233	CLA	OBD-CAD	3.55	1.28	1.22
14	b	1221	CLA	C1B-NB	-3.55	1.33	1.37
14	a	1124	CLA	CHC-C4B	3.55	1.47	1.39
14	A	1120	CLA	CHB-C1B	3.55	1.47	1.39
14	B	1231	CLA	OBD-CAD	3.55	1.28	1.22
14	B	1205	CLA	C1B-NB	-3.55	1.33	1.37
14	G	1012	CLA	CHD-C4C	3.55	1.47	1.39
14	a	1114	CLA	OBD-CAD	3.55	1.28	1.22
14	A	1115	CLA	CHC-C4B	3.55	1.47	1.39
14	A	1130	CLA	CHD-C4C	3.55	1.47	1.39
14	A	1102	CLA	CHC-C4B	3.55	1.47	1.39
14	B	1208	CLA	CHC-C4B	3.55	1.47	1.39
15	b	1238	F6C	CHD-C1D	3.55	1.45	1.38
14	b	1234	CLA	C1B-NB	-3.55	1.33	1.37
14	a	1102	CLA	CHC-C4B	3.55	1.47	1.39
14	A	1106	CLA	CHC-C4B	3.55	1.47	1.39
14	L	1502	CLA	CHC-C4B	3.55	1.47	1.39
14	G	1106	CLA	CHC-C4B	3.55	1.47	1.39
14	G	1132	CLA	CHC-C4B	3.55	1.47	1.39
14	A	1111	CLA	C1D-ND	-3.55	1.33	1.37
14	A	1126	CLA	C1B-NB	-3.54	1.33	1.37
14	B	1233	CLA	CHB-C1B	3.54	1.47	1.39
14	a	1113	CLA	CHD-C4C	3.54	1.47	1.39
14	H	1222	CLA	CHD-C4C	3.54	1.47	1.39
14	a	1103	CLA	CHD-C4C	3.54	1.47	1.39
14	a	1130	CLA	CHD-C4C	3.54	1.47	1.39
14	B	1233	CLA	OBD-CAD	3.54	1.28	1.22
14	H	1236	CLA	CHD-C4C	3.54	1.47	1.39
14	b	1223	CLA	C1D-ND	-3.54	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1102	CLA	CHC-C4B	3.54	1.47	1.39
14	a	1115	CLA	CHC-C4B	3.54	1.47	1.39
14	G	1111	CLA	C1D-ND	-3.54	1.33	1.37
15	b	1238	F6C	C1C-NC	-3.54	1.33	1.37
14	H	1206	CLA	C1C-NC	-3.54	1.32	1.37
14	k	1401	CLA	OBD-CAD	3.54	1.28	1.22
14	H	1208	CLA	CHC-C4B	3.54	1.47	1.39
14	G	1126	CLA	C1B-NB	-3.54	1.33	1.37
14	A	1104	CLA	C1B-NB	-3.54	1.33	1.37
14	a	1012	CLA	CHD-C4C	3.54	1.47	1.39
14	b	1225	CLA	MG-ND	-3.54	1.98	2.05
14	A	1106	CLA	CHD-C4C	3.54	1.47	1.39
14	l	1501	CLA	C1B-NB	-3.54	1.33	1.37
14	L	1501	CLA	C1B-NB	-3.54	1.33	1.37
14	b	1211	CLA	CHC-C4B	3.54	1.47	1.39
14	H	1224	CLA	C1B-NB	-3.54	1.33	1.37
14	b	1236	CLA	CHD-C4C	3.53	1.47	1.39
14	b	1233	CLA	CHB-C1B	3.53	1.47	1.39
14	a	1129	CLA	CHD-C4C	3.53	1.47	1.39
14	b	1222	CLA	CHD-C4C	3.53	1.47	1.39
14	A	1135	CLA	CHD-C4C	3.53	1.47	1.39
14	B	1222	CLA	CHD-C4C	3.53	1.47	1.39
14	A	1103	CLA	CHD-C4C	3.53	1.47	1.39
14	H	1235	CLA	CHC-C4B	3.53	1.47	1.39
14	B	1211	CLA	CHC-C4B	3.53	1.47	1.39
14	G	1123	CLA	CHB-C1B	3.53	1.47	1.39
14	A	1012	CLA	CHD-C4C	3.53	1.47	1.39
14	H	1202	CLA	CHC-C4B	3.53	1.47	1.39
14	G	1117	CLA	C1B-NB	-3.53	1.33	1.37
14	b	1022	CLA	MG-ND	-3.53	1.98	2.05
14	B	1224	CLA	C1B-NB	-3.53	1.33	1.37
14	G	1137	CLA	CHD-C4C	3.53	1.47	1.39
14	G	1108	CLA	C1D-ND	-3.53	1.33	1.37
14	A	1107	CLA	CHB-C1B	3.53	1.47	1.39
14	A	1117	CLA	C1D-ND	-3.53	1.33	1.37
14	B	1223	CLA	C1D-ND	-3.53	1.33	1.37
14	A	1117	CLA	C1B-NB	-3.53	1.33	1.37
18	H	4016	BCR	C11-C12	-3.53	1.25	1.34
14	a	1123	CLA	CHB-C1B	3.53	1.47	1.39
14	W	1701	CLA	C1D-ND	-3.52	1.33	1.37
14	H	1210	CLA	OBD-CAD	3.52	1.28	1.22
14	G	1125	CLA	C1B-NB	-3.52	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1137	CLA	C4B-NB	-3.52	1.33	1.37
14	B	1219	CLA	OBD-CAD	3.52	1.28	1.22
14	l	1502	CLA	CHC-C4B	3.52	1.47	1.39
14	H	1233	CLA	OBD-CAD	3.52	1.28	1.22
14	B	1225	CLA	MG-ND	-3.52	1.98	2.05
14	G	1106	CLA	CHD-C4C	3.52	1.47	1.39
14	H	1219	CLA	OBD-CAD	3.52	1.28	1.22
14	a	1134	CLA	CHB-C1B	3.52	1.47	1.39
14	U	1502	CLA	CHC-C4B	3.52	1.47	1.39
14	b	1232	CLA	CHC-C4B	3.52	1.47	1.39
14	A	1111	CLA	CHC-C4B	3.52	1.47	1.39
14	B	1221	CLA	MG-ND	-3.52	1.98	2.05
14	X	1701	CLA	C1D-ND	-3.52	1.33	1.37
14	a	1138	CLA	CHC-C4B	3.52	1.47	1.39
14	A	1129	CLA	CHD-C4C	3.52	1.47	1.39
14	a	1107	CLA	CHD-C4C	3.52	1.47	1.39
14	B	1211	CLA	C1D-ND	-3.52	1.33	1.37
14	H	1211	CLA	CHC-C4B	3.52	1.47	1.39
14	B	1231	CLA	CHB-C1B	3.52	1.47	1.39
14	G	1130	CLA	CHD-C4C	3.52	1.47	1.39
14	a	1108	CLA	C1D-ND	-3.52	1.33	1.37
14	b	1202	CLA	CHC-C4B	3.52	1.47	1.39
14	a	1125	CLA	C1B-NB	-3.51	1.33	1.37
14	B	1021	CLA	CHD-C1D	3.51	1.45	1.38
14	a	1132	CLA	CHC-C4B	3.51	1.47	1.39
14	H	1211	CLA	C1D-ND	-3.51	1.33	1.37
14	H	1232	CLA	CHC-C4B	3.51	1.47	1.39
14	a	1111	CLA	C1D-ND	-3.51	1.33	1.37
14	G	1138	CLA	CHC-C4B	3.51	1.47	1.39
14	b	1235	CLA	CHC-C4B	3.51	1.47	1.39
14	A	1138	CLA	CHC-C4B	3.51	1.47	1.39
14	G	1107	CLA	CHD-C4C	3.51	1.47	1.39
14	a	1103	CLA	C1B-NB	-3.51	1.33	1.37
14	H	1231	CLA	CHB-C1B	3.51	1.47	1.39
14	B	1235	CLA	CHC-C4B	3.51	1.47	1.39
14	A	1132	CLA	CHC-C4B	3.51	1.47	1.39
14	G	1107	CLA	CHB-C1B	3.51	1.47	1.39
14	B	1234	CLA	C1B-NB	-3.51	1.33	1.37
14	G	1120	CLA	CHC-C4B	3.51	1.47	1.39
14	a	1111	CLA	CHC-C4B	3.51	1.47	1.39
14	H	1223	CLA	C1B-NB	-3.51	1.33	1.37
14	l	1503	CLA	CHB-C1B	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1106	CLA	CHD-C4C	3.51	1.47	1.39
14	A	1110	CLA	CHB-C1B	3.51	1.47	1.39
14	a	1132	CLA	OBD-CAD	3.51	1.28	1.22
14	A	1126	CLA	C4B-NB	-3.51	1.33	1.37
14	H	1234	CLA	C1B-NB	-3.50	1.33	1.37
14	H	1233	CLA	CHB-C1B	3.50	1.47	1.39
14	A	1133	CLA	CHB-C1B	3.50	1.47	1.39
14	a	1137	CLA	CHD-C4C	3.50	1.47	1.39
14	a	1107	CLA	CHB-C1B	3.50	1.47	1.39
14	A	1137	CLA	C4B-NB	-3.50	1.33	1.37
14	A	1137	CLA	CHD-C4C	3.50	1.47	1.39
14	A	1105	CLA	OBD-CAD	3.50	1.28	1.22
14	b	1206	CLA	C1C-NC	-3.50	1.32	1.37
14	b	1221	CLA	MG-ND	-3.50	1.98	2.05
18	B	4016	BCR	C11-C12	-3.50	1.25	1.34
14	B	1206	CLA	C1C-NC	-3.50	1.32	1.37
14	b	1205	CLA	C1B-NB	-3.50	1.33	1.37
14	b	1219	CLA	OBD-CAD	3.50	1.28	1.22
14	H	1221	CLA	MG-ND	-3.50	1.98	2.05
14	A	1123	CLA	CHB-C1B	3.50	1.47	1.39
14	H	1210	CLA	C1B-NB	-3.49	1.33	1.37
14	a	1117	CLA	C1D-ND	-3.49	1.33	1.37
14	G	1108	CLA	CHC-C4B	3.49	1.47	1.39
14	b	1211	CLA	C1D-ND	-3.49	1.33	1.37
14	B	1232	CLA	CHC-C4B	3.49	1.47	1.39
14	b	1212	CLA	CHC-C4B	3.49	1.47	1.39
14	b	1232	CLA	OBD-CAD	3.49	1.28	1.22
14	A	1108	CLA	CHC-C4B	3.49	1.47	1.39
14	x	1701	CLA	C1D-ND	-3.49	1.33	1.37
14	a	1120	CLA	CHC-C4B	3.49	1.47	1.39
14	A	1120	CLA	CHC-C4B	3.49	1.47	1.39
14	G	1104	CLA	C1B-NB	-3.49	1.33	1.37
14	A	1127	CLA	CHB-C1B	3.49	1.47	1.39
14	b	1231	CLA	CHB-C1B	3.49	1.47	1.39
14	B	1202	CLA	CHC-C4B	3.49	1.47	1.39
14	H	1022	CLA	C1B-NB	-3.49	1.33	1.37
14	A	1103	CLA	C1B-NB	-3.49	1.33	1.37
14	A	1125	CLA	C1B-NB	-3.49	1.33	1.37
14	a	1126	CLA	C1B-NB	-3.49	1.33	1.37
14	H	1021	CLA	CHD-C1D	3.49	1.45	1.38
18	b	4016	BCR	C11-C12	-3.49	1.25	1.34
14	B	1022	CLA	C1B-NB	-3.49	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1105	CLA	OBD-CAD	3.49	1.28	1.22
14	b	1216	CLA	C1D-ND	-3.49	1.33	1.37
14	A	1114	CLA	C1B-NB	-3.49	1.33	1.37
14	A	1104	CLA	CHD-C4C	3.48	1.47	1.39
14	G	1111	CLA	CHC-C4B	3.48	1.47	1.39
15	B	1207	F6C	CHD-C4C	3.48	1.47	1.39
15	B	1230	F6C	OBD-CAD	3.48	1.28	1.22
14	a	1140	CLA	CHB-C1B	3.48	1.47	1.39
14	L	1503	CLA	CHB-C1B	3.48	1.47	1.39
14	A	1107	CLA	CHD-C4C	3.48	1.47	1.39
14	B	1205	CLA	MG-ND	-3.48	1.98	2.05
14	A	1108	CLA	C1D-ND	-3.48	1.33	1.37
14	a	1127	CLA	CHB-C1B	3.48	1.47	1.39
14	B	1227	CLA	C1B-NB	-3.48	1.33	1.37
14	G	1140	CLA	CHB-C1B	3.47	1.47	1.39
14	b	1216	CLA	OBD-CAD	3.47	1.28	1.22
14	G	1136	CLA	CHC-C4B	3.47	1.47	1.39
14	H	1212	CLA	CHB-C1B	3.47	1.47	1.39
15	a	1121	F6C	C1C-NC	-3.47	1.33	1.37
14	a	1105	CLA	OBD-CAD	3.47	1.28	1.22
14	A	1136	CLA	CHC-C4B	3.47	1.47	1.39
14	B	1021	CLA	CHB-C1B	3.47	1.47	1.39
14	a	1130	CLA	MG-ND	-3.47	1.98	2.05
14	G	1012	CLA	C1B-NB	-3.47	1.33	1.37
14	H	1216	CLA	C1D-ND	-3.47	1.33	1.37
14	a	1110	CLA	CHB-C1B	3.47	1.47	1.39
14	b	1021	CLA	CHB-C1B	3.47	1.47	1.39
14	H	1234	CLA	CHD-C1D	3.47	1.45	1.38
14	B	1216	CLA	OBD-CAD	3.47	1.28	1.22
14	b	1234	CLA	CHD-C1D	3.47	1.45	1.38
14	a	1136	CLA	CHC-C4B	3.47	1.47	1.39
14	B	1234	CLA	CHD-C1D	3.47	1.45	1.38
14	H	1212	CLA	CHC-C4B	3.47	1.47	1.39
14	U	1503	CLA	CHB-C1B	3.46	1.47	1.39
14	A	1140	CLA	CHB-C1B	3.46	1.47	1.39
15	b	1207	F6C	CHD-C4C	3.46	1.47	1.39
14	a	1114	CLA	C1B-NB	-3.46	1.33	1.37
14	b	1022	CLA	C1B-NB	-3.46	1.33	1.37
14	b	1225	CLA	CHC-C4B	3.46	1.47	1.39
14	b	1021	CLA	CHD-C1D	3.46	1.45	1.38
14	G	1132	CLA	OBD-CAD	3.46	1.28	1.22
14	a	1102	CLA	C1B-NB	-3.46	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1012	CLA	C1B-NB	-3.46	1.33	1.37
14	A	1111	CLA	C1B-NB	-3.46	1.33	1.37
14	G	1133	CLA	CHB-C1B	3.46	1.47	1.39
14	b	1212	CLA	CHB-C1B	3.46	1.47	1.39
14	B	1212	CLA	CHC-C4B	3.46	1.47	1.39
14	a	1120	CLA	CHD-C4C	3.46	1.47	1.39
14	A	1115	CLA	CHB-C1B	3.46	1.47	1.39
14	b	1227	CLA	CHC-C4B	3.46	1.47	1.39
14	A	1120	CLA	CHD-C4C	3.46	1.47	1.39
14	a	1115	CLA	OBD-CAD	3.46	1.28	1.22
14	H	1205	CLA	MG-ND	-3.46	1.98	2.05
14	B	1227	CLA	CHC-C4B	3.46	1.47	1.39
14	a	1012	CLA	C1B-NB	-3.46	1.33	1.37
14	G	1130	CLA	MG-ND	-3.46	1.98	2.05
14	G	1110	CLA	CHB-C1B	3.46	1.47	1.39
14	H	1021	CLA	CHB-C1B	3.46	1.47	1.39
14	H	1225	CLA	CHC-C4B	3.46	1.47	1.39
14	a	1108	CLA	CHC-C4B	3.46	1.47	1.39
14	H	1232	CLA	OBD-CAD	3.46	1.28	1.22
14	a	1133	CLA	CHB-C1B	3.45	1.47	1.39
14	A	1126	CLA	MG-ND	-3.45	1.98	2.05
15	b	1237	F6C	C1D-ND	-3.45	1.32	1.37
14	A	1104	CLA	CHB-C1B	3.45	1.47	1.39
14	b	1223	CLA	C1B-NB	-3.45	1.33	1.37
14	A	1112	CLA	OBD-CAD	3.45	1.28	1.22
14	a	1012	CLA	C4B-NB	-3.45	1.33	1.37
14	G	1126	CLA	C4B-NB	-3.45	1.33	1.37
13	a	1011	CL0	MG-ND	-3.45	1.98	2.05
14	A	1137	CLA	MG-ND	-3.45	1.98	2.05
13	G	1011	CL0	MG-ND	-3.45	1.98	2.05
14	A	1130	CLA	MG-ND	-3.45	1.98	2.05
14	B	1223	CLA	C1B-NB	-3.45	1.33	1.37
14	a	1107	CLA	CHC-C4B	3.45	1.47	1.39
14	A	1132	CLA	OBD-CAD	3.45	1.28	1.22
14	a	1123	CLA	MG-ND	-3.45	1.99	2.05
14	G	1103	CLA	C1B-NB	-3.45	1.33	1.37
15	H	1207	F6C	CHD-C4C	3.45	1.47	1.39
14	H	1226	CLA	C1C-NC	-3.45	1.32	1.37
14	A	1133	CLA	OBD-CAD	3.45	1.28	1.22
14	H	1216	CLA	OBD-CAD	3.45	1.28	1.22
14	b	1210	CLA	CHC-C4B	3.45	1.47	1.39
14	A	1104	CLA	CHC-C4B	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1114	CLA	C1B-NB	-3.44	1.33	1.37
14	b	1211	CLA	C1B-NB	-3.44	1.33	1.37
14	G	1107	CLA	CHC-C4B	3.44	1.47	1.39
14	G	1120	CLA	CHD-C4C	3.44	1.47	1.39
14	G	1123	CLA	CHD-C4C	3.44	1.47	1.39
14	G	1127	CLA	CHB-C1B	3.44	1.47	1.39
15	H	1230	F6C	OBD-CAD	3.44	1.28	1.22
14	G	1123	CLA	MG-ND	-3.44	1.99	2.05
14	H	1023	CLA	CHD-C4C	3.44	1.47	1.39
14	H	1227	CLA	CHC-C4B	3.44	1.47	1.39
14	a	1125	CLA	CHD-C1D	3.44	1.45	1.38
14	a	1101	CLA	CHB-C1B	3.44	1.47	1.39
14	a	1104	CLA	CHC-C4B	3.44	1.47	1.39
14	B	1232	CLA	OBD-CAD	3.44	1.28	1.22
14	b	1218	CLA	C1B-NB	-3.44	1.33	1.37
14	a	1125	CLA	CHB-C1B	3.44	1.47	1.39
14	G	1104	CLA	CHD-C4C	3.44	1.47	1.39
14	B	1218	CLA	C1B-NB	-3.44	1.33	1.37
14	a	1112	CLA	OBD-CAD	3.44	1.28	1.22
14	G	1111	CLA	C1B-NB	-3.44	1.33	1.37
14	G	1112	CLA	OBD-CAD	3.44	1.28	1.22
14	U	1501	CLA	CHB-C1B	3.44	1.47	1.39
18	H	4006	BCR	C11-C12	-3.44	1.25	1.34
14	G	1122	CLA	C1C-NC	-3.44	1.32	1.37
14	b	1205	CLA	C1C-NC	-3.44	1.32	1.37
14	a	1104	CLA	CHD-C4C	3.44	1.47	1.39
14	b	1210	CLA	C1B-NB	-3.44	1.33	1.37
18	b	4006	BCR	C11-C12	-3.44	1.25	1.34
14	B	1225	CLA	CHC-C4B	3.44	1.47	1.39
14	a	1123	CLA	CHC-C4B	3.44	1.47	1.39
14	B	1227	CLA	OBD-CAD	3.44	1.28	1.22
14	B	1212	CLA	CHB-C1B	3.44	1.47	1.39
14	H	1218	CLA	C1B-NB	-3.44	1.33	1.37
14	H	1227	CLA	C1B-NB	-3.44	1.33	1.37
14	H	1229	CLA	C1D-ND	-3.44	1.33	1.37
14	G	1104	CLA	CHC-C4B	3.44	1.47	1.39
14	H	1210	CLA	CHC-C4B	3.44	1.47	1.39
14	G	1133	CLA	OBD-CAD	3.44	1.28	1.22
14	G	1126	CLA	MG-ND	-3.44	1.99	2.05
15	G	1121	F6C	C1C-NC	-3.44	1.33	1.37
14	H	1208	CLA	CHB-C1B	3.44	1.47	1.39
14	a	1126	CLA	MG-ND	-3.43	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1115	CLA	CHB-C1B	3.43	1.47	1.39
14	G	1123	CLA	CHC-C4B	3.43	1.47	1.39
14	a	1109	CLA	CHB-C1B	3.43	1.47	1.39
14	a	1111	CLA	C1B-NB	-3.43	1.33	1.37
14	B	1023	CLA	CHD-C4C	3.43	1.47	1.39
13	G	1011	CL0	C3B-C2B	3.43	1.45	1.40
14	G	1125	CLA	CHB-C1B	3.43	1.47	1.39
18	B	4006	BCR	C11-C12	-3.43	1.25	1.34
14	G	1125	CLA	CHD-C1D	3.43	1.45	1.38
14	G	1127	CLA	MG-ND	-3.43	1.99	2.05
14	b	1203	CLA	C4B-NB	-3.43	1.33	1.37
14	A	1125	CLA	CHB-C1B	3.43	1.47	1.39
14	H	1223	CLA	MG-ND	-3.43	1.99	2.05
14	a	1133	CLA	OBD-CAD	3.43	1.28	1.22
14	A	1115	CLA	OBD-CAD	3.43	1.28	1.22
14	H	1236	CLA	C1B-NB	-3.43	1.33	1.37
14	L	1503	CLA	CHC-C4B	3.43	1.47	1.39
14	a	1013	CLA	OBD-CAD	3.43	1.28	1.22
14	b	1227	CLA	C1B-NB	-3.43	1.33	1.37
14	A	1012	CLA	C4B-NB	-3.43	1.33	1.37
14	B	1218	CLA	OBD-CAD	3.43	1.28	1.22
15	H	1237	F6C	C1D-ND	-3.43	1.32	1.37
18	A	4003	BCR	C11-C12	-3.43	1.25	1.34
14	L	1501	CLA	CHB-C1B	3.43	1.47	1.39
15	b	1230	F6C	OBD-CAD	3.43	1.28	1.22
14	A	1123	CLA	MG-ND	-3.43	1.99	2.05
14	a	1104	CLA	CHB-C1B	3.43	1.47	1.39
14	B	1220	CLA	OBD-CAD	3.43	1.28	1.22
14	a	1138	CLA	C1B-NB	-3.43	1.33	1.37
14	b	1205	CLA	MG-ND	-3.43	1.99	2.05
14	B	1236	CLA	C1B-NB	-3.43	1.33	1.37
14	b	1023	CLA	CHD-C4C	3.43	1.47	1.39
14	B	1223	CLA	MG-ND	-3.43	1.99	2.05
14	A	1128	CLA	C1C-NC	-3.43	1.32	1.37
18	B	4009	BCR	C11-C12	-3.42	1.25	1.34
14	A	1106	CLA	C1B-NB	-3.42	1.33	1.37
14	G	1117	CLA	C1C-NC	-3.42	1.32	1.37
14	A	1117	CLA	C1C-NC	-3.42	1.32	1.37
14	b	1226	CLA	OBD-CAD	3.42	1.28	1.22
14	b	1224	CLA	CHC-C4B	3.42	1.47	1.39
13	A	1011	CL0	MG-ND	-3.42	1.99	2.05
14	A	1127	CLA	MG-ND	-3.42	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1119	CLA	C1D-ND	-3.42	1.33	1.37
14	b	1218	CLA	OBD-CAD	3.42	1.28	1.22
18	b	4009	BCR	C11-C12	-3.42	1.25	1.34
14	B	1210	CLA	CHC-C4B	3.42	1.47	1.39
14	G	1104	CLA	CHB-C1B	3.42	1.47	1.39
14	A	1127	CLA	CHC-C4B	3.42	1.47	1.39
14	b	1229	CLA	C1D-ND	-3.42	1.33	1.37
14	b	1212	CLA	CHD-C4C	3.42	1.47	1.39
15	A	1121	F6C	C1C-NC	-3.42	1.33	1.37
14	H	1227	CLA	OBD-CAD	3.42	1.28	1.22
18	H	4009	BCR	C11-C12	-3.42	1.25	1.34
14	a	1130	CLA	CHC-C4B	3.42	1.47	1.39
14	G	1130	CLA	CHC-C4B	3.42	1.47	1.39
14	a	1126	CLA	CHC-C4B	3.42	1.47	1.39
14	H	1213	CLA	C1D-ND	-3.42	1.33	1.37
14	G	1129	CLA	MG-ND	-3.42	1.99	2.05
14	a	1127	CLA	MG-ND	-3.42	1.99	2.05
15	a	1121	F6C	CHC-C1C	3.41	1.47	1.39
14	G	1102	CLA	C1B-NB	-3.41	1.33	1.37
14	b	1232	CLA	C1B-NB	-3.41	1.33	1.37
14	b	1227	CLA	OBD-CAD	3.41	1.28	1.22
14	H	1228	CLA	CHB-C1B	3.41	1.47	1.39
14	H	1212	CLA	CHD-C4C	3.41	1.47	1.39
14	B	1219	CLA	C1D-ND	-3.41	1.33	1.37
14	G	1115	CLA	OBD-CAD	3.41	1.28	1.22
14	H	1218	CLA	OBD-CAD	3.41	1.28	1.22
14	A	1013	CLA	OBD-CAD	3.41	1.28	1.22
14	b	1213	CLA	C1D-ND	-3.41	1.33	1.37
14	A	1102	CLA	C1B-NB	-3.41	1.33	1.37
18	a	4003	BCR	C11-C12	-3.41	1.25	1.34
14	A	1125	CLA	CHD-C1D	3.41	1.45	1.38
14	G	1128	CLA	C1C-NC	-3.41	1.32	1.37
14	a	1118	CLA	CHB-C1B	3.41	1.47	1.39
14	A	1138	CLA	C1B-NB	-3.41	1.33	1.37
14	A	1126	CLA	CHC-C4B	3.41	1.47	1.39
14	b	1227	CLA	CHB-C1B	3.41	1.47	1.39
15	b	1230	F6C	CHC-C1C	3.41	1.47	1.39
14	G	1138	CLA	C1B-NB	-3.41	1.33	1.37
14	B	1213	CLA	C1D-ND	-3.41	1.33	1.37
14	B	1216	CLA	C1D-ND	-3.41	1.33	1.37
14	L	1501	CLA	CHD-C4C	3.41	1.47	1.39
14	b	1226	CLA	C1C-NC	-3.41	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1211	CLA	CHB-C1B	3.41	1.47	1.39
14	a	1129	CLA	MG-ND	-3.41	1.99	2.05
14	A	1129	CLA	MG-ND	-3.41	1.99	2.05
14	b	1221	CLA	CHC-C4B	3.41	1.47	1.39
14	B	1228	CLA	CHB-C1B	3.41	1.47	1.39
14	H	1221	CLA	CHD-C4C	3.41	1.47	1.39
14	a	1128	CLA	CHD-C4C	3.41	1.47	1.39
14	a	1117	CLA	C1C-NC	-3.41	1.32	1.37
15	G	1121	F6C	CHC-C1C	3.41	1.47	1.39
14	G	1109	CLA	CHC-C4B	3.41	1.47	1.39
14	b	1208	CLA	CHB-C1B	3.41	1.47	1.39
14	A	1107	CLA	CHC-C4B	3.41	1.47	1.39
14	A	1129	CLA	CHC-C4B	3.41	1.47	1.39
14	B	1232	CLA	C1B-NB	-3.41	1.33	1.37
14	A	1128	CLA	CHD-C4C	3.41	1.47	1.39
14	U	1503	CLA	CHC-C4B	3.41	1.47	1.39
15	H	1237	F6C	CHD-C4C	3.41	1.47	1.39
14	A	1135	CLA	MG-ND	-3.41	1.99	2.05
14	B	1210	CLA	C1B-NB	-3.41	1.33	1.37
14	a	1109	CLA	CHC-C4B	3.40	1.47	1.39
14	b	1228	CLA	CHB-C1B	3.40	1.47	1.39
14	l	1501	CLA	CHD-C4C	3.40	1.46	1.39
14	H	1211	CLA	C1B-NB	-3.40	1.33	1.37
14	l	1503	CLA	C1B-NB	-3.40	1.33	1.37
15	b	1237	F6C	CHD-C4C	3.40	1.47	1.39
14	G	1012	CLA	C4B-NB	-3.40	1.33	1.37
14	A	1103	CLA	C1C-NC	-3.40	1.32	1.37
14	H	1211	CLA	CHB-C1B	3.40	1.47	1.39
14	a	1115	CLA	CHB-C1B	3.40	1.47	1.39
14	a	1131	CLA	CHC-C4B	3.40	1.47	1.39
14	b	1232	CLA	CHB-C1B	3.40	1.47	1.39
14	B	1227	CLA	CHB-C1B	3.40	1.47	1.39
14	a	1127	CLA	CHC-C4B	3.40	1.47	1.39
14	B	1229	CLA	C1D-ND	-3.40	1.33	1.37
14	H	1221	CLA	CHC-C4B	3.40	1.47	1.39
14	a	1103	CLA	C1C-NC	-3.40	1.32	1.37
14	G	1013	CLA	OBD-CAD	3.40	1.28	1.22
14	H	1226	CLA	OBD-CAD	3.40	1.28	1.22
14	a	1123	CLA	CHD-C4C	3.40	1.46	1.39
14	G	1127	CLA	CHC-C4B	3.40	1.47	1.39
14	A	1109	CLA	CHB-C1B	3.40	1.47	1.39
14	A	1109	CLA	CHC-C4B	3.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1201	CLA	CHC-C4B	3.40	1.47	1.39
14	a	1102	CLA	MG-ND	-3.40	1.99	2.05
14	G	1109	CLA	CHB-C1B	3.40	1.47	1.39
14	a	1122	CLA	C1C-NC	-3.40	1.32	1.37
14	G	1126	CLA	CHC-C4B	3.40	1.47	1.39
14	G	1128	CLA	CHD-C4C	3.40	1.46	1.39
14	H	1205	CLA	C1C-NC	-3.40	1.32	1.37
14	A	1130	CLA	CHC-C4B	3.40	1.47	1.39
14	B	1208	CLA	CHB-C1B	3.40	1.47	1.39
14	A	1101	CLA	CHB-C1B	3.39	1.47	1.39
14	H	1213	CLA	OBD-CAD	3.39	1.28	1.22
14	H	1227	CLA	CHB-C1B	3.39	1.47	1.39
14	a	1135	CLA	C4B-NB	-3.39	1.33	1.37
14	G	1112	CLA	CHC-C4B	3.39	1.47	1.39
18	G	4003	BCR	C11-C12	-3.39	1.25	1.34
14	G	1113	CLA	C1D-ND	-3.39	1.33	1.37
14	a	1128	CLA	C1C-NC	-3.39	1.32	1.37
14	a	1106	CLA	C1B-NB	-3.39	1.33	1.37
15	B	1237	F6C	C1D-ND	-3.39	1.32	1.37
14	H	1228	CLA	OBD-CAD	3.39	1.28	1.22
14	l	1501	CLA	CHB-C1B	3.39	1.47	1.39
14	a	1137	CLA	MG-ND	-3.39	1.99	2.05
14	H	1224	CLA	CHC-C4B	3.39	1.47	1.39
14	B	1205	CLA	C1C-NC	-3.39	1.32	1.37
14	B	1221	CLA	CHD-C4C	3.39	1.46	1.39
14	a	1107	CLA	MG-ND	-3.39	1.99	2.05
14	B	1221	CLA	CHC-C4B	3.39	1.47	1.39
14	B	1202	CLA	C1B-NB	-3.39	1.33	1.37
14	B	1239	CLA	C1C-NC	-3.39	1.32	1.37
14	G	1131	CLA	CHC-C4B	3.39	1.47	1.39
14	l	1503	CLA	CHC-C4B	3.39	1.47	1.39
14	A	1135	CLA	CHB-C1B	3.39	1.47	1.39
14	A	1123	CLA	CHD-C4C	3.39	1.46	1.39
14	H	1232	CLA	CHB-C1B	3.39	1.47	1.39
14	a	1135	CLA	CHB-C1B	3.39	1.47	1.39
14	a	1129	CLA	CHB-C1B	3.39	1.47	1.39
15	A	1121	F6C	CHC-C1C	3.39	1.47	1.39
14	A	1119	CLA	C1D-ND	-3.39	1.33	1.37
14	A	1131	CLA	CHC-C4B	3.39	1.47	1.39
14	G	1118	CLA	OBD-CAD	3.38	1.28	1.22
14	H	1202	CLA	C1B-NB	-3.38	1.33	1.37
14	a	1131	CLA	C1B-NB	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1140	CLA	CHD-C4C	3.38	1.46	1.39
14	B	1226	CLA	C1C-NC	-3.38	1.32	1.37
14	B	1224	CLA	CHC-C4B	3.38	1.47	1.39
14	B	1214	CLA	CHC-C4B	3.38	1.47	1.39
14	H	1224	CLA	CHD-C4C	3.38	1.46	1.39
14	b	1221	CLA	CHD-C4C	3.38	1.46	1.39
14	G	1135	CLA	C4B-NB	-3.38	1.33	1.37
14	b	1220	CLA	OBD-CAD	3.38	1.28	1.22
14	A	1122	CLA	C1C-NC	-3.38	1.32	1.37
14	G	1124	CLA	C1C-NC	-3.38	1.32	1.37
14	G	1103	CLA	C1C-NC	-3.38	1.32	1.37
14	H	1232	CLA	C1B-NB	-3.38	1.33	1.37
14	B	1212	CLA	CHD-C4C	3.38	1.46	1.39
14	U	1501	CLA	CHD-C4C	3.38	1.46	1.39
14	G	1105	CLA	CHB-C1B	3.38	1.47	1.39
14	G	1129	CLA	CHC-C4B	3.38	1.47	1.39
14	H	1239	CLA	C1C-NC	-3.38	1.32	1.37
14	G	1137	CLA	MG-ND	-3.38	1.99	2.05
14	A	1129	CLA	CHB-C1B	3.38	1.47	1.39
14	G	1101	CLA	CHB-C1B	3.38	1.47	1.39
14	b	1228	CLA	OBD-CAD	3.37	1.28	1.22
14	L	1503	CLA	C1B-NB	-3.37	1.33	1.37
14	A	1131	CLA	MG-ND	-3.37	1.99	2.05
14	A	1108	CLA	CHB-C1B	3.37	1.47	1.39
14	a	1129	CLA	CHC-C4B	3.37	1.47	1.39
14	B	1232	CLA	CHB-C1B	3.37	1.47	1.39
14	B	1211	CLA	CHB-C1B	3.37	1.47	1.39
14	H	1210	CLA	C1C-NC	-3.37	1.32	1.37
14	A	1118	CLA	CHB-C1B	3.37	1.47	1.39
15	B	1237	F6C	CHD-C4C	3.37	1.47	1.39
14	G	1122	CLA	C4B-NB	-3.37	1.33	1.37
14	G	1111	CLA	OBD-CAD	3.37	1.28	1.22
14	A	1013	CLA	CHD-C1D	3.37	1.45	1.38
14	A	1123	CLA	CHC-C4B	3.37	1.47	1.39
14	G	1118	CLA	CHB-C1B	3.37	1.47	1.39
14	G	1135	CLA	CHB-C1B	3.37	1.47	1.39
14	a	1130	CLA	C4B-NB	-3.37	1.33	1.37
14	G	1135	CLA	MG-ND	-3.37	1.99	2.05
14	B	1203	CLA	C4B-NB	-3.37	1.33	1.37
14	B	1211	CLA	C1B-NB	-3.37	1.33	1.37
14	W	1701	CLA	OBD-CAD	3.37	1.28	1.22
14	a	1112	CLA	CHC-C4B	3.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1108	CLA	CHB-C1B	3.37	1.47	1.39
14	G	1119	CLA	C1D-ND	-3.37	1.33	1.37
14	b	1210	CLA	C1C-NC	-3.37	1.32	1.37
14	B	1229	CLA	CHB-C1B	3.37	1.47	1.39
14	H	1217	CLA	C1D-ND	-3.37	1.33	1.37
14	H	1214	CLA	CHC-C4B	3.37	1.47	1.39
14	A	1112	CLA	CHC-C4B	3.37	1.47	1.39
15	B	1230	F6C	CHC-C1C	3.37	1.47	1.39
14	a	1102	CLA	OBD-CAD	3.37	1.28	1.22
14	b	1224	CLA	CHD-C4C	3.37	1.46	1.39
14	A	1128	CLA	CHB-C1B	3.37	1.47	1.39
14	a	1113	CLA	C1B-NB	-3.37	1.33	1.37
14	a	1122	CLA	C4B-NB	-3.37	1.33	1.37
14	a	1013	CLA	CHD-C1D	3.37	1.45	1.38
14	b	1201	CLA	CHC-C4B	3.37	1.47	1.39
14	G	1107	CLA	MG-ND	-3.37	1.99	2.05
14	a	1140	CLA	CHD-C4C	3.37	1.46	1.39
14	B	1223	CLA	CHD-C4C	3.37	1.46	1.39
14	A	1122	CLA	C4B-NB	-3.37	1.33	1.37
14	B	1226	CLA	OBD-CAD	3.37	1.28	1.22
14	H	1223	CLA	CHD-C4C	3.37	1.46	1.39
14	b	1213	CLA	OBD-CAD	3.36	1.28	1.22
14	b	1202	CLA	CHD-C4C	3.36	1.46	1.39
14	H	1229	CLA	OBD-CAD	3.36	1.28	1.22
14	B	1224	CLA	CHD-C4C	3.36	1.46	1.39
14	G	1102	CLA	MG-ND	-3.36	1.99	2.05
14	a	1111	CLA	OBD-CAD	3.36	1.28	1.22
14	a	1113	CLA	C1D-ND	-3.36	1.33	1.37
14	A	1102	CLA	MG-ND	-3.36	1.99	2.05
14	H	1201	CLA	CHC-C4B	3.36	1.47	1.39
14	a	1135	CLA	OBD-CAD	3.36	1.28	1.22
13	a	1011	CL0	C3B-C2B	3.36	1.44	1.40
13	A	1011	CL0	C3B-C2B	3.36	1.44	1.40
14	a	1101	CLA	OBD-CAD	3.36	1.28	1.22
14	a	1128	CLA	CHB-C1B	3.36	1.47	1.39
15	H	1230	F6C	CHC-C1C	3.36	1.47	1.39
14	A	1102	CLA	OBD-CAD	3.36	1.28	1.22
14	A	1107	CLA	MG-ND	-3.36	1.99	2.05
14	B	1215	CLA	MG-ND	-3.36	1.99	2.05
14	a	1105	CLA	CHB-C1B	3.36	1.47	1.39
14	B	1215	CLA	CHC-C4B	3.36	1.46	1.39
14	H	1219	CLA	C1D-ND	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1101	CLA	OBD-CAD	3.36	1.28	1.22
14	b	1223	CLA	CHD-C4C	3.36	1.46	1.39
14	b	1210	CLA	C4B-NB	-3.36	1.33	1.37
14	b	1239	CLA	CHC-C4B	3.36	1.46	1.39
14	H	1203	CLA	C4B-NB	-3.36	1.33	1.37
14	B	1208	CLA	OBD-CAD	3.36	1.28	1.22
14	A	1124	CLA	C1C-NC	-3.36	1.32	1.37
14	H	1229	CLA	CHB-C1B	3.36	1.46	1.39
14	G	1102	CLA	OBD-CAD	3.36	1.28	1.22
14	a	1112	CLA	C1D-ND	-3.36	1.33	1.37
14	H	1215	CLA	MG-ND	-3.35	1.99	2.05
14	b	1215	CLA	MG-ND	-3.35	1.99	2.05
14	H	1202	CLA	CHB-C1B	3.35	1.46	1.39
14	a	1140	CLA	C1B-NB	-3.35	1.33	1.37
14	A	1132	CLA	C4B-NB	-3.35	1.33	1.37
14	H	1220	CLA	OBD-CAD	3.35	1.28	1.22
14	G	1140	CLA	CHD-C4C	3.35	1.46	1.39
14	G	1108	CLA	CHB-C1B	3.35	1.46	1.39
14	A	1114	CLA	CHC-C4B	3.35	1.46	1.39
14	a	1118	CLA	MG-ND	-3.35	1.99	2.05
14	a	1135	CLA	MG-ND	-3.35	1.99	2.05
14	G	1106	CLA	C1B-NB	-3.35	1.33	1.37
14	B	1021	CLA	C1C-NC	-3.35	1.32	1.37
14	G	1130	CLA	C4B-NB	-3.35	1.33	1.37
14	a	1118	CLA	OBD-CAD	3.35	1.28	1.22
14	G	1131	CLA	MG-ND	-3.35	1.99	2.05
14	G	1106	CLA	CHB-C1B	3.35	1.46	1.39
14	b	1223	CLA	MG-ND	-3.35	1.99	2.05
14	H	1210	CLA	C4B-NB	-3.35	1.33	1.37
14	B	1217	CLA	C1D-ND	-3.35	1.33	1.37
14	H	1202	CLA	CHD-C4C	3.35	1.46	1.39
14	a	1106	CLA	CHB-C1B	3.35	1.46	1.39
14	G	1113	CLA	CHB-C1B	3.35	1.46	1.39
14	H	1239	CLA	CHC-C4B	3.35	1.46	1.39
14	G	1140	CLA	C1B-NB	-3.35	1.33	1.37
14	A	1131	CLA	C1B-NB	-3.35	1.33	1.37
14	A	1118	CLA	OBD-CAD	3.35	1.28	1.22
14	A	1140	CLA	C1B-NB	-3.35	1.33	1.37
14	A	1113	CLA	CHB-C1B	3.35	1.46	1.39
14	a	1124	CLA	C1C-NC	-3.35	1.32	1.37
14	b	1239	CLA	C1C-NC	-3.35	1.32	1.37
14	G	1131	CLA	C1B-NB	-3.35	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1111	CLA	OBD-CAD	3.35	1.28	1.22
14	G	1013	CLA	CHD-C1D	3.34	1.44	1.38
14	A	1133	CLA	CHC-C4B	3.34	1.46	1.39
14	b	1214	CLA	CHC-C4B	3.34	1.46	1.39
14	b	1219	CLA	C1D-ND	-3.34	1.33	1.37
14	G	1129	CLA	CHB-C1B	3.34	1.46	1.39
14	A	1105	CLA	CHB-C1B	3.34	1.46	1.39
14	G	1110	CLA	OBD-CAD	3.34	1.28	1.22
14	A	1135	CLA	C4B-NB	-3.34	1.33	1.37
14	a	1139	CLA	CHD-C4C	3.34	1.46	1.39
14	A	1122	CLA	CHB-C1B	3.34	1.46	1.39
14	B	1202	CLA	CHD-C4C	3.34	1.46	1.39
14	b	1021	CLA	C1C-NC	-3.34	1.32	1.37
14	G	1101	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1229	CLA	OBD-CAD	3.34	1.28	1.22
14	b	1236	CLA	C1B-NB	-3.34	1.33	1.37
14	A	1108	CLA	C1B-NB	-3.34	1.33	1.37
14	a	1103	CLA	CHB-C1B	3.34	1.46	1.39
15	b	1230	F6C	CHD-C4C	3.34	1.46	1.39
14	a	1119	CLA	OBD-CAD	3.34	1.28	1.22
14	G	1113	CLA	C1B-NB	-3.34	1.33	1.37
14	H	1228	CLA	C1B-NB	-3.34	1.33	1.37
14	B	1210	CLA	C4B-NB	-3.34	1.33	1.37
14	U	1503	CLA	C1B-NB	-3.34	1.33	1.37
14	A	1124	CLA	C4B-NB	-3.34	1.33	1.37
14	b	1214	CLA	MG-ND	-3.34	1.99	2.05
14	B	1236	CLA	CHB-C1B	3.34	1.46	1.39
14	A	1113	CLA	C1B-NB	-3.34	1.33	1.37
14	a	1131	CLA	MG-ND	-3.33	1.99	2.05
14	L	1501	CLA	MG-ND	-3.33	1.99	2.05
14	B	1201	CLA	OBD-CAD	3.33	1.28	1.22
14	b	1217	CLA	C1D-ND	-3.33	1.33	1.37
14	B	1239	CLA	CHC-C4B	3.33	1.46	1.39
14	b	1222	CLA	CHB-C1B	3.33	1.46	1.39
14	G	1122	CLA	CHB-C1B	3.33	1.46	1.39
14	b	1229	CLA	CHB-C1B	3.33	1.46	1.39
14	G	1103	CLA	CHB-C1B	3.33	1.46	1.39
14	G	1116	CLA	OBD-CAD	3.33	1.28	1.22
14	A	1139	CLA	CHD-C4C	3.33	1.46	1.39
15	b	1237	F6C	CHB-C1B	3.33	1.46	1.39
14	A	1110	CLA	C1B-NB	-3.33	1.33	1.37
14	H	1221	CLA	CHB-C1B	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1237	F6C	CHB-C1B	3.33	1.46	1.39
14	a	1132	CLA	C4B-NB	-3.33	1.33	1.37
14	B	1224	CLA	C4B-NB	-3.33	1.33	1.37
14	G	1133	CLA	CHC-C4B	3.33	1.46	1.39
14	G	1135	CLA	OBD-CAD	3.33	1.28	1.22
14	H	1239	CLA	MG-ND	-3.33	1.99	2.05
14	A	1119	CLA	OBD-CAD	3.33	1.28	1.22
14	A	1135	CLA	OBD-CAD	3.33	1.28	1.22
14	b	1215	CLA	CHC-C4B	3.33	1.46	1.39
14	B	1210	CLA	C1C-NC	-3.33	1.32	1.37
14	B	1209	CLA	OBD-CAD	3.33	1.28	1.22
14	H	1215	CLA	CHC-C4B	3.33	1.46	1.39
14	A	1103	CLA	CHB-C1B	3.33	1.46	1.39
14	B	1239	CLA	C1B-NB	-3.33	1.33	1.37
14	a	1013	CLA	CHD-C4C	3.33	1.46	1.39
14	b	1225	CLA	CHD-C4C	3.33	1.46	1.39
14	G	1120	CLA	C1B-NB	-3.33	1.33	1.37
14	a	1114	CLA	CHC-C4B	3.33	1.46	1.39
14	H	1209	CLA	OBD-CAD	3.33	1.28	1.22
14	b	1214	CLA	CHB-C1B	3.32	1.46	1.39
14	A	1113	CLA	C1D-ND	-3.32	1.33	1.37
14	a	1110	CLA	OBD-CAD	3.32	1.28	1.22
14	A	1137	CLA	CHC-C4B	3.32	1.46	1.39
14	H	1021	CLA	C1C-NC	-3.32	1.32	1.37
14	a	1120	CLA	C1B-NB	-3.32	1.33	1.37
14	A	1130	CLA	C4B-NB	-3.32	1.33	1.37
14	G	1128	CLA	CHB-C1B	3.32	1.46	1.39
14	B	1215	CLA	OBD-CAD	3.32	1.28	1.22
15	H	1230	F6C	CHD-C4C	3.32	1.46	1.39
14	A	1118	CLA	MG-ND	-3.32	1.99	2.05
14	A	1116	CLA	OBD-CAD	3.32	1.28	1.22
14	B	1229	CLA	OBD-CAD	3.32	1.28	1.22
14	H	1201	CLA	OBD-CAD	3.32	1.28	1.22
14	X	1701	CLA	OBD-CAD	3.32	1.28	1.22
14	G	1118	CLA	MG-ND	-3.32	1.99	2.05
14	l	1501	CLA	MG-ND	-3.32	1.99	2.05
14	a	1122	CLA	CHB-C1B	3.32	1.46	1.39
14	b	1223	CLA	CHB-C1B	3.32	1.46	1.39
14	b	1220	CLA	C1B-NB	-3.32	1.33	1.37
14	b	1209	CLA	OBD-CAD	3.32	1.28	1.22
14	A	1103	CLA	MG-ND	-3.32	1.99	2.05
14	A	1140	CLA	MG-ND	-3.32	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1222	CLA	CHB-C1B	3.32	1.46	1.39
15	B	1237	F6C	CHB-C1B	3.32	1.46	1.39
14	B	1221	CLA	CHB-C1B	3.32	1.46	1.39
14	b	1228	CLA	C1B-NB	-3.32	1.33	1.37
14	b	1205	CLA	C4B-NB	-3.32	1.33	1.37
14	A	1106	CLA	CHB-C1B	3.32	1.46	1.39
14	G	1112	CLA	C1B-NB	-3.32	1.33	1.37
14	L	1501	CLA	C4B-NB	-3.31	1.33	1.37
14	a	1133	CLA	CHC-C4B	3.31	1.46	1.39
14	G	1139	CLA	CHD-C4C	3.31	1.46	1.39
14	H	1214	CLA	MG-ND	-3.31	1.99	2.05
14	G	1013	CLA	CHD-C4C	3.31	1.46	1.39
14	A	1013	CLA	CHD-C4C	3.31	1.46	1.39
14	B	1239	CLA	MG-ND	-3.31	1.99	2.05
14	B	1205	CLA	CHC-C4B	3.31	1.46	1.39
14	B	1235	CLA	CHB-C1B	3.31	1.46	1.39
14	G	1101	CLA	C1D-ND	-3.31	1.33	1.37
14	B	1228	CLA	C1B-NB	-3.31	1.33	1.37
14	x	1701	CLA	OBD-CAD	3.31	1.28	1.22
14	b	1235	CLA	CHB-C1B	3.31	1.46	1.39
14	H	1208	CLA	OBD-CAD	3.31	1.28	1.22
14	G	1114	CLA	CHC-C4B	3.31	1.46	1.39
14	a	1116	CLA	OBD-CAD	3.31	1.28	1.22
14	A	1101	CLA	C1D-ND	-3.31	1.33	1.37
18	H	4013	BCR	C11-C12	-3.31	1.26	1.34
14	H	1220	CLA	C1C-NC	-3.31	1.32	1.37
14	a	1101	CLA	C1D-ND	-3.31	1.33	1.37
14	b	1202	CLA	CHB-C1B	3.31	1.46	1.39
14	b	1205	CLA	CHC-C4B	3.31	1.46	1.39
14	G	1106	CLA	C4B-NB	-3.31	1.33	1.37
14	H	1236	CLA	CHB-C1B	3.31	1.46	1.39
14	A	1105	CLA	CHC-C4B	3.31	1.46	1.39
14	H	1215	CLA	OBD-CAD	3.31	1.28	1.22
14	G	1132	CLA	C4B-NB	-3.31	1.33	1.37
15	B	1230	F6C	CHD-C4C	3.31	1.46	1.39
14	H	1203	CLA	MG-ND	-3.31	1.99	2.05
14	B	1209	CLA	CHB-C1B	3.31	1.46	1.39
14	B	1228	CLA	OBD-CAD	3.31	1.28	1.22
14	a	1113	CLA	CHB-C1B	3.31	1.46	1.39
14	A	1120	CLA	C1B-NB	-3.30	1.33	1.37
14	b	1201	CLA	OBD-CAD	3.30	1.28	1.22
14	G	1108	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	1108	CLA	C1B-NB	-3.30	1.33	1.37
14	B	1203	CLA	CHD-C4C	3.30	1.46	1.39
14	b	1234	CLA	CHB-C1B	3.30	1.46	1.39
14	b	1236	CLA	CHB-C1B	3.30	1.46	1.39
14	a	1140	CLA	MG-ND	-3.30	1.99	2.05
15	H	1237	F6C	C4C-NC	-3.30	1.33	1.37
14	H	1214	CLA	CHB-C1B	3.30	1.46	1.39
14	B	1205	CLA	CHD-C4C	3.30	1.46	1.39
14	b	1208	CLA	OBD-CAD	3.30	1.28	1.22
14	A	1110	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1224	CLA	OBD-CAD	3.30	1.28	1.22
15	H	1238	F6C	CHD-C4C	3.30	1.46	1.39
14	a	1117	CLA	OBD-CAD	3.30	1.28	1.22
14	H	1220	CLA	C1B-NB	-3.30	1.33	1.37
14	b	1221	CLA	CHB-C1B	3.30	1.46	1.39
14	b	1215	CLA	OBD-CAD	3.30	1.28	1.22
14	H	1205	CLA	C4B-NB	-3.30	1.33	1.37
14	G	1120	CLA	OBD-CAD	3.30	1.28	1.22
14	a	1127	CLA	OBD-CAD	3.30	1.28	1.22
14	A	1126	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1213	CLA	OBD-CAD	3.30	1.28	1.22
14	b	1239	CLA	C1B-NB	-3.30	1.33	1.37
18	b	4013	BCR	C11-C12	-3.30	1.26	1.34
14	A	1117	CLA	OBD-CAD	3.30	1.28	1.22
14	B	1023	CLA	OBD-CAD	3.30	1.28	1.22
15	b	1237	F6C	C4C-NC	-3.30	1.33	1.37
14	G	1124	CLA	OBD-CAD	3.30	1.28	1.22
14	H	1235	CLA	CHB-C1B	3.30	1.46	1.39
14	B	1225	CLA	CHB-C1B	3.30	1.46	1.39
14	H	1213	CLA	CHB-C1B	3.30	1.46	1.39
14	H	1236	CLA	C1C-NC	-3.30	1.32	1.37
14	B	1239	CLA	OBD-CAD	3.30	1.28	1.22
14	b	1213	CLA	CHB-C1B	3.30	1.46	1.39
14	U	1501	CLA	MG-ND	-3.30	1.99	2.05
14	G	1119	CLA	OBD-CAD	3.30	1.28	1.22
14	b	1206	CLA	C4B-NB	-3.30	1.33	1.37
14	A	1139	CLA	C1C-NC	-3.30	1.32	1.37
14	H	1208	CLA	C1B-NB	-3.29	1.33	1.37
14	G	1137	CLA	CHC-C4B	3.29	1.46	1.39
14	a	1105	CLA	CHC-C4B	3.29	1.46	1.39
14	A	1120	CLA	OBD-CAD	3.29	1.28	1.22
14	H	1205	CLA	CHC-C4B	3.29	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	1501	CLA	C4B-NB	-3.29	1.33	1.37
14	G	1117	CLA	OBD-CAD	3.29	1.28	1.22
14	a	1120	CLA	OBD-CAD	3.29	1.28	1.22
14	L	1501	CLA	OBD-CAD	3.29	1.28	1.22
14	b	1209	CLA	CHB-C1B	3.29	1.46	1.39
14	A	1124	CLA	OBD-CAD	3.29	1.28	1.22
14	B	1220	CLA	C1B-NB	-3.29	1.33	1.37
14	a	1103	CLA	MG-ND	-3.29	1.99	2.05
18	B	4013	BCR	C11-C12	-3.29	1.26	1.34
14	a	1117	CLA	MG-ND	-3.29	1.99	2.05
14	B	1202	CLA	CHB-C1B	3.29	1.46	1.39
14	H	1223	CLA	CHB-C1B	3.29	1.46	1.39
14	b	1220	CLA	C1C-NC	-3.29	1.32	1.37
14	b	1023	CLA	OBD-CAD	3.29	1.28	1.22
14	A	1116	CLA	MG-ND	-3.29	1.99	2.05
14	H	1227	CLA	MG-ND	-3.29	1.99	2.05
14	H	1234	CLA	CHD-C4C	3.29	1.46	1.39
14	b	1202	CLA	C1B-NB	-3.28	1.33	1.37
14	b	1227	CLA	MG-ND	-3.28	1.99	2.05
14	H	1225	CLA	CHD-C4C	3.28	1.46	1.39
14	B	1225	CLA	CHD-C4C	3.28	1.46	1.39
14	B	1228	CLA	CHC-C4B	3.28	1.46	1.39
14	B	1223	CLA	CHB-C1B	3.28	1.46	1.39
14	a	1110	CLA	C1B-NB	-3.28	1.33	1.37
14	A	1112	CLA	C1D-ND	-3.28	1.33	1.37
14	A	1116	CLA	C1B-NB	-3.28	1.33	1.37
14	H	1205	CLA	CHD-C4C	3.28	1.46	1.39
14	b	1203	CLA	CHD-C4C	3.28	1.46	1.39
14	G	1119	CLA	MG-ND	-3.28	1.99	2.05
14	H	1216	CLA	C1B-NB	-3.28	1.33	1.37
14	G	1116	CLA	MG-ND	-3.28	1.99	2.05
14	A	1119	CLA	MG-ND	-3.28	1.99	2.05
14	b	1234	CLA	CHD-C4C	3.28	1.46	1.39
14	A	1106	CLA	C4B-NB	-3.28	1.33	1.37
14	A	1139	CLA	OBD-CAD	3.28	1.28	1.22
15	G	1121	F6C	OBD-CAD	3.28	1.28	1.22
14	b	1228	CLA	CHC-C4B	3.28	1.46	1.39
14	a	1119	CLA	C4B-NB	-3.28	1.33	1.37
15	A	1121	F6C	OBD-CAD	3.28	1.28	1.22
14	l	1501	CLA	CHC-C4B	3.28	1.46	1.39
14	B	1209	CLA	C1D-ND	-3.28	1.33	1.37
14	B	1235	CLA	C1B-NB	-3.28	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1234	CLA	CHB-C1B	3.28	1.46	1.39
14	A	1127	CLA	OBD-CAD	3.28	1.28	1.22
14	a	1137	CLA	C1B-NB	-3.28	1.33	1.37
14	b	1216	CLA	C1B-NB	-3.28	1.33	1.37
14	b	1222	CLA	MG-ND	-3.28	1.99	2.05
14	a	1124	CLA	OBD-CAD	3.28	1.28	1.22
14	H	1236	CLA	OBD-CAD	3.28	1.28	1.22
14	B	1201	CLA	C1B-NB	-3.28	1.33	1.37
14	B	1227	CLA	MG-ND	-3.28	1.99	2.05
14	G	1112	CLA	C1D-ND	-3.28	1.33	1.37
14	H	1209	CLA	C1D-ND	-3.28	1.33	1.37
14	H	1232	CLA	C1D-ND	-3.28	1.33	1.37
14	H	1239	CLA	C1B-NB	-3.28	1.33	1.37
15	G	1121	F6C	MG-NC	3.27	2.12	2.05
14	a	1126	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1229	CLA	C1B-NB	-3.27	1.33	1.37
14	U	1501	CLA	OBD-CAD	3.27	1.28	1.22
15	a	1121	F6C	OBD-CAD	3.27	1.28	1.22
14	U	1501	CLA	CHC-C4B	3.27	1.46	1.39
14	H	1235	CLA	C1B-NB	-3.27	1.33	1.37
14	a	1112	CLA	C1B-NB	-3.27	1.33	1.37
14	H	1225	CLA	CHB-C1B	3.27	1.46	1.39
14	a	1139	CLA	C1C-NC	-3.27	1.32	1.37
14	H	1222	CLA	MG-ND	-3.27	1.99	2.05
14	b	1224	CLA	OBD-CAD	3.27	1.28	1.22
14	G	1105	CLA	CHC-C4B	3.27	1.46	1.39
14	A	1122	CLA	C1B-NB	-3.27	1.33	1.37
14	a	1137	CLA	CHC-C4B	3.27	1.46	1.39
14	B	1222	CLA	MG-ND	-3.27	1.99	2.05
14	G	1140	CLA	MG-ND	-3.27	1.99	2.05
14	L	1501	CLA	CHC-C4B	3.27	1.46	1.39
14	H	1023	CLA	OBD-CAD	3.27	1.28	1.22
14	L	1503	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1234	CLA	CHB-C1B	3.27	1.46	1.39
14	b	1239	CLA	OBD-CAD	3.27	1.28	1.22
14	A	1122	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1203	CLA	MG-ND	-3.27	1.99	2.05
15	a	1121	F6C	MG-NC	3.27	2.12	2.05
14	H	1222	CLA	C4B-NB	-3.27	1.33	1.37
14	b	1208	CLA	C1B-NB	-3.27	1.33	1.37
14	G	1137	CLA	C1C-NC	-3.27	1.32	1.37
14	G	1117	CLA	MG-ND	-3.27	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1203	CLA	MG-ND	-3.27	1.99	2.05
14	a	1111	CLA	CHB-C1B	3.27	1.46	1.39
14	H	1224	CLA	OBD-CAD	3.27	1.28	1.22
14	b	1212	CLA	OBD-CAD	3.27	1.28	1.22
14	B	1211	CLA	OBD-CAD	3.27	1.28	1.22
15	B	1237	F6C	C4C-NC	-3.27	1.33	1.37
14	H	1228	CLA	CHC-C4B	3.27	1.46	1.39
14	G	1103	CLA	MG-ND	-3.27	1.99	2.05
14	a	1122	CLA	OBD-CAD	3.27	1.28	1.22
14	A	1117	CLA	MG-ND	-3.27	1.99	2.05
14	H	1201	CLA	C1B-NB	-3.27	1.33	1.37
14	B	1234	CLA	CHD-C4C	3.26	1.46	1.39
14	a	1119	CLA	MG-ND	-3.26	1.99	2.05
14	a	1124	CLA	C4B-NB	-3.26	1.33	1.37
14	A	1112	CLA	C1B-NB	-3.26	1.33	1.37
14	H	1209	CLA	CHB-C1B	3.26	1.46	1.39
14	B	1213	CLA	CHB-C1B	3.26	1.46	1.39
14	H	1203	CLA	CHD-C4C	3.26	1.46	1.39
14	B	1222	CLA	CHB-C1B	3.26	1.46	1.39
14	G	1126	CLA	OBD-CAD	3.26	1.28	1.22
14	G	1110	CLA	C1B-NB	-3.26	1.33	1.37
14	a	1109	CLA	C1B-NB	-3.26	1.33	1.37
14	b	1205	CLA	CHD-C4C	3.26	1.46	1.39
14	G	1104	CLA	OBD-CAD	3.26	1.28	1.22
14	B	1212	CLA	OBD-CAD	3.26	1.28	1.22
14	a	1116	CLA	MG-ND	-3.26	1.99	2.05
14	l	1503	CLA	OBD-CAD	3.26	1.28	1.22
14	A	1109	CLA	OBD-CAD	3.26	1.28	1.22
14	a	1106	CLA	OBD-CAD	3.26	1.28	1.22
14	H	1203	CLA	CHC-C4B	3.26	1.46	1.39
14	B	1214	CLA	CHB-C1B	3.26	1.46	1.39
14	B	1214	CLA	MG-ND	-3.26	1.99	2.05
14	A	1119	CLA	C4B-NB	-3.26	1.33	1.37
14	a	1116	CLA	CHB-C1B	3.26	1.46	1.39
14	b	1021	CLA	CHC-C4B	3.26	1.46	1.39
14	H	1224	CLA	C4B-NB	-3.26	1.33	1.37
14	a	1127	CLA	CHD-C4C	3.26	1.46	1.39
14	b	1203	CLA	CHC-C4B	3.26	1.46	1.39
14	H	1211	CLA	OBD-CAD	3.26	1.28	1.22
18	B	4004	BCR	C11-C12	-3.26	1.26	1.34
14	G	1127	CLA	CHD-C4C	3.26	1.46	1.39
14	b	1239	CLA	MG-ND	-3.26	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	H	4004	BCR	C11-C12	-3.25	1.26	1.34
15	b	1238	F6C	CHD-C4C	3.25	1.46	1.39
14	a	1104	CLA	OBD-CAD	3.25	1.28	1.22
18	b	4004	BCR	C11-C12	-3.25	1.26	1.34
14	a	1139	CLA	OBD-CAD	3.25	1.28	1.22
14	G	1119	CLA	C4B-NB	-3.25	1.33	1.37
14	H	1021	CLA	CHC-C4B	3.25	1.46	1.39
14	B	1206	CLA	C4B-NB	-3.25	1.33	1.37
14	H	1210	CLA	CHB-C1B	3.25	1.46	1.39
14	H	1239	CLA	OBD-CAD	3.25	1.28	1.22
14	H	1206	CLA	C4B-NB	-3.25	1.33	1.37
14	B	1203	CLA	CHB-C1B	3.25	1.46	1.39
14	A	1137	CLA	C1C-NC	-3.25	1.32	1.37
15	A	1121	F6C	MG-NC	3.25	2.12	2.05
14	G	1139	CLA	OBD-CAD	3.25	1.28	1.22
14	a	1117	CLA	C4B-NB	-3.25	1.33	1.37
15	H	1238	F6C	C4C-NC	-3.25	1.33	1.37
14	b	1235	CLA	C1B-NB	-3.25	1.33	1.37
14	l	1501	CLA	OBD-CAD	3.25	1.28	1.22
14	U	1501	CLA	C4B-NB	-3.25	1.33	1.37
14	b	1201	CLA	C1C-NC	-3.25	1.32	1.37
14	b	1224	CLA	C4B-NB	-3.25	1.33	1.37
14	a	1117	CLA	CHB-C1B	3.25	1.46	1.39
14	B	1231	CLA	C1B-NB	-3.25	1.33	1.37
14	b	1203	CLA	CHB-C1B	3.25	1.46	1.39
14	G	1137	CLA	C1B-NB	-3.24	1.33	1.37
14	b	1209	CLA	C1D-ND	-3.24	1.33	1.37
14	b	1219	CLA	C1B-NB	-3.24	1.33	1.37
14	A	1103	CLA	CHC-C4B	3.24	1.46	1.39
15	a	1121	F6C	CHB-C1B	3.24	1.46	1.39
14	H	1212	CLA	OBD-CAD	3.24	1.28	1.22
14	A	1106	CLA	OBD-CAD	3.24	1.28	1.22
14	A	1111	CLA	CHB-C1B	3.24	1.46	1.39
15	B	1238	F6C	CHD-C4C	3.24	1.46	1.39
14	A	1137	CLA	C1B-NB	-3.24	1.33	1.37
14	A	1116	CLA	CHB-C1B	3.24	1.46	1.39
14	U	1503	CLA	OBD-CAD	3.24	1.28	1.22
14	b	1222	CLA	C4B-NB	-3.24	1.33	1.37
14	B	1201	CLA	MG-ND	-3.24	1.99	2.05
14	H	1219	CLA	C1B-NB	-3.24	1.33	1.37
14	a	1106	CLA	C4B-NB	-3.24	1.33	1.37
14	A	1133	CLA	C4B-NB	-3.24	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1205	CLA	C4B-NB	-3.24	1.33	1.37
14	G	1103	CLA	CHC-C4B	3.24	1.46	1.39
14	G	1139	CLA	C1C-NC	-3.24	1.32	1.37
14	L	1503	CLA	C1C-NC	-3.24	1.32	1.37
14	G	1109	CLA	OBD-CAD	3.24	1.28	1.22
14	a	1112	CLA	CHB-C1B	3.24	1.46	1.39
15	b	1207	F6C	MG-NC	3.24	2.12	2.05
14	B	1210	CLA	CHB-C1B	3.24	1.46	1.39
14	G	1112	CLA	CHB-C1B	3.24	1.46	1.39
14	b	1201	CLA	MG-ND	-3.23	1.99	2.05
14	A	1117	CLA	CHB-C1B	3.23	1.46	1.39
14	G	1127	CLA	OBD-CAD	3.23	1.28	1.22
14	H	1212	CLA	C1B-NB	-3.23	1.33	1.37
14	B	1223	CLA	C4B-NB	-3.23	1.33	1.37
14	b	1202	CLA	MG-ND	-3.23	1.99	2.05
14	B	1222	CLA	C4B-NB	-3.23	1.33	1.37
14	G	1106	CLA	OBD-CAD	3.23	1.28	1.22
14	B	1236	CLA	OBD-CAD	3.23	1.28	1.22
14	a	1103	CLA	CHC-C4B	3.23	1.46	1.39
14	b	1210	CLA	CHB-C1B	3.23	1.46	1.39
15	B	1230	F6C	MG-NC	3.23	2.12	2.05
14	b	1225	CLA	C4B-NB	-3.23	1.33	1.37
14	b	1225	CLA	C1C-NC	-3.23	1.32	1.37
14	B	1220	CLA	C1C-NC	-3.23	1.32	1.37
14	a	1122	CLA	C1B-NB	-3.23	1.33	1.37
14	G	1133	CLA	C1B-NB	-3.23	1.33	1.37
14	B	1022	CLA	C4B-NB	-3.23	1.33	1.37
14	H	1201	CLA	MG-ND	-3.23	1.99	2.05
14	G	1118	CLA	C1B-NB	-3.23	1.33	1.37
14	G	1111	CLA	CHB-C1B	3.23	1.46	1.39
14	l	1503	CLA	C1C-NC	-3.23	1.32	1.37
15	G	1121	F6C	CHB-C1B	3.23	1.46	1.39
14	G	1109	CLA	C1B-NB	-3.23	1.33	1.37
14	B	1208	CLA	C1B-NB	-3.23	1.33	1.37
14	G	1122	CLA	C1B-NB	-3.23	1.33	1.37
14	B	1232	CLA	C1D-ND	-3.23	1.33	1.37
14	a	1109	CLA	OBD-CAD	3.23	1.28	1.22
14	a	1116	CLA	C1B-NB	-3.22	1.33	1.37
14	b	1225	CLA	CHB-C1B	3.22	1.46	1.39
14	B	1021	CLA	CHC-C4B	3.22	1.46	1.39
14	A	1130	CLA	C1C-NC	-3.22	1.32	1.37
14	H	1022	CLA	C4B-NB	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	1230	F6C	MG-NC	3.22	2.12	2.05
14	a	1118	CLA	C1B-NB	-3.22	1.33	1.37
14	b	1232	CLA	C1D-ND	-3.22	1.33	1.37
14	B	1219	CLA	C1B-NB	-3.22	1.33	1.37
14	b	1211	CLA	OBD-CAD	3.22	1.28	1.22
14	b	1236	CLA	OBD-CAD	3.22	1.28	1.22
14	a	1013	CLA	C4B-NB	-3.22	1.33	1.37
14	a	1107	CLA	C1B-NB	-3.22	1.33	1.37
14	b	1223	CLA	C4B-NB	-3.22	1.33	1.37
14	B	1203	CLA	CHC-C4B	3.22	1.46	1.39
14	G	1122	CLA	OBD-CAD	3.22	1.28	1.22
14	A	1127	CLA	CHD-C4C	3.22	1.46	1.39
14	G	1013	CLA	MG-ND	-3.22	1.99	2.05
14	H	1202	CLA	MG-ND	-3.22	1.99	2.05
14	A	1117	CLA	C4B-NB	-3.22	1.33	1.37
14	G	1116	CLA	CHB-C1B	3.22	1.46	1.39
15	B	1207	F6C	MG-NC	3.22	2.12	2.05
15	A	1121	F6C	CHB-C1B	3.22	1.46	1.39
14	G	1117	CLA	CHB-C1B	3.22	1.46	1.39
14	B	1204	CLA	CHC-C4B	3.22	1.46	1.39
14	A	1138	CLA	OBD-CAD	3.22	1.28	1.22
14	a	1013	CLA	MG-ND	-3.22	1.99	2.05
15	H	1207	F6C	MG-NC	3.22	2.12	2.05
14	G	1127	CLA	C4B-NB	-3.22	1.33	1.37
14	a	1137	CLA	CHB-C1B	3.22	1.46	1.39
14	H	1218	CLA	CHD-C4C	3.22	1.46	1.39
14	G	1124	CLA	C4B-NB	-3.22	1.33	1.37
14	a	1115	CLA	MG-ND	-3.22	1.99	2.05
14	a	1137	CLA	C1C-NC	-3.21	1.32	1.37
14	L	1502	CLA	C1B-NB	-3.21	1.33	1.37
14	H	1202	CLA	OBD-CAD	3.21	1.28	1.22
14	A	1133	CLA	MG-ND	-3.21	1.99	2.05
14	a	1133	CLA	C1B-NB	-3.21	1.33	1.37
14	B	1216	CLA	C1B-NB	-3.21	1.33	1.37
14	b	1208	CLA	MG-ND	-3.21	1.99	2.05
14	G	1013	CLA	C4B-NB	-3.21	1.33	1.37
14	G	1116	CLA	C1B-NB	-3.21	1.33	1.37
14	b	1201	CLA	C1B-NB	-3.21	1.33	1.37
14	H	1229	CLA	C1B-NB	-3.21	1.33	1.37
14	H	1201	CLA	C1C-NC	-3.21	1.32	1.37
14	H	1226	CLA	CHB-C1B	3.21	1.46	1.39
14	G	1133	CLA	MG-ND	-3.21	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1138	CLA	OBD-CAD	3.21	1.28	1.22
14	b	1214	CLA	OBD-CAD	3.21	1.28	1.22
14	b	1228	CLA	C1C-NC	-3.21	1.32	1.37
14	l	1502	CLA	C1B-NB	-3.21	1.33	1.37
14	H	1219	CLA	CHB-C1B	3.21	1.46	1.39
15	H	1230	F6C	MG-NC	3.21	2.12	2.05
14	A	1105	CLA	C1B-NB	-3.21	1.33	1.37
14	H	1228	CLA	C1C-NC	-3.21	1.32	1.37
14	B	1228	CLA	C1C-NC	-3.21	1.32	1.37
14	b	1229	CLA	C1B-NB	-3.21	1.33	1.37
14	B	1219	CLA	CHB-C1B	3.21	1.46	1.39
14	G	1105	CLA	C1B-NB	-3.21	1.33	1.37
14	B	1220	CLA	C4B-NB	-3.21	1.33	1.37
18	a	4002	BCR	C11-C12	-3.20	1.26	1.34
14	A	1126	CLA	C1C-NC	-3.20	1.32	1.37
14	b	1231	CLA	C1B-NB	-3.20	1.33	1.37
14	b	1226	CLA	CHB-C1B	3.20	1.46	1.39
15	H	1238	F6C	MG-NC	3.20	2.12	2.05
14	G	1107	CLA	C1B-NB	-3.20	1.33	1.37
14	G	1115	CLA	C1B-NB	-3.20	1.33	1.37
14	A	1115	CLA	C1B-NB	-3.20	1.33	1.37
14	A	1112	CLA	CHB-C1B	3.20	1.46	1.39
14	A	1109	CLA	C1B-NB	-3.20	1.33	1.37
14	A	1104	CLA	OBD-CAD	3.20	1.28	1.22
14	b	1224	CLA	CHB-C1B	3.20	1.46	1.39
14	A	1137	CLA	CHB-C1B	3.20	1.46	1.39
14	G	1139	CLA	C1B-NB	-3.20	1.33	1.37
14	H	1208	CLA	MG-ND	-3.20	1.99	2.05
14	H	1203	CLA	CHB-C1B	3.20	1.46	1.39
14	a	1114	CLA	CHB-C1B	3.20	1.46	1.39
14	b	1236	CLA	C1C-NC	-3.20	1.32	1.37
14	G	1137	CLA	CHB-C1B	3.20	1.46	1.39
14	a	1135	CLA	CHC-C4B	3.20	1.46	1.39
14	a	1130	CLA	C1C-NC	-3.20	1.32	1.37
14	B	1236	CLA	C1C-NC	-3.20	1.32	1.37
14	b	1232	CLA	MG-ND	-3.20	1.99	2.05
14	H	1201	CLA	CHB-C1B	3.20	1.46	1.39
14	H	1225	CLA	C1C-NC	-3.20	1.32	1.37
14	a	1126	CLA	C1C-NC	-3.20	1.32	1.37
14	G	1132	CLA	C1B-NB	-3.20	1.33	1.37
14	B	1218	CLA	CHD-C4C	3.20	1.46	1.39
14	G	1125	CLA	CHC-C4B	3.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1220	CLA	C4B-NB	-3.20	1.33	1.37
15	B	1207	F6C	C4C-NC	-3.20	1.33	1.37
14	U	1503	CLA	C1C-NC	-3.20	1.32	1.37
14	a	1133	CLA	C4B-NB	-3.20	1.33	1.37
14	B	1202	CLA	MG-ND	-3.20	1.99	2.05
14	a	1107	CLA	OBD-CAD	3.20	1.28	1.22
14	G	1135	CLA	CHC-C4B	3.20	1.46	1.39
14	a	1105	CLA	C4B-NB	-3.20	1.33	1.37
14	B	1226	CLA	CHB-C1B	3.19	1.46	1.39
14	A	1013	CLA	MG-ND	-3.19	1.99	2.05
14	H	1234	CLA	MG-ND	-3.19	1.99	2.05
14	A	1123	CLA	OBD-CAD	3.19	1.28	1.22
14	b	1233	CLA	C1D-ND	-3.19	1.33	1.37
14	a	1133	CLA	MG-ND	-3.19	1.99	2.05
14	B	1201	CLA	CHB-C1B	3.19	1.46	1.39
14	G	1123	CLA	OBD-CAD	3.19	1.28	1.22
14	B	1202	CLA	OBD-CAD	3.19	1.28	1.22
14	H	1223	CLA	C4B-NB	-3.19	1.33	1.37
14	b	1204	CLA	CHC-C4B	3.19	1.46	1.39
14	H	1022	CLA	CHD-C4C	3.19	1.46	1.39
15	b	1207	F6C	C4C-NC	-3.19	1.33	1.37
14	B	1222	CLA	C1C-NC	-3.19	1.32	1.37
14	G	1114	CLA	CHB-C1B	3.19	1.46	1.39
14	G	1107	CLA	OBD-CAD	3.19	1.28	1.22
14	G	1117	CLA	C4B-NB	-3.19	1.33	1.37
14	A	1133	CLA	C1B-NB	-3.19	1.33	1.37
14	a	1122	CLA	CHC-C4B	3.19	1.46	1.39
14	A	1122	CLA	CHC-C4B	3.19	1.46	1.39
14	a	1114	CLA	C1D-ND	-3.19	1.33	1.37
14	a	1115	CLA	C1B-NB	-3.19	1.33	1.37
14	A	1107	CLA	C1B-NB	-3.19	1.33	1.37
14	a	1111	CLA	C1C-NC	-3.19	1.32	1.37
14	G	1012	CLA	OBD-CAD	3.19	1.28	1.22
14	B	1224	CLA	CHB-C1B	3.19	1.46	1.39
14	b	1218	CLA	CHD-C4C	3.19	1.46	1.39
14	G	1115	CLA	MG-ND	-3.19	1.99	2.05
15	B	1238	F6C	OBD-CAD	3.19	1.28	1.22
14	H	1220	CLA	CHC-C4B	3.19	1.46	1.39
14	b	1234	CLA	MG-ND	-3.19	1.99	2.05
14	G	1122	CLA	CHC-C4B	3.19	1.46	1.39
14	b	1223	CLA	C1C-NC	-3.19	1.32	1.37
14	G	1133	CLA	C4B-NB	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1220	CLA	CHC-C4B	3.19	1.46	1.39
18	G	4002	BCR	C11-C12	-3.18	1.26	1.34
14	H	1225	CLA	C4B-NB	-3.18	1.33	1.37
14	B	1022	CLA	CHB-C1B	3.18	1.46	1.39
15	b	1237	F6C	CHC-C1C	3.18	1.46	1.39
14	a	1125	CLA	CHC-C4B	3.18	1.46	1.39
14	B	1217	CLA	OBD-CAD	3.18	1.28	1.22
14	A	1013	CLA	C4B-NB	-3.18	1.33	1.37
14	G	1101	CLA	C1B-NB	-3.18	1.33	1.37
14	a	1101	CLA	C1B-NB	-3.18	1.33	1.37
14	B	1223	CLA	C1C-NC	-3.18	1.32	1.37
14	b	1022	CLA	CHD-C4C	3.18	1.46	1.39
14	H	1204	CLA	C1C-NC	-3.18	1.32	1.37
14	b	1022	CLA	C4B-NB	-3.18	1.33	1.37
14	G	1138	CLA	MG-ND	-3.18	1.99	2.05
14	a	1102	CLA	CHB-C1B	3.18	1.46	1.39
14	b	1220	CLA	CHC-C4B	3.18	1.46	1.39
14	H	1221	CLA	C1C-NC	-3.18	1.32	1.37
14	B	1225	CLA	C1C-NC	-3.18	1.32	1.37
14	A	1115	CLA	MG-ND	-3.18	1.99	2.05
15	B	1237	F6C	CHC-C1C	3.18	1.46	1.39
14	A	1138	CLA	MG-ND	-3.18	1.99	2.05
14	B	1234	CLA	MG-ND	-3.18	1.99	2.05
14	b	1202	CLA	OBD-CAD	3.18	1.28	1.22
14	A	1012	CLA	OBD-CAD	3.18	1.28	1.22
14	B	1022	CLA	CHD-C4C	3.18	1.46	1.39
14	a	1127	CLA	C4B-NB	-3.18	1.33	1.37
14	b	1201	CLA	CHB-C1B	3.17	1.46	1.39
14	G	1126	CLA	C1C-NC	-3.17	1.32	1.37
14	x	1701	CLA	MG-ND	-3.17	1.99	2.05
15	H	1237	F6C	CHC-C1C	3.17	1.46	1.39
14	A	1105	CLA	C4B-NB	-3.17	1.33	1.37
14	A	1111	CLA	C1C-NC	-3.17	1.32	1.37
14	a	1131	CLA	OBD-CAD	3.17	1.27	1.22
14	A	1131	CLA	OBD-CAD	3.17	1.27	1.22
14	G	1140	CLA	C1C-NC	-3.17	1.32	1.37
14	G	1131	CLA	CHB-C1B	3.17	1.46	1.39
14	W	1701	CLA	MG-ND	-3.17	1.99	2.05
14	U	1502	CLA	C1B-NB	-3.17	1.33	1.37
14	B	1216	CLA	CHB-C1B	3.17	1.46	1.39
14	a	1111	CLA	C4B-NB	-3.17	1.33	1.37
14	A	1118	CLA	C1B-NB	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	X	1701	CLA	MG-ND	-3.17	1.99	2.05
14	A	1127	CLA	C4B-NB	-3.17	1.33	1.37
14	B	1225	CLA	C4B-NB	-3.17	1.33	1.37
14	B	1214	CLA	OBD-CAD	3.17	1.27	1.22
14	a	1139	CLA	MG-ND	-3.17	1.99	2.05
15	B	1238	F6C	MG-NC	3.17	2.12	2.05
14	b	1203	CLA	C1C-NC	-3.17	1.32	1.37
14	B	1221	CLA	C1C-NC	-3.17	1.32	1.37
14	H	1224	CLA	CHB-C1B	3.17	1.46	1.39
15	H	1207	F6C	MG-ND	-3.17	1.98	2.06
15	b	1207	F6C	MG-ND	-3.17	1.98	2.06
14	U	1503	CLA	MG-ND	-3.17	1.99	2.05
14	A	1101	CLA	C1B-NB	-3.17	1.33	1.37
14	B	1208	CLA	MG-ND	-3.17	1.99	2.05
15	B	1207	F6C	MG-ND	-3.17	1.98	2.06
14	b	1201	CLA	C4B-NB	-3.17	1.33	1.37
14	G	1131	CLA	C1C-NC	-3.17	1.32	1.37
14	G	1132	CLA	CHB-C1B	3.16	1.46	1.39
15	B	1238	F6C	C4C-NC	-3.16	1.33	1.37
14	H	1214	CLA	OBD-CAD	3.16	1.27	1.22
14	A	1131	CLA	C1C-NC	-3.16	1.32	1.37
14	a	1103	CLA	C4B-NB	-3.16	1.33	1.37
14	a	1131	CLA	CHB-C1B	3.16	1.46	1.39
14	B	1211	CLA	C4B-NB	-3.16	1.33	1.37
14	B	1201	CLA	C1C-NC	-3.16	1.32	1.37
14	H	1231	CLA	C1B-NB	-3.16	1.33	1.37
15	b	1238	F6C	C4C-NC	-3.16	1.33	1.37
14	H	1222	CLA	C1C-NC	-3.16	1.32	1.37
14	A	1140	CLA	C1C-NC	-3.16	1.32	1.37
14	A	1107	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1139	CLA	MG-ND	-3.16	1.99	2.05
14	b	1219	CLA	CHB-C1B	3.16	1.46	1.39
14	G	1131	CLA	OBD-CAD	3.16	1.27	1.22
14	A	1114	CLA	CHB-C1B	3.16	1.46	1.39
14	a	1136	CLA	C1C-NC	-3.16	1.32	1.37
14	B	1232	CLA	MG-ND	-3.16	1.99	2.05
14	A	1135	CLA	C1C-NC	-3.16	1.32	1.37
14	L	1501	CLA	C1C-NC	-3.16	1.32	1.37
14	a	1012	CLA	CHC-C4B	3.16	1.46	1.39
14	H	1218	CLA	C3D-C2D	3.16	1.47	1.39
14	B	1203	CLA	C1C-NC	-3.16	1.32	1.37
14	b	1022	CLA	CHB-C1B	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	1501	CLA	C1C-NC	-3.16	1.32	1.37
14	a	1138	CLA	C4B-NB	-3.16	1.33	1.37
15	H	1207	F6C	C4C-NC	-3.16	1.33	1.37
14	H	1232	CLA	MG-ND	-3.16	1.99	2.05
14	a	1012	CLA	OBD-CAD	3.16	1.27	1.22
14	G	1130	CLA	C1C-NC	-3.15	1.32	1.37
14	H	1205	CLA	CHB-C1B	3.15	1.46	1.39
14	A	1125	CLA	CHC-C4B	3.15	1.46	1.39
14	G	1129	CLA	OBD-CAD	3.15	1.27	1.22
14	b	1217	CLA	OBD-CAD	3.15	1.27	1.22
14	H	1204	CLA	CHC-C4B	3.15	1.46	1.39
14	H	1211	CLA	C4B-NB	-3.15	1.33	1.37
14	A	1103	CLA	C4B-NB	-3.15	1.33	1.37
14	A	1132	CLA	C1B-NB	-3.15	1.33	1.37
14	A	1139	CLA	C1B-NB	-3.15	1.33	1.37
14	H	1201	CLA	C4B-NB	-3.15	1.33	1.37
14	H	1021	CLA	OBD-CAD	3.15	1.27	1.22
15	B	1237	F6C	OBD-CAD	3.15	1.27	1.22
14	G	1104	CLA	C4B-NB	-3.15	1.33	1.37
14	b	1213	CLA	MG-ND	-3.15	1.99	2.05
18	A	4002	BCR	C11-C12	-3.15	1.26	1.34
14	A	1135	CLA	CHC-C4B	3.15	1.46	1.39
14	G	1112	CLA	MG-ND	-3.15	1.99	2.05
14	G	1103	CLA	C4B-NB	-3.15	1.33	1.37
14	H	1022	CLA	CHB-C1B	3.15	1.46	1.39
14	G	1111	CLA	C1C-NC	-3.15	1.32	1.37
14	b	1221	CLA	C1C-NC	-3.15	1.32	1.37
14	B	1204	CLA	C1C-NC	-3.15	1.32	1.37
14	a	1104	CLA	C4B-NB	-3.15	1.33	1.37
14	A	1112	CLA	MG-ND	-3.15	1.99	2.05
14	G	1138	CLA	OBD-CAD	3.15	1.27	1.22
14	H	1213	CLA	MG-ND	-3.15	1.99	2.05
14	B	1201	CLA	C4B-NB	-3.15	1.33	1.37
14	A	1132	CLA	CHB-C1B	3.14	1.46	1.39
14	H	1213	CLA	C1B-NB	-3.14	1.33	1.37
14	H	1223	CLA	C1C-NC	-3.14	1.32	1.37
14	A	1136	CLA	C1C-NC	-3.14	1.32	1.37
14	B	1021	CLA	C4B-NB	-3.14	1.33	1.37
14	B	1021	CLA	OBD-CAD	3.14	1.27	1.22
14	G	1106	CLA	C1C-NC	-3.14	1.32	1.37
14	b	1204	CLA	C1C-NC	-3.14	1.32	1.37
14	H	1225	CLA	OBD-CAD	3.14	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1113	CLA	C1C-NC	-3.14	1.32	1.37
14	G	1102	CLA	CHB-C1B	3.14	1.46	1.39
14	B	1218	CLA	C3D-C2D	3.14	1.47	1.39
14	G	1114	CLA	C1D-ND	-3.14	1.33	1.37
14	H	1021	CLA	C4B-NB	-3.14	1.33	1.37
15	b	1238	F6C	MG-NC	3.14	2.12	2.05
14	G	1136	CLA	C1C-NC	-3.14	1.32	1.37
14	H	1203	CLA	C1C-NC	-3.14	1.32	1.37
15	H	1238	F6C	OBD-CAD	3.14	1.27	1.22
14	a	1106	CLA	C1C-NC	-3.14	1.32	1.37
14	A	1139	CLA	MG-ND	-3.14	1.99	2.05
14	H	1234	CLA	C1C-NC	-3.14	1.32	1.37
14	b	1225	CLA	OBD-CAD	3.14	1.27	1.22
14	B	1213	CLA	MG-ND	-3.14	1.99	2.05
14	H	1220	CLA	C4B-NB	-3.14	1.33	1.37
14	H	1233	CLA	C1D-ND	-3.14	1.33	1.37
14	b	1212	CLA	C1B-NB	-3.14	1.33	1.37
14	b	1204	CLA	OBD-CAD	3.14	1.27	1.22
14	G	1138	CLA	C4B-NB	-3.14	1.33	1.37
14	A	1131	CLA	CHB-C1B	3.14	1.46	1.39
14	H	1217	CLA	OBD-CAD	3.14	1.27	1.22
14	B	1225	CLA	OBD-CAD	3.14	1.27	1.22
15	b	1238	F6C	OBD-CAD	3.13	1.27	1.22
14	a	1112	CLA	C1C-NC	-3.13	1.32	1.37
14	a	1135	CLA	C1C-NC	-3.13	1.32	1.37
15	b	1237	F6C	OBD-CAD	3.13	1.27	1.22
14	G	1111	CLA	C4B-NB	-3.13	1.33	1.37
14	A	1112	CLA	C4B-NB	-3.13	1.33	1.37
14	G	1140	CLA	OBD-CAD	3.13	1.27	1.22
15	A	1121	F6C	C1D-ND	-3.13	1.33	1.37
14	G	1108	CLA	MG-ND	-3.13	1.99	2.05
14	a	1136	CLA	OBD-CAD	3.13	1.27	1.22
14	b	1218	CLA	C3D-C2D	3.13	1.47	1.39
14	H	1204	CLA	C4B-NB	-3.13	1.33	1.37
14	B	1233	CLA	C1D-ND	-3.13	1.33	1.37
14	B	1212	CLA	C1B-NB	-3.13	1.33	1.37
14	b	1222	CLA	OBD-CAD	3.13	1.27	1.22
14	A	1140	CLA	OBD-CAD	3.13	1.27	1.22
14	G	1112	CLA	C1C-NC	-3.13	1.33	1.37
14	a	1112	CLA	MG-ND	-3.13	1.99	2.05
14	a	1139	CLA	C1B-NB	-3.13	1.33	1.37
14	B	1204	CLA	OBD-CAD	3.13	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1138	CLA	C4B-NB	-3.13	1.33	1.37
14	a	1131	CLA	C1C-NC	-3.13	1.33	1.37
14	U	1501	CLA	C1C-NC	-3.13	1.33	1.37
15	H	1237	F6C	OBD-CAD	3.13	1.27	1.22
14	a	1123	CLA	OBD-CAD	3.13	1.27	1.22
14	a	1129	CLA	OBD-CAD	3.13	1.27	1.22
14	l	1503	CLA	MG-ND	-3.13	1.99	2.05
14	a	1105	CLA	C1B-NB	-3.13	1.33	1.37
14	b	1211	CLA	C4B-NB	-3.13	1.33	1.37
14	A	1114	CLA	C1D-ND	-3.13	1.33	1.37
14	b	1213	CLA	C1B-NB	-3.13	1.33	1.37
14	b	1222	CLA	C1C-NC	-3.13	1.33	1.37
14	H	1231	CLA	MG-ND	-3.13	1.99	2.05
14	A	1108	CLA	MG-ND	-3.13	1.99	2.05
14	B	1235	CLA	MG-ND	-3.13	1.99	2.05
14	A	1102	CLA	CHB-C1B	3.12	1.46	1.39
14	G	1108	CLA	C1C-NC	-3.12	1.33	1.37
14	a	1108	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1224	CLA	C1C-NC	-3.12	1.33	1.37
14	G	1108	CLA	C4B-NB	-3.12	1.33	1.37
14	H	1222	CLA	OBD-CAD	3.12	1.27	1.22
14	a	1113	CLA	OBD-CAD	3.12	1.27	1.22
14	A	1113	CLA	OBD-CAD	3.12	1.27	1.22
14	A	1129	CLA	OBD-CAD	3.12	1.27	1.22
14	a	1140	CLA	OBD-CAD	3.12	1.27	1.22
14	B	1205	CLA	CHB-C1B	3.12	1.46	1.39
14	L	1503	CLA	MG-ND	-3.12	1.99	2.05
14	a	1128	CLA	OBD-CAD	3.12	1.27	1.22
14	B	1231	CLA	MG-ND	-3.12	1.99	2.05
14	b	1229	CLA	C4B-NB	-3.12	1.33	1.37
14	b	1216	CLA	CHB-C1B	3.12	1.46	1.39
14	a	1132	CLA	CHB-C1B	3.12	1.46	1.39
14	G	1105	CLA	C4B-NB	-3.12	1.33	1.37
14	H	1235	CLA	MG-ND	-3.12	1.99	2.05
14	B	1213	CLA	C1B-NB	-3.12	1.33	1.37
14	G	1135	CLA	C1C-NC	-3.12	1.33	1.37
14	A	1106	CLA	C1C-NC	-3.12	1.33	1.37
14	A	1012	CLA	CHC-C4B	3.12	1.46	1.39
14	b	1234	CLA	C1C-NC	-3.12	1.33	1.37
14	H	1216	CLA	CHB-C1B	3.12	1.46	1.39
14	b	1205	CLA	CHB-C1B	3.12	1.46	1.39
14	b	1220	CLA	MG-ND	-3.12	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	5007	LMG	C43-C42	-3.12	1.32	1.51
14	G	1012	CLA	CHC-C4B	3.11	1.46	1.39
14	a	1113	CLA	C1C-NC	-3.11	1.33	1.37
14	b	1235	CLA	MG-ND	-3.11	1.99	2.05
14	B	1204	CLA	C4B-NB	-3.11	1.33	1.37
14	G	1109	CLA	MG-ND	-3.11	1.99	2.05
14	B	1228	CLA	MG-ND	-3.11	1.99	2.05
14	b	1204	CLA	C4B-NB	-3.11	1.33	1.37
14	G	1112	CLA	C4B-NB	-3.11	1.33	1.37
14	b	1235	CLA	C4B-NB	-3.11	1.33	1.37
14	x	1701	CLA	C1B-NB	-3.11	1.33	1.37
14	H	1228	CLA	MG-ND	-3.11	1.99	2.05
20	U	5007	LMG	C43-C42	-3.11	1.32	1.51
20	l	5007	LMG	C43-C42	-3.11	1.32	1.51
14	A	1108	CLA	C4B-NB	-3.11	1.33	1.37
14	b	1231	CLA	MG-ND	-3.11	1.99	2.05
14	b	1021	CLA	OBD-CAD	3.11	1.27	1.22
14	a	1112	CLA	C4B-NB	-3.11	1.33	1.37
14	a	1132	CLA	C1B-NB	-3.11	1.33	1.37
14	a	1104	CLA	C1C-NC	-3.11	1.33	1.37
14	a	1123	CLA	C4B-NB	-3.10	1.33	1.37
14	G	1128	CLA	OBD-CAD	3.10	1.27	1.22
14	A	1128	CLA	OBD-CAD	3.10	1.27	1.22
14	a	1138	CLA	MG-ND	-3.10	1.99	2.05
14	b	1228	CLA	MG-ND	-3.10	1.99	2.05
14	B	1229	CLA	C4B-NB	-3.10	1.33	1.37
14	H	1211	CLA	C1C-NC	-3.10	1.33	1.37
14	G	1132	CLA	C1C-NC	-3.10	1.33	1.37
14	a	1012	CLA	C1C-NC	-3.10	1.33	1.37
14	a	1109	CLA	MG-ND	-3.10	1.99	2.05
14	a	1140	CLA	C1C-NC	-3.10	1.33	1.37
15	H	1207	F6C	C1D-ND	-3.10	1.33	1.37
14	A	1132	CLA	C1C-NC	-3.10	1.33	1.37
14	b	1212	CLA	MG-ND	-3.10	1.99	2.05
14	A	1111	CLA	C4B-NB	-3.10	1.33	1.37
14	B	1220	CLA	MG-ND	-3.10	1.99	2.05
14	B	1234	CLA	C1C-NC	-3.10	1.33	1.37
14	G	1136	CLA	MG-ND	-3.09	1.99	2.05
14	A	1129	CLA	C4B-NB	-3.09	1.33	1.37
14	A	1112	CLA	C1C-NC	-3.09	1.33	1.37
14	l	1502	CLA	C1C-NC	-3.09	1.33	1.37
15	b	1207	F6C	C1D-ND	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1206	CLA	CHB-C1B	3.09	1.46	1.39
14	a	1136	CLA	CHB-C1B	3.09	1.46	1.39
14	a	1108	CLA	MG-ND	-3.09	1.99	2.05
14	A	1104	CLA	C1C-NC	-3.09	1.33	1.37
14	A	1110	CLA	MG-ND	-3.09	1.99	2.05
14	A	1108	CLA	C1C-NC	-3.09	1.33	1.37
14	B	1212	CLA	MG-ND	-3.09	1.99	2.05
14	A	1104	CLA	C4B-NB	-3.09	1.33	1.37
14	G	1122	CLA	MG-ND	-3.09	1.99	2.05
14	A	1122	CLA	MG-ND	-3.09	1.99	2.05
14	G	1117	CLA	CHC-C4B	3.09	1.46	1.39
14	G	1110	CLA	MG-ND	-3.09	1.99	2.05
15	H	1237	F6C	MG-NC	3.09	2.11	2.05
14	H	1220	CLA	MG-ND	-3.09	1.99	2.05
14	H	1235	CLA	C4B-NB	-3.09	1.33	1.37
14	G	1113	CLA	OBD-CAD	3.09	1.27	1.22
14	G	1136	CLA	OBD-CAD	3.09	1.27	1.22
14	A	1136	CLA	CHB-C1B	3.09	1.46	1.39
14	B	1226	CLA	C3D-C2D	3.09	1.47	1.39
14	B	1209	CLA	C1B-NB	-3.08	1.33	1.37
14	b	1211	CLA	C1C-NC	-3.08	1.33	1.37
14	b	1224	CLA	C1C-NC	-3.08	1.33	1.37
14	b	1226	CLA	C3D-C2D	3.08	1.47	1.39
14	A	1109	CLA	MG-ND	-3.08	1.99	2.05
15	a	1121	F6C	C1D-ND	-3.08	1.33	1.37
14	U	1503	CLA	C4B-NB	-3.08	1.33	1.37
14	G	1138	CLA	CHB-C1B	3.08	1.46	1.39
14	a	1117	CLA	CHC-C4B	3.08	1.46	1.39
14	A	1113	CLA	MG-ND	-3.08	1.99	2.05
14	L	1502	CLA	C1C-NC	-3.08	1.33	1.37
14	H	1226	CLA	C3D-C2D	3.08	1.47	1.39
15	B	1207	F6C	C1D-ND	-3.08	1.33	1.37
14	G	1012	CLA	C1C-NC	-3.07	1.33	1.37
15	B	1238	F6C	CHB-C1B	3.07	1.46	1.39
14	H	1212	CLA	MG-ND	-3.07	1.99	2.05
14	a	1122	CLA	MG-ND	-3.07	1.99	2.05
14	a	1119	CLA	C3D-C2D	3.07	1.47	1.39
14	A	1123	CLA	C4B-NB	-3.07	1.33	1.37
14	L	1503	CLA	C4B-NB	-3.07	1.33	1.37
14	G	1109	CLA	C1C-NC	-3.07	1.33	1.37
15	b	1238	F6C	CHB-C1B	3.07	1.46	1.39
14	X	1701	CLA	C1B-NB	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1229	CLA	C4B-NB	-3.07	1.33	1.37
14	H	1236	CLA	MG-ND	-3.07	1.99	2.05
14	l	1503	CLA	C4B-NB	-3.07	1.33	1.37
15	G	1121	F6C	C1D-ND	-3.07	1.33	1.37
14	H	1204	CLA	OBD-CAD	3.07	1.27	1.22
15	b	1238	F6C	MG-ND	-3.07	1.99	2.06
14	H	1022	CLA	OBD-CAD	3.07	1.27	1.22
14	G	1129	CLA	C4B-NB	-3.07	1.33	1.37
14	B	1217	CLA	MG-ND	-3.07	1.99	2.05
14	B	1236	CLA	MG-ND	-3.07	1.99	2.05
14	G	1113	CLA	C1C-NC	-3.07	1.33	1.37
15	H	1238	F6C	CHB-C1B	3.07	1.46	1.39
14	G	1111	CLA	MG-ND	-3.06	1.99	2.05
14	a	1130	CLA	CHB-C1B	3.06	1.46	1.39
14	a	1110	CLA	MG-ND	-3.06	1.99	2.05
14	B	1211	CLA	C1C-NC	-3.06	1.33	1.37
14	G	1136	CLA	CHB-C1B	3.06	1.46	1.39
14	A	1119	CLA	C3D-C2D	3.06	1.47	1.39
14	a	1129	CLA	C4B-NB	-3.06	1.33	1.37
15	H	1238	F6C	MG-ND	-3.06	1.99	2.06
14	l	1502	CLA	CHB-C1B	3.06	1.46	1.39
14	A	1117	CLA	CHC-C4B	3.06	1.46	1.39
14	a	1108	CLA	C4B-NB	-3.06	1.33	1.37
14	H	1217	CLA	MG-ND	-3.06	1.99	2.05
14	B	1235	CLA	C4B-NB	-3.06	1.33	1.37
14	L	1502	CLA	CHB-C1B	3.06	1.46	1.39
14	B	1224	CLA	C1C-NC	-3.06	1.33	1.37
14	a	1113	CLA	MG-ND	-3.06	1.99	2.05
14	a	1132	CLA	C1C-NC	-3.06	1.33	1.37
15	B	1237	F6C	MG-NC	3.06	2.11	2.05
14	H	1206	CLA	CHB-C1B	3.06	1.46	1.39
14	b	1021	CLA	C4B-NB	-3.06	1.33	1.37
14	G	1106	CLA	MG-ND	-3.05	1.99	2.05
14	b	1206	CLA	CHB-C1B	3.05	1.46	1.39
14	a	1124	CLA	MG-ND	-3.05	1.99	2.05
14	A	1106	CLA	MG-ND	-3.05	1.99	2.05
14	H	1209	CLA	C1B-NB	-3.05	1.33	1.37
14	W	1701	CLA	C1B-NB	-3.05	1.33	1.37
14	U	1502	CLA	CHB-C1B	3.05	1.46	1.39
14	a	1138	CLA	CHB-C1B	3.05	1.46	1.39
14	b	1231	CLA	C1C-NC	-3.05	1.33	1.37
14	A	1012	CLA	C1C-NC	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1222	CLA	OBD-CAD	3.05	1.27	1.22
14	G	1123	CLA	C4B-NB	-3.05	1.33	1.37
14	G	1012	CLA	CHB-C1B	3.05	1.46	1.39
14	A	1119	CLA	CHB-C1B	3.05	1.46	1.39
14	a	1106	CLA	MG-ND	-3.05	1.99	2.05
14	a	1136	CLA	MG-ND	-3.05	1.99	2.05
15	b	1207	F6C	OBD-CAD	3.05	1.27	1.22
15	b	1237	F6C	MG-NC	3.05	2.11	2.05
14	G	1130	CLA	CHB-C1B	3.05	1.46	1.39
14	a	1120	CLA	MG-ND	-3.05	1.99	2.05
14	b	1209	CLA	C1B-NB	-3.05	1.33	1.37
14	G	1104	CLA	C1C-NC	-3.05	1.33	1.37
14	G	1124	CLA	MG-ND	-3.04	1.99	2.05
14	A	1111	CLA	MG-ND	-3.04	1.99	2.05
14	U	1502	CLA	C1C-NC	-3.04	1.33	1.37
14	b	1021	CLA	CHD-C4C	3.04	1.46	1.39
14	A	1120	CLA	MG-ND	-3.04	1.99	2.05
14	a	1012	CLA	CHB-C1B	3.04	1.46	1.39
14	A	1105	CLA	C1C-NC	-3.04	1.33	1.37
15	B	1207	F6C	OBD-CAD	3.04	1.27	1.22
14	A	1012	CLA	C3D-C2D	3.04	1.47	1.39
14	b	1022	CLA	OBD-CAD	3.04	1.27	1.22
15	B	1238	F6C	MG-ND	-3.04	1.99	2.06
14	G	1120	CLA	MG-ND	-3.04	1.99	2.05
14	H	1023	CLA	CHB-C1B	3.04	1.46	1.39
14	G	1012	CLA	C3D-C2D	3.04	1.47	1.39
14	A	1012	CLA	CHB-C1B	3.04	1.46	1.39
14	b	1023	CLA	CHB-C1B	3.03	1.46	1.39
15	H	1207	F6C	OBD-CAD	3.03	1.27	1.22
14	A	1132	CLA	MG-ND	-3.03	1.99	2.05
14	G	1107	CLA	C4B-NB	-3.03	1.33	1.37
14	A	1134	CLA	C3D-C2D	3.03	1.47	1.39
14	A	1107	CLA	C1C-NC	-3.03	1.33	1.37
14	B	1212	CLA	C1C-NC	-3.03	1.33	1.37
14	A	1136	CLA	MG-ND	-3.03	1.99	2.05
14	G	1119	CLA	CHB-C1B	3.03	1.46	1.39
14	B	1023	CLA	CHB-C1B	3.03	1.46	1.39
14	a	1107	CLA	C4B-NB	-3.03	1.33	1.37
14	B	1202	CLA	C1C-NC	-3.03	1.33	1.37
14	A	1124	CLA	MG-ND	-3.03	1.99	2.05
14	a	1105	CLA	C1C-NC	-3.03	1.33	1.37
14	B	1215	CLA	C1C-NC	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1132	CLA	MG-ND	-3.03	1.99	2.05
14	a	1134	CLA	MG-NC	3.03	2.13	2.06
14	b	1215	CLA	C1C-NC	-3.03	1.33	1.37
14	B	1206	CLA	CHC-C4B	3.03	1.46	1.39
14	A	1138	CLA	CHB-C1B	3.03	1.46	1.39
14	G	1113	CLA	MG-ND	-3.03	1.99	2.05
14	a	1105	CLA	MG-ND	-3.03	1.99	2.05
14	b	1221	CLA	C4B-NB	-3.02	1.33	1.37
14	a	1132	CLA	MG-ND	-3.02	1.99	2.05
14	B	1216	CLA	MG-ND	-3.02	1.99	2.05
14	A	1136	CLA	OBD-CAD	3.02	1.27	1.22
14	a	1012	CLA	C3D-C2D	3.02	1.47	1.39
14	a	1111	CLA	MG-ND	-3.02	1.99	2.05
14	H	1216	CLA	C1C-NC	-3.02	1.33	1.37
14	b	1212	CLA	C4B-NB	-3.02	1.33	1.37
14	G	1119	CLA	C3D-C2D	3.02	1.47	1.39
14	G	1134	CLA	MG-NC	3.02	2.13	2.06
14	G	1105	CLA	C1C-NC	-3.02	1.33	1.37
14	a	1134	CLA	C3D-C2D	3.02	1.47	1.39
15	b	1207	F6C	CHC-C1C	3.02	1.46	1.39
14	B	1231	CLA	C1C-NC	-3.02	1.33	1.37
15	B	1207	F6C	CHC-C1C	3.02	1.46	1.39
14	b	1236	CLA	MG-ND	-3.02	1.99	2.05
14	A	1134	CLA	MG-NC	3.02	2.13	2.06
14	H	1206	CLA	C3D-C2D	3.01	1.47	1.39
14	k	1401	CLA	MG-NC	3.01	2.13	2.06
15	B	1237	F6C	C3B-C2B	3.01	1.46	1.39
14	a	1114	CLA	MG-ND	-3.01	1.99	2.05
14	G	1134	CLA	C3D-C2D	3.01	1.47	1.39
14	a	1119	CLA	CHB-C1B	3.01	1.46	1.39
15	H	1237	F6C	C3B-C2B	3.01	1.46	1.39
14	A	1130	CLA	CHB-C1B	3.01	1.46	1.39
14	b	1217	CLA	MG-ND	-3.01	1.99	2.05
14	B	1210	CLA	MG-ND	-3.01	1.99	2.05
14	A	1115	CLA	C4B-NB	-3.01	1.33	1.37
14	b	1206	CLA	CHC-C4B	3.01	1.46	1.39
14	H	1206	CLA	CHC-C4B	3.01	1.46	1.39
14	a	1109	CLA	C1C-NC	-3.01	1.33	1.37
14	b	1210	CLA	MG-ND	-3.01	1.99	2.05
14	H	1212	CLA	C1C-NC	-3.01	1.33	1.37
14	H	1216	CLA	MG-ND	-3.01	1.99	2.05
14	A	1105	CLA	MG-ND	-3.01	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1128	CLA	C4B-NB	-3.01	1.33	1.37
14	H	1210	CLA	MG-ND	-3.01	1.99	2.05
14	B	1216	CLA	C1C-NC	-3.01	1.33	1.37
14	A	1128	CLA	C4B-NB	-3.01	1.33	1.37
14	B	1212	CLA	C4B-NB	-3.01	1.33	1.37
14	H	1231	CLA	C1C-NC	-3.01	1.33	1.37
14	b	1212	CLA	C1C-NC	-3.01	1.33	1.37
14	B	1022	CLA	OBD-CAD	3.00	1.27	1.22
14	b	1206	CLA	C3D-C2D	3.00	1.47	1.39
14	B	1221	CLA	C4B-NB	-3.00	1.33	1.37
14	b	1216	CLA	MG-ND	-3.00	1.99	2.05
14	H	1202	CLA	C1C-NC	-3.00	1.33	1.37
14	b	1216	CLA	C1C-NC	-3.00	1.33	1.37
14	b	1208	CLA	C4B-NB	-3.00	1.33	1.37
14	a	1123	CLA	MG-NC	3.00	2.13	2.06
14	G	1107	CLA	C1C-NC	-3.00	1.33	1.37
14	b	1205	CLA	OBD-CAD	3.00	1.27	1.22
15	H	1237	F6C	C4B-NB	-3.00	1.33	1.37
14	G	1123	CLA	MG-NC	3.00	2.13	2.06
14	H	1215	CLA	C1C-NC	-3.00	1.33	1.37
14	G	1127	CLA	C1C-NC	-3.00	1.33	1.37
14	B	1231	CLA	C4B-NB	-3.00	1.33	1.37
14	U	1501	CLA	C3D-C2D	3.00	1.47	1.39
14	b	1208	CLA	C1C-NC	-3.00	1.33	1.37
14	A	1114	CLA	MG-ND	-2.99	1.99	2.05
14	L	1501	CLA	C3D-C2D	2.99	1.47	1.39
14	H	1231	CLA	C4B-NB	-2.99	1.33	1.37
14	H	1209	CLA	MG-ND	-2.99	1.99	2.05
14	B	1021	CLA	CHD-C4C	2.99	1.46	1.39
14	G	1103	CLA	OBD-CAD	2.99	1.27	1.22
14	H	1221	CLA	C4B-NB	-2.99	1.33	1.37
14	A	1109	CLA	C1C-NC	-2.99	1.33	1.37
14	H	1021	CLA	CHD-C4C	2.99	1.46	1.39
18	i	4018	BCR	C30-C25	-2.99	1.50	1.53
14	B	1209	CLA	MG-ND	-2.99	1.99	2.05
14	b	1209	CLA	MG-ND	-2.99	1.99	2.05
14	G	1105	CLA	MG-ND	-2.99	1.99	2.05
14	b	1226	CLA	CHC-C4B	2.99	1.46	1.39
15	A	1121	F6C	C4C-NC	-2.99	1.33	1.37
14	H	1233	CLA	C3D-C2D	2.99	1.47	1.39
14	H	1211	CLA	MG-ND	-2.99	1.99	2.05
18	b	4005	BCR	C30-C25	-2.99	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1120	CLA	C1C-NC	-2.99	1.33	1.37
14	G	1114	CLA	MG-ND	-2.99	1.99	2.05
15	H	1207	F6C	CHC-C1C	2.99	1.46	1.39
14	l	1501	CLA	C3D-C2D	2.98	1.47	1.39
14	G	1118	CLA	C1C-NC	-2.98	1.33	1.37
14	G	1013	CLA	C1C-NC	-2.98	1.33	1.37
14	A	1128	CLA	CHC-C4B	2.98	1.46	1.39
14	G	1115	CLA	C4B-NB	-2.98	1.33	1.37
14	G	1134	CLA	C1B-NB	-2.98	1.33	1.37
14	A	1131	CLA	C4B-NB	-2.98	1.33	1.37
14	a	1013	CLA	C1C-NC	-2.98	1.33	1.37
14	A	1123	CLA	MG-NC	2.98	2.13	2.06
14	B	1213	CLA	C1C-NC	-2.98	1.33	1.37
14	a	1128	CLA	C4B-NB	-2.98	1.33	1.37
14	H	1213	CLA	C1C-NC	-2.98	1.33	1.37
14	b	1202	CLA	C1C-NC	-2.98	1.33	1.37
14	U	1502	CLA	MG-ND	-2.98	1.99	2.05
14	K	1401	CLA	MG-NC	2.98	2.13	2.06
14	a	1131	CLA	C4B-NB	-2.98	1.33	1.37
14	H	1228	CLA	C4B-NB	-2.98	1.33	1.37
14	a	1107	CLA	C1C-NC	-2.98	1.33	1.37
14	a	1134	CLA	C1B-NB	-2.98	1.34	1.37
14	G	1101	CLA	C1C-NC	-2.98	1.33	1.37
14	G	1129	CLA	C1C-NC	-2.98	1.33	1.37
15	a	1121	F6C	C4C-NC	-2.98	1.34	1.37
15	b	1237	F6C	C4B-NB	-2.98	1.33	1.37
14	b	1231	CLA	C4B-NB	-2.98	1.34	1.37
14	B	1226	CLA	CHC-C4B	2.97	1.46	1.39
14	A	1107	CLA	C4B-NB	-2.97	1.34	1.37
14	l	1502	CLA	MG-ND	-2.97	1.99	2.05
14	L	1502	CLA	MG-ND	-2.97	1.99	2.05
14	H	1226	CLA	CHC-C4B	2.97	1.46	1.39
14	B	1206	CLA	C3D-C2D	2.97	1.47	1.39
14	T	1401	CLA	MG-NC	2.97	2.13	2.06
14	B	1233	CLA	C3D-C2D	2.97	1.47	1.39
14	L	1502	CLA	OBD-CAD	2.97	1.27	1.22
14	B	1208	CLA	C1C-NC	-2.97	1.33	1.37
15	H	1207	F6C	CHB-C4A	-2.97	1.32	1.38
14	b	1213	CLA	C1C-NC	-2.97	1.33	1.37
14	B	1205	CLA	OBD-CAD	2.96	1.27	1.22
14	B	1229	CLA	C1C-NC	-2.96	1.33	1.37
15	H	1230	F6C	C1D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1208	CLA	C1C-NC	-2.96	1.33	1.37
14	b	1227	CLA	C4B-NB	-2.96	1.34	1.37
14	H	1022	CLA	C1C-NC	-2.96	1.33	1.37
14	H	1205	CLA	OBD-CAD	2.96	1.27	1.22
14	b	1233	CLA	C3D-C2D	2.96	1.47	1.39
20	U	5007	LMG	C22-C21	-2.96	1.33	1.51
14	b	1239	CLA	C4B-NB	-2.96	1.34	1.37
15	b	1237	F6C	C3B-C2B	2.96	1.46	1.39
15	G	1121	F6C	C4C-NC	-2.96	1.34	1.37
14	H	1213	CLA	C4B-NB	-2.96	1.34	1.37
18	B	4005	BCR	C30-C25	-2.96	1.50	1.53
14	H	1217	CLA	C1B-NB	-2.96	1.34	1.37
14	A	1138	CLA	C1C-NC	-2.96	1.33	1.37
14	b	1211	CLA	MG-ND	-2.96	1.99	2.05
14	B	1204	CLA	CHB-C1B	2.95	1.46	1.39
14	A	1129	CLA	C1C-NC	-2.95	1.33	1.37
14	b	1216	CLA	C3D-C2D	2.95	1.47	1.39
20	L	5007	LMG	C22-C21	-2.95	1.33	1.51
14	b	1229	CLA	C1C-NC	-2.95	1.33	1.37
14	b	1204	CLA	CHB-C1B	2.95	1.46	1.39
14	b	1215	CLA	CHB-C1B	2.95	1.46	1.39
15	b	1230	F6C	C1D-ND	-2.95	1.33	1.37
14	b	1228	CLA	C4B-NB	-2.95	1.34	1.37
15	b	1207	F6C	CHB-C4A	-2.95	1.32	1.38
14	H	1208	CLA	C4B-NB	-2.95	1.34	1.37
14	B	1215	CLA	C3D-C2D	2.95	1.47	1.39
14	B	1217	CLA	C1B-NB	-2.95	1.34	1.37
15	b	1230	F6C	C3B-C2B	2.95	1.46	1.39
15	B	1237	F6C	C4B-NB	-2.95	1.33	1.37
14	a	1127	CLA	C1C-NC	-2.95	1.33	1.37
14	A	1118	CLA	C1C-NC	-2.95	1.33	1.37
14	H	1233	CLA	C1B-NB	-2.95	1.34	1.37
14	H	1229	CLA	C1C-NC	-2.95	1.33	1.37
14	A	1101	CLA	C1C-NC	-2.95	1.33	1.37
20	l	5007	LMG	C22-C21	-2.95	1.33	1.51
14	B	1023	CLA	CHC-C4B	2.95	1.46	1.39
14	A	1134	CLA	C1B-NB	-2.95	1.34	1.37
14	G	1128	CLA	CHC-C4B	2.95	1.46	1.39
14	b	1219	CLA	MG-ND	-2.95	1.99	2.05
15	B	1207	F6C	CHB-C4A	-2.95	1.32	1.38
14	H	1216	CLA	C3D-C2D	2.95	1.47	1.39
14	a	1101	CLA	C1C-NC	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1013	CLA	C1C-NC	-2.95	1.33	1.37
14	H	1023	CLA	CHC-C4B	2.95	1.46	1.39
14	K	1401	CLA	C1D-ND	-2.94	1.34	1.37
14	a	1118	CLA	C1C-NC	-2.94	1.33	1.37
14	G	1120	CLA	C3D-C2D	2.94	1.47	1.39
15	H	1230	F6C	C3B-C2B	2.94	1.46	1.39
14	H	1219	CLA	MG-ND	-2.94	2.00	2.05
14	B	1216	CLA	C3D-C2D	2.94	1.47	1.39
14	b	1022	CLA	MG-NC	2.94	2.13	2.06
14	B	1218	CLA	MG-NC	2.94	2.13	2.06
14	b	1221	CLA	OBD-CAD	2.94	1.27	1.22
14	a	1138	CLA	C1C-NC	-2.94	1.33	1.37
15	B	1230	F6C	C1D-ND	-2.94	1.33	1.37
14	B	1228	CLA	C4B-NB	-2.94	1.34	1.37
14	H	1239	CLA	C4B-NB	-2.94	1.34	1.37
14	a	1128	CLA	CHC-C4B	2.94	1.46	1.39
14	k	1401	CLA	C3D-C2D	2.94	1.47	1.39
14	a	1103	CLA	OBD-CAD	2.94	1.27	1.22
14	G	1120	CLA	C1C-NC	-2.94	1.33	1.37
14	B	1022	CLA	MG-NC	2.94	2.13	2.06
14	A	1102	CLA	C4B-NB	-2.94	1.34	1.37
14	A	1120	CLA	C1C-NC	-2.94	1.33	1.37
14	B	1235	CLA	C1C-NC	-2.93	1.33	1.37
14	B	1211	CLA	MG-ND	-2.93	2.00	2.05
14	G	1115	CLA	C1C-NC	-2.93	1.33	1.37
14	B	1214	CLA	C3D-C2D	2.93	1.47	1.39
14	G	1131	CLA	C4B-NB	-2.93	1.34	1.37
14	b	1212	CLA	C3D-C2D	2.93	1.47	1.39
14	A	1103	CLA	OBD-CAD	2.93	1.27	1.22
14	G	1133	CLA	C1C-NC	-2.93	1.33	1.37
14	a	1129	CLA	C1C-NC	-2.93	1.33	1.37
15	B	1230	F6C	C3B-C2B	2.93	1.46	1.39
18	I	4018	BCR	C30-C25	-2.93	1.50	1.53
14	H	1204	CLA	CHB-C1B	2.93	1.46	1.39
14	A	1109	CLA	C4B-NB	-2.93	1.34	1.37
18	R	4018	BCR	C30-C25	-2.93	1.50	1.53
14	A	1115	CLA	C1C-NC	-2.93	1.33	1.37
14	H	1212	CLA	C3D-C2D	2.93	1.47	1.39
14	b	1023	CLA	CHC-C4B	2.93	1.46	1.39
14	H	1235	CLA	C3D-C2D	2.93	1.47	1.39
14	H	1212	CLA	C4B-NB	-2.93	1.34	1.37
13	A	1011	CL0	C4A-C3A	-2.93	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1124	CLA	CHB-C1B	2.93	1.46	1.39
14	B	1022	CLA	C1C-NC	-2.93	1.33	1.37
14	T	1401	CLA	C1D-ND	-2.92	1.34	1.37
15	H	1237	F6C	MG-ND	-2.92	1.99	2.06
14	b	1215	CLA	C3D-C2D	2.92	1.47	1.39
14	B	1219	CLA	MG-ND	-2.92	2.00	2.05
14	b	1226	CLA	C4B-NB	-2.92	1.34	1.37
14	A	1138	CLA	C3D-C2D	2.92	1.47	1.39
14	G	1112	CLA	C3D-C2D	2.92	1.47	1.39
14	B	1212	CLA	C3D-C2D	2.92	1.47	1.39
14	A	1124	CLA	CHB-C1B	2.92	1.46	1.39
14	G	1110	CLA	C1C-NC	-2.92	1.33	1.37
14	G	1138	CLA	C1C-NC	-2.92	1.33	1.37
15	B	1237	F6C	MG-ND	-2.92	1.99	2.06
14	H	1235	CLA	C1C-NC	-2.92	1.33	1.37
14	a	1133	CLA	C1C-NC	-2.92	1.33	1.37
14	a	1134	CLA	C1D-ND	-2.92	1.34	1.37
14	B	1233	CLA	C1B-NB	-2.92	1.34	1.37
14	K	1401	CLA	C3D-C2D	2.92	1.46	1.39
14	a	1115	CLA	C4B-NB	-2.92	1.34	1.37
14	B	1227	CLA	C4B-NB	-2.92	1.34	1.37
14	U	1502	CLA	OBD-CAD	2.92	1.27	1.22
14	l	1502	CLA	OBD-CAD	2.92	1.27	1.22
14	A	1127	CLA	C1C-NC	-2.92	1.33	1.37
14	G	1138	CLA	C3D-C2D	2.91	1.46	1.39
14	b	1218	CLA	MG-NC	2.91	2.13	2.06
13	a	1011	CL0	C4A-C3A	-2.91	1.45	1.51
18	H	4005	BCR	C30-C25	-2.91	1.50	1.53
14	G	1109	CLA	C4B-NB	-2.91	1.34	1.37
14	a	1120	CLA	C3D-C2D	2.91	1.46	1.39
14	b	1213	CLA	C4B-NB	-2.91	1.34	1.37
14	a	1138	CLA	C3D-C2D	2.91	1.46	1.39
14	H	1215	CLA	C3D-C2D	2.91	1.46	1.39
14	H	1215	CLA	CHB-C1B	2.91	1.45	1.39
14	a	1124	CLA	CHB-C1B	2.91	1.45	1.39
14	A	1120	CLA	C3D-C2D	2.91	1.46	1.39
14	H	1214	CLA	C3D-C2D	2.91	1.46	1.39
14	T	1401	CLA	C3D-C2D	2.91	1.46	1.39
14	B	1221	CLA	OBD-CAD	2.91	1.27	1.22
14	B	1226	CLA	C4B-NB	-2.91	1.34	1.37
14	b	1217	CLA	C1B-NB	-2.91	1.34	1.37
14	B	1213	CLA	C4B-NB	-2.91	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	k	1401	CLA	C1D-ND	-2.90	1.34	1.37
14	b	1235	CLA	C1C-NC	-2.90	1.33	1.37
14	K	1401	CLA	C4D-CHA	2.90	1.48	1.38
14	b	1022	CLA	C1C-NC	-2.90	1.33	1.37
14	H	1226	CLA	C4B-NB	-2.90	1.34	1.37
14	a	1115	CLA	C1C-NC	-2.90	1.33	1.37
14	b	1235	CLA	C3D-C2D	2.90	1.46	1.39
14	H	1217	CLA	MG-NC	2.90	2.13	2.06
14	H	1221	CLA	OBD-CAD	2.90	1.27	1.22
14	b	1234	CLA	C4B-NB	-2.90	1.34	1.37
14	A	1112	CLA	C3D-C2D	2.90	1.46	1.39
14	G	1102	CLA	C4B-NB	-2.90	1.34	1.37
14	a	1109	CLA	C4B-NB	-2.90	1.34	1.37
13	G	1011	CL0	C4A-C3A	-2.90	1.45	1.51
14	G	1128	CLA	C3D-C2D	2.90	1.46	1.39
14	H	1228	CLA	C3D-C2D	2.90	1.46	1.39
14	b	1214	CLA	C3D-C2D	2.90	1.46	1.39
14	b	1235	CLA	OBD-CAD	2.90	1.27	1.22
14	H	1022	CLA	MG-NC	2.90	2.13	2.06
14	B	1234	CLA	C4B-NB	-2.89	1.34	1.37
14	k	1401	CLA	C4D-CHA	2.89	1.48	1.38
14	B	1215	CLA	CHB-C1B	2.89	1.45	1.39
14	B	1235	CLA	C3D-C2D	2.89	1.46	1.39
14	a	1110	CLA	C1C-NC	-2.89	1.33	1.37
14	a	1128	CLA	C3D-C2D	2.89	1.46	1.39
14	L	1502	CLA	C4B-NB	-2.89	1.34	1.37
14	a	1102	CLA	C4B-NB	-2.89	1.34	1.37
14	B	1208	CLA	C3D-C2D	2.89	1.46	1.39
14	a	1134	CLA	C4D-CHA	2.89	1.48	1.38
14	B	1239	CLA	C4B-NB	-2.89	1.34	1.37
14	G	1134	CLA	C4D-CHA	2.89	1.48	1.38
14	H	1218	CLA	MG-NC	2.88	2.13	2.06
14	A	1134	CLA	C4D-CHA	2.88	1.48	1.38
14	A	1128	CLA	C3D-C2D	2.88	1.46	1.39
14	b	1208	CLA	C3D-C2D	2.88	1.46	1.39
14	T	1401	CLA	C4D-CHA	2.88	1.48	1.38
14	B	1228	CLA	C3D-C2D	2.88	1.46	1.39
14	B	1208	CLA	C4B-NB	-2.88	1.34	1.37
14	A	1110	CLA	C1C-NC	-2.88	1.33	1.37
14	H	1219	CLA	C3D-C2D	2.88	1.46	1.39
14	H	1227	CLA	C4B-NB	-2.88	1.34	1.37
14	X	1701	CLA	MG-NC	2.87	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1221	CLA	C3D-C2D	2.87	1.46	1.39
14	H	1235	CLA	OBD-CAD	2.87	1.27	1.22
14	a	1114	CLA	C3D-C2D	2.87	1.46	1.39
14	a	1108	CLA	C3D-C2D	2.87	1.46	1.39
14	A	1133	CLA	C1C-NC	-2.87	1.33	1.37
14	a	1112	CLA	C3D-C2D	2.87	1.46	1.39
14	B	1219	CLA	C3D-C2D	2.87	1.46	1.39
14	l	1502	CLA	C4B-NB	-2.87	1.34	1.37
15	b	1237	F6C	MG-ND	-2.87	1.99	2.06
14	b	1228	CLA	C3D-C2D	2.87	1.46	1.39
14	b	1217	CLA	MG-NC	2.86	2.13	2.06
14	U	1502	CLA	C3D-C2D	2.86	1.46	1.39
14	H	1227	CLA	C1C-NC	-2.86	1.33	1.37
14	B	1235	CLA	OBD-CAD	2.86	1.27	1.22
14	H	1234	CLA	C4B-NB	-2.86	1.34	1.37
14	G	1114	CLA	C4D-CHA	2.86	1.48	1.38
14	G	1117	CLA	C3D-C2D	2.86	1.46	1.39
14	G	1116	CLA	C4B-NB	-2.86	1.34	1.37
14	a	1114	CLA	C4D-CHA	2.86	1.48	1.38
14	A	1117	CLA	C3D-C2D	2.86	1.46	1.39
14	H	1208	CLA	C3D-C2D	2.86	1.46	1.39
14	b	1221	CLA	C3D-C2D	2.86	1.46	1.39
14	G	1119	CLA	CHC-C4B	2.86	1.45	1.39
14	A	1114	CLA	C3D-C2D	2.86	1.46	1.39
14	W	1701	CLA	MG-NC	2.86	2.13	2.06
14	H	1220	CLA	C3D-C2D	2.86	1.46	1.39
14	B	1233	CLA	MG-NC	2.86	2.13	2.06
14	A	1114	CLA	C4D-CHA	2.86	1.48	1.38
14	H	1232	CLA	MG-NC	2.86	2.13	2.06
14	a	1117	CLA	C4D-CHA	2.85	1.48	1.38
14	b	1233	CLA	C1B-NB	-2.85	1.34	1.37
14	B	1232	CLA	MG-NC	2.85	2.13	2.06
15	G	1121	F6C	C3D-C2D	2.85	1.46	1.39
14	A	1116	CLA	C4B-NB	-2.85	1.34	1.37
14	A	1134	CLA	C1D-ND	-2.85	1.34	1.37
14	A	1126	CLA	CHB-C1B	2.85	1.45	1.39
14	G	1117	CLA	C4D-CHA	2.85	1.48	1.38
14	G	1126	CLA	CHB-C1B	2.85	1.45	1.39
14	B	1214	CLA	C4B-NB	-2.85	1.34	1.37
14	A	1117	CLA	C4D-CHA	2.85	1.48	1.38
14	L	1502	CLA	C3D-C2D	2.85	1.46	1.39
15	B	1238	F6C	C4B-NB	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	x	1701	CLA	MG-NC	2.85	2.13	2.06
14	H	1221	CLA	C3D-C2D	2.85	1.46	1.39
14	l	1502	CLA	C3D-C2D	2.85	1.46	1.39
14	A	1118	CLA	MG-NC	2.85	2.13	2.06
14	B	1217	CLA	MG-NC	2.85	2.13	2.06
14	X	1701	CLA	C1C-NC	-2.85	1.33	1.37
14	G	1114	CLA	C3D-C2D	2.85	1.46	1.39
14	b	1219	CLA	C3D-C2D	2.85	1.46	1.39
14	U	1502	CLA	C4B-NB	-2.84	1.34	1.37
14	G	1118	CLA	MG-NC	2.84	2.13	2.06
14	A	1108	CLA	C3D-C2D	2.84	1.46	1.39
14	a	1125	CLA	CHD-C4C	2.84	1.45	1.39
14	G	1108	CLA	C3D-C2D	2.84	1.46	1.39
14	a	1101	CLA	MG-ND	-2.84	2.00	2.05
14	a	1116	CLA	C4B-NB	-2.84	1.34	1.37
14	b	1232	CLA	C4B-NB	-2.84	1.34	1.37
14	H	1227	CLA	MG-NC	2.84	2.13	2.06
14	b	1233	CLA	MG-NC	2.84	2.13	2.06
14	b	1232	CLA	MG-NC	2.84	2.13	2.06
15	H	1207	F6C	CHB-C1B	2.84	1.45	1.39
14	B	1233	CLA	MG-ND	-2.83	2.00	2.05
14	b	1219	CLA	MG-NC	2.83	2.13	2.06
14	B	1219	CLA	MG-NC	2.83	2.13	2.06
14	a	1013	CLA	C3D-C2D	2.83	1.46	1.39
14	a	1126	CLA	CHB-C1B	2.83	1.45	1.39
14	G	1101	CLA	MG-ND	-2.83	2.00	2.05
14	a	1117	CLA	C3D-C2D	2.83	1.46	1.39
15	a	1121	F6C	C3D-C2D	2.83	1.46	1.39
14	A	1119	CLA	CHC-C4B	2.83	1.45	1.39
14	b	1220	CLA	C3D-C2D	2.83	1.46	1.39
14	A	1125	CLA	CHD-C4C	2.83	1.45	1.39
14	G	1013	CLA	C3D-C2D	2.83	1.46	1.39
14	A	1107	CLA	MG-NC	2.83	2.13	2.06
14	B	1214	CLA	MG-NC	2.83	2.13	2.06
14	H	1234	CLA	OBD-CAD	2.83	1.27	1.22
14	B	1232	CLA	C4B-NB	-2.83	1.34	1.37
14	H	1219	CLA	MG-NC	2.83	2.13	2.06
14	H	1233	CLA	MG-NC	2.83	2.13	2.06
14	a	1125	CLA	OBD-CAD	2.82	1.27	1.22
14	H	1215	CLA	C4D-CHA	2.82	1.48	1.38
14	B	1220	CLA	C3D-C2D	2.82	1.46	1.39
14	H	1233	CLA	MG-ND	-2.82	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1134	CLA	C1D-ND	-2.82	1.34	1.37
14	B	1227	CLA	C1C-NC	-2.82	1.33	1.37
14	a	1105	CLA	C3D-C2D	2.82	1.46	1.39
14	b	1227	CLA	MG-NC	2.82	2.13	2.06
15	b	1207	F6C	CHB-C1B	2.82	1.45	1.39
14	A	1113	CLA	C3D-C2D	2.82	1.46	1.39
14	A	1013	CLA	C3D-C2D	2.82	1.46	1.39
15	B	1237	F6C	C3D-C2D	2.82	1.46	1.39
18	a	4007	BCR	C1-C6	-2.82	1.50	1.53
14	G	1138	CLA	C4D-CHA	2.82	1.48	1.38
14	a	1137	CLA	OBD-CAD	2.81	1.27	1.22
14	a	1119	CLA	CHC-C4B	2.81	1.45	1.39
14	A	1105	CLA	C3D-C2D	2.81	1.46	1.39
14	A	1101	CLA	MG-ND	-2.81	2.00	2.05
14	B	1231	CLA	C3D-C2D	2.81	1.46	1.39
14	G	1105	CLA	C3D-C2D	2.81	1.46	1.39
14	a	1140	CLA	C3D-C2D	2.81	1.46	1.39
14	B	1227	CLA	MG-NC	2.81	2.13	2.06
14	a	1107	CLA	MG-NC	2.81	2.12	2.06
14	B	1223	CLA	OBD-CAD	2.81	1.27	1.22
14	a	1113	CLA	C3D-C2D	2.81	1.46	1.39
14	A	1133	CLA	C3D-C2D	2.81	1.46	1.39
14	H	1214	CLA	C4B-NB	-2.81	1.34	1.37
15	A	1121	F6C	C3D-C2D	2.81	1.46	1.39
14	B	1209	CLA	C1C-NC	-2.81	1.33	1.37
15	B	1207	F6C	CHB-C1B	2.81	1.45	1.39
14	W	1701	CLA	C1C-NC	-2.81	1.33	1.37
14	A	1140	CLA	C3D-C2D	2.81	1.46	1.39
15	H	1237	F6C	C3D-C2D	2.81	1.46	1.39
14	a	1118	CLA	MG-NC	2.81	2.12	2.06
14	b	1215	CLA	C4D-CHA	2.81	1.48	1.38
15	H	1238	F6C	C4B-NB	-2.81	1.33	1.37
14	G	1125	CLA	CHD-C4C	2.81	1.45	1.39
14	A	1118	CLA	C3D-C2D	2.80	1.46	1.39
14	B	1215	CLA	C4D-CHA	2.80	1.48	1.38
14	x	1701	CLA	C1C-NC	-2.80	1.33	1.37
14	b	1022	CLA	C3D-C2D	2.80	1.46	1.39
14	H	1214	CLA	MG-NC	2.80	2.12	2.06
15	b	1238	F6C	C3B-C2B	2.80	1.46	1.39
14	G	1113	CLA	C3D-C2D	2.80	1.46	1.39
14	A	1138	CLA	C4D-CHA	2.80	1.48	1.38
14	b	1214	CLA	C4B-NB	-2.80	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1118	CLA	C3D-C2D	2.80	1.46	1.39
15	b	1237	F6C	C3D-C2D	2.80	1.46	1.39
14	H	1213	CLA	C4D-CHA	2.80	1.48	1.38
14	G	1140	CLA	C3D-C2D	2.80	1.46	1.39
15	b	1238	F6C	C4B-NB	-2.80	1.33	1.37
14	G	1133	CLA	C3D-C2D	2.80	1.46	1.39
14	b	1234	CLA	OBD-CAD	2.80	1.27	1.22
14	b	1231	CLA	C3D-C2D	2.80	1.46	1.39
14	b	1209	CLA	C1C-NC	-2.79	1.33	1.37
14	H	1209	CLA	C1C-NC	-2.79	1.33	1.37
14	b	1227	CLA	C1C-NC	-2.79	1.33	1.37
14	G	1104	CLA	MG-ND	-2.79	2.00	2.05
18	G	4007	BCR	C1-C6	-2.79	1.50	1.53
14	A	1136	CLA	C3D-C2D	2.79	1.46	1.39
14	a	1138	CLA	C4D-CHA	2.79	1.48	1.38
14	B	1213	CLA	C4D-CHA	2.79	1.48	1.38
14	B	1219	CLA	C4D-CHA	2.79	1.48	1.38
14	a	1106	CLA	C3D-C2D	2.79	1.46	1.39
14	A	1134	CLA	MG-ND	-2.79	2.00	2.05
14	b	1233	CLA	MG-ND	-2.79	2.00	2.05
14	G	1118	CLA	C3D-C2D	2.79	1.46	1.39
14	A	1106	CLA	C3D-C2D	2.79	1.46	1.39
14	G	1127	CLA	MG-NC	2.79	2.12	2.06
14	A	1137	CLA	OBD-CAD	2.79	1.27	1.22
14	a	1133	CLA	C3D-C2D	2.79	1.46	1.39
15	B	1238	F6C	C3B-C2B	2.79	1.45	1.39
14	b	1213	CLA	C4D-CHA	2.79	1.47	1.38
14	G	1134	CLA	MG-ND	-2.79	2.00	2.05
14	b	1214	CLA	MG-NC	2.79	2.12	2.06
14	H	1231	CLA	C3D-C2D	2.79	1.46	1.39
14	A	1123	CLA	C1C-NC	-2.78	1.33	1.37
14	A	1104	CLA	MG-ND	-2.78	2.00	2.05
15	G	1121	F6C	MG-ND	-2.78	1.99	2.06
15	B	1207	F6C	C4B-NB	-2.78	1.33	1.37
14	B	1232	CLA	C4D-CHA	2.78	1.47	1.38
15	b	1230	F6C	C3D-C2D	2.78	1.46	1.39
15	A	1121	F6C	MG-ND	-2.78	1.99	2.06
14	b	1209	CLA	C3D-C2D	2.78	1.46	1.39
14	b	1223	CLA	OBD-CAD	2.78	1.27	1.22
14	a	1104	CLA	MG-ND	-2.78	2.00	2.05
14	B	1234	CLA	OBD-CAD	2.78	1.27	1.22
14	H	1211	CLA	C3D-C2D	2.78	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1219	CLA	C4D-CHA	2.78	1.47	1.38
15	B	1238	F6C	CHB-C4A	-2.78	1.32	1.38
14	H	1209	CLA	C3D-C2D	2.78	1.46	1.39
14	b	1210	CLA	C3D-C2D	2.78	1.46	1.39
14	b	1232	CLA	C4D-CHA	2.77	1.47	1.38
15	a	1121	F6C	MG-ND	-2.77	1.99	2.06
14	H	1022	CLA	C3D-C2D	2.77	1.46	1.39
15	H	1238	F6C	C3B-C2B	2.77	1.45	1.39
14	H	1232	CLA	C4B-NB	-2.77	1.34	1.37
14	U	1503	CLA	C3D-C2D	2.77	1.46	1.39
14	B	1022	CLA	C3D-C2D	2.77	1.46	1.39
15	B	1230	F6C	C3D-C2D	2.77	1.46	1.39
14	G	1107	CLA	MG-NC	2.77	2.12	2.06
14	G	1137	CLA	OBD-CAD	2.77	1.27	1.22
15	H	1238	F6C	CHB-C4A	-2.77	1.32	1.38
14	B	1210	CLA	C3D-C2D	2.77	1.46	1.39
14	H	1232	CLA	C4D-CHA	2.77	1.47	1.38
14	G	1111	CLA	C3D-C2D	2.77	1.46	1.39
14	G	1125	CLA	OBD-CAD	2.77	1.27	1.22
14	G	1106	CLA	C3D-C2D	2.77	1.46	1.39
15	b	1238	F6C	CHB-C4A	-2.77	1.32	1.38
14	G	1112	CLA	C4D-CHA	2.77	1.47	1.38
14	H	1223	CLA	OBD-CAD	2.77	1.27	1.22
14	G	1136	CLA	C4B-NB	-2.77	1.34	1.37
14	A	1136	CLA	C4B-NB	-2.77	1.34	1.37
14	l	1501	CLA	C4D-CHA	2.76	1.47	1.38
14	H	1219	CLA	C4D-CHA	2.76	1.47	1.38
14	A	1125	CLA	OBD-CAD	2.76	1.27	1.22
14	a	1134	CLA	MG-ND	-2.76	2.00	2.05
14	B	1209	CLA	C3D-C2D	2.76	1.46	1.39
14	B	1211	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1136	CLA	C3D-C2D	2.76	1.46	1.39
14	A	1116	CLA	C3D-C2D	2.76	1.46	1.39
14	X	1701	CLA	C4D-CHA	2.76	1.47	1.38
14	H	1239	CLA	C3D-C2D	2.76	1.46	1.39
14	U	1501	CLA	C4D-CHA	2.76	1.47	1.38
14	H	1023	CLA	C3D-C2D	2.76	1.46	1.39
14	G	1115	CLA	C3D-C2D	2.76	1.46	1.39
18	A	4007	BCR	C1-C6	-2.76	1.50	1.53
14	H	1205	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1123	CLA	C1C-NC	-2.76	1.33	1.37
15	b	1207	F6C	C4B-NB	-2.76	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1210	CLA	C3D-C2D	2.76	1.46	1.39
14	G	1136	CLA	C3D-C2D	2.76	1.46	1.39
14	L	1503	CLA	C3D-C2D	2.76	1.46	1.39
14	a	1013	CLA	CHB-C1B	2.76	1.45	1.39
14	H	1212	CLA	C4D-CHA	2.76	1.47	1.38
14	L	1501	CLA	C4D-CHA	2.76	1.47	1.38
14	B	1232	CLA	C3D-C2D	2.76	1.46	1.39
15	H	1207	F6C	C3B-C2B	2.75	1.45	1.39
14	b	1211	CLA	C3D-C2D	2.75	1.46	1.39
14	W	1701	CLA	C4D-CHA	2.75	1.47	1.38
14	A	1115	CLA	C3D-C2D	2.75	1.46	1.39
14	a	1111	CLA	C3D-C2D	2.75	1.46	1.39
14	b	1201	CLA	C3D-C2D	2.75	1.46	1.39
14	x	1701	CLA	C4D-CHA	2.75	1.47	1.38
14	A	1112	CLA	C4D-CHA	2.75	1.47	1.38
14	B	1239	CLA	C3D-C2D	2.75	1.46	1.39
14	B	1201	CLA	C3D-C2D	2.75	1.46	1.39
14	B	1212	CLA	C4D-CHA	2.75	1.47	1.38
14	b	1232	CLA	C3D-C2D	2.75	1.46	1.39
14	a	1136	CLA	C4B-NB	-2.75	1.34	1.37
14	a	1112	CLA	C4D-CHA	2.75	1.47	1.38
14	b	1239	CLA	C3D-C2D	2.75	1.46	1.39
15	H	1230	F6C	C3D-C2D	2.75	1.46	1.39
14	G	1127	CLA	C3D-C2D	2.75	1.46	1.39
15	B	1207	F6C	C3B-C2B	2.75	1.45	1.39
14	b	1222	CLA	C3D-C2D	2.75	1.46	1.39
14	B	1229	CLA	C3D-C2D	2.75	1.46	1.39
14	l	1503	CLA	C3D-C2D	2.75	1.46	1.39
14	A	1013	CLA	CHB-C1B	2.74	1.45	1.39
14	B	1213	CLA	C3D-C2D	2.74	1.46	1.39
14	k	1401	CLA	C1B-NB	-2.74	1.34	1.37
15	b	1207	F6C	C3B-C2B	2.74	1.45	1.39
14	b	1214	CLA	C1C-NC	-2.74	1.33	1.37
14	H	1201	CLA	C3D-C2D	2.74	1.46	1.39
14	H	1213	CLA	C3D-C2D	2.74	1.46	1.39
14	b	1213	CLA	C3D-C2D	2.74	1.46	1.39
14	A	1127	CLA	MG-NC	2.74	2.12	2.06
14	a	1116	CLA	C3D-C2D	2.74	1.46	1.39
15	H	1207	F6C	C4B-NB	-2.74	1.33	1.37
14	a	1115	CLA	C3D-C2D	2.74	1.46	1.39
14	b	1217	CLA	C3D-C2D	2.74	1.46	1.39
14	A	1108	CLA	C4D-CHA	2.74	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1218	CLA	C1C-NC	-2.74	1.33	1.37
14	G	1102	CLA	MG-NC	2.74	2.12	2.06
14	b	1229	CLA	C3D-C2D	2.74	1.46	1.39
14	B	1217	CLA	C3D-C2D	2.74	1.46	1.39
14	a	1127	CLA	MG-NC	2.74	2.12	2.06
14	H	1217	CLA	C3D-C2D	2.74	1.46	1.39
14	H	1233	CLA	C4D-CHA	2.74	1.47	1.38
14	b	1212	CLA	C4D-CHA	2.74	1.47	1.38
14	a	1127	CLA	C3D-C2D	2.73	1.46	1.39
14	a	1122	CLA	C4D-CHA	2.73	1.47	1.38
14	G	1116	CLA	C3D-C2D	2.73	1.46	1.39
14	A	1122	CLA	C4D-CHA	2.73	1.47	1.38
14	A	1102	CLA	C4D-CHA	2.73	1.47	1.38
14	G	1102	CLA	C1C-NC	-2.73	1.33	1.37
14	G	1131	CLA	C3D-C2D	2.73	1.46	1.39
14	A	1131	CLA	C3D-C2D	2.73	1.46	1.39
14	B	1233	CLA	C4D-CHA	2.73	1.47	1.38
14	X	1701	CLA	C3D-C2D	2.73	1.46	1.39
14	G	1122	CLA	C4D-CHA	2.73	1.47	1.38
14	T	1401	CLA	MG-ND	-2.73	2.00	2.05
14	b	1224	CLA	C3D-C2D	2.73	1.46	1.39
14	a	1115	CLA	C4D-CHA	2.73	1.47	1.38
14	A	1115	CLA	C4D-CHA	2.73	1.47	1.38
21	A	6001	LMT	O3'-C3'	-2.73	1.36	1.43
14	a	1108	CLA	C4D-CHA	2.73	1.47	1.38
14	G	1101	CLA	C3D-C2D	2.73	1.46	1.39
14	A	1127	CLA	C3D-C2D	2.73	1.46	1.39
14	A	1101	CLA	C3D-C2D	2.73	1.46	1.39
14	G	1123	CLA	C1C-NC	-2.73	1.33	1.37
14	a	1102	CLA	MG-NC	2.73	2.12	2.06
14	a	1116	CLA	MG-NC	2.73	2.12	2.06
14	B	1023	CLA	C3D-C2D	2.73	1.46	1.39
14	A	1102	CLA	MG-NC	2.73	2.12	2.06
14	G	1013	CLA	CHB-C1B	2.73	1.45	1.39
14	B	1224	CLA	C3D-C2D	2.73	1.46	1.39
14	H	1232	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1205	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1233	CLA	C4D-CHA	2.72	1.47	1.38
14	b	1218	CLA	C4B-NB	-2.72	1.34	1.37
14	x	1701	CLA	C3D-C2D	2.72	1.46	1.39
14	a	1101	CLA	C3D-C2D	2.72	1.46	1.39
14	b	1206	CLA	OBD-CAD	2.72	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1218	CLA	C4B-NB	-2.72	1.34	1.37
14	B	1217	CLA	C4D-CHA	2.72	1.47	1.38
14	a	1102	CLA	C4D-CHA	2.72	1.47	1.38
14	a	1123	CLA	C4D-CHA	2.72	1.47	1.38
14	G	1116	CLA	MG-NC	2.72	2.12	2.06
14	H	1214	CLA	C1C-NC	-2.72	1.33	1.37
14	b	1023	CLA	C3D-C2D	2.72	1.46	1.39
14	H	1218	CLA	C1C-NC	-2.72	1.33	1.37
14	H	1220	CLA	C4D-CHA	2.72	1.47	1.38
14	b	1229	CLA	MG-ND	-2.72	2.00	2.05
14	A	1123	CLA	C4D-CHA	2.72	1.47	1.38
14	T	1401	CLA	C1B-NB	-2.72	1.34	1.37
14	H	1217	CLA	C1C-NC	-2.72	1.33	1.37
14	B	1214	CLA	C1C-NC	-2.72	1.33	1.37
14	G	1115	CLA	C4D-CHA	2.72	1.47	1.38
14	H	1229	CLA	C3D-C2D	2.72	1.46	1.39
14	H	1222	CLA	C3D-C2D	2.71	1.46	1.39
14	a	1123	CLA	C3D-C2D	2.71	1.46	1.39
14	B	1222	CLA	C3D-C2D	2.71	1.46	1.39
14	K	1401	CLA	C1B-NB	-2.71	1.34	1.37
14	B	1216	CLA	C4D-CHA	2.71	1.47	1.38
14	a	1116	CLA	C1C-NC	-2.71	1.33	1.37
14	W	1701	CLA	C3D-C2D	2.71	1.46	1.39
14	G	1123	CLA	C4D-CHA	2.71	1.47	1.38
14	H	1217	CLA	C4D-CHA	2.71	1.47	1.38
14	b	1220	CLA	C4D-CHA	2.71	1.47	1.38
14	a	1114	CLA	C1C-NC	-2.71	1.33	1.37
14	b	1213	CLA	MG-NC	2.71	2.12	2.06
14	A	1139	CLA	MG-NC	2.71	2.12	2.06
14	A	1012	CLA	MG-NC	2.71	2.12	2.06
14	B	1232	CLA	C1C-NC	-2.71	1.33	1.37
14	G	1113	CLA	C4D-CHA	2.71	1.47	1.38
14	H	1206	CLA	OBD-CAD	2.71	1.27	1.22
14	G	1108	CLA	C4D-CHA	2.71	1.47	1.38
14	A	1114	CLA	C1C-NC	-2.71	1.33	1.37
14	H	1223	CLA	C4D-CHA	2.71	1.47	1.38
21	a	6001	LMT	O3'-C3'	-2.71	1.36	1.43
14	a	1122	CLA	C3D-C2D	2.71	1.46	1.39
14	G	1111	CLA	C4D-CHA	2.71	1.47	1.38
14	b	1217	CLA	C4D-CHA	2.71	1.47	1.38
14	G	1123	CLA	C3D-C2D	2.71	1.46	1.39
14	B	1205	CLA	C3D-C2D	2.71	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1102	CLA	C3D-C2D	2.71	1.46	1.39
14	a	1102	CLA	C1C-NC	-2.71	1.33	1.37
14	H	1224	CLA	C3D-C2D	2.71	1.46	1.39
14	H	1222	CLA	MG-NC	2.71	2.12	2.06
14	k	1401	CLA	MG-ND	-2.71	2.00	2.05
14	W	1701	CLA	C4B-NB	-2.71	1.34	1.37
15	b	1230	F6C	C4C-NC	-2.71	1.34	1.37
14	A	1111	CLA	C3D-C2D	2.71	1.46	1.39
14	K	1401	CLA	MG-ND	-2.71	2.00	2.05
14	A	1109	CLA	C3D-C2D	2.70	1.46	1.39
14	H	1201	CLA	C4D-CHA	2.70	1.47	1.38
14	H	1216	CLA	C4D-CHA	2.70	1.47	1.38
14	G	1113	CLA	C4B-NB	-2.70	1.34	1.37
14	b	1218	CLA	C1C-NC	-2.70	1.33	1.37
14	a	1137	CLA	C3D-C2D	2.70	1.46	1.39
14	B	1229	CLA	MG-ND	-2.70	2.00	2.05
15	B	1230	F6C	MG-ND	-2.70	1.99	2.06
14	A	1113	CLA	C4D-CHA	2.70	1.47	1.38
14	B	1213	CLA	MG-NC	2.70	2.12	2.06
14	G	1133	CLA	C4D-CHA	2.70	1.47	1.38
14	A	1116	CLA	C1C-NC	-2.70	1.33	1.37
14	a	1131	CLA	C3D-C2D	2.70	1.46	1.39
14	H	1224	CLA	MG-NC	2.70	2.12	2.06
14	b	1216	CLA	C4D-CHA	2.70	1.47	1.38
14	B	1201	CLA	C4D-CHA	2.70	1.47	1.38
14	B	1220	CLA	C4D-CHA	2.70	1.47	1.38
14	G	1102	CLA	C4D-CHA	2.70	1.47	1.38
15	b	1230	F6C	MG-ND	-2.70	1.99	2.06
14	H	1231	CLA	MG-NC	2.70	2.12	2.06
14	G	1116	CLA	C4D-CHA	2.70	1.47	1.38
14	H	1218	CLA	C4B-NB	-2.70	1.34	1.37
14	a	1133	CLA	C4D-CHA	2.70	1.47	1.38
14	A	1115	CLA	MG-NC	2.70	2.12	2.06
14	A	1133	CLA	C4D-CHA	2.70	1.47	1.38
15	H	1230	F6C	C4B-NB	-2.70	1.33	1.37
14	l	1501	CLA	MG-NC	2.69	2.12	2.06
14	A	1111	CLA	C4D-CHA	2.69	1.47	1.38
14	G	1107	CLA	C3D-C2D	2.69	1.46	1.39
14	H	1236	CLA	C4B-NB	-2.69	1.34	1.37
14	k	1401	CLA	C1B-C2B	2.69	1.49	1.43
14	a	1102	CLA	C3D-C2D	2.69	1.46	1.39
14	B	1217	CLA	C1C-NC	-2.69	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1231	CLA	C4D-CHA	2.69	1.47	1.38
14	G	1107	CLA	C4D-CHA	2.69	1.47	1.38
14	A	1136	CLA	C4D-CHA	2.69	1.47	1.38
14	a	1107	CLA	C3D-C2D	2.69	1.46	1.39
14	T	1401	CLA	C1B-C2B	2.69	1.49	1.43
14	b	1231	CLA	C4D-CHA	2.69	1.47	1.38
21	G	6002	LMT	O3B-C3B	-2.69	1.36	1.43
14	b	1217	CLA	C1C-NC	-2.69	1.33	1.37
14	B	1218	CLA	C4D-CHA	2.69	1.47	1.38
14	a	1101	CLA	C4B-NB	-2.69	1.34	1.37
14	a	1111	CLA	C4D-CHA	2.69	1.47	1.38
14	A	1122	CLA	C3D-C2D	2.69	1.46	1.39
14	a	1101	CLA	C4D-CHA	2.69	1.47	1.38
14	b	1201	CLA	C4D-CHA	2.69	1.47	1.38
14	b	1236	CLA	C4B-NB	-2.69	1.34	1.37
14	G	1128	CLA	C4D-CHA	2.69	1.47	1.38
14	G	1136	CLA	C4D-CHA	2.69	1.47	1.38
14	b	1223	CLA	C4D-CHA	2.69	1.47	1.38
14	A	1107	CLA	C4D-CHA	2.69	1.47	1.38
14	b	1231	CLA	MG-NC	2.69	2.12	2.06
14	H	1208	CLA	C4D-CHA	2.69	1.47	1.38
14	a	1136	CLA	C4D-CHA	2.69	1.47	1.38
14	H	1216	CLA	C4B-NB	-2.69	1.34	1.37
14	A	1116	CLA	MG-NC	2.69	2.12	2.06
14	a	1107	CLA	C4D-CHA	2.69	1.47	1.38
15	H	1230	F6C	MG-ND	-2.69	1.99	2.06
14	G	1109	CLA	C3D-C2D	2.69	1.46	1.39
14	H	1229	CLA	MG-ND	-2.69	2.00	2.05
14	G	1116	CLA	C1C-NC	-2.69	1.33	1.37
14	G	1137	CLA	C3D-C2D	2.69	1.46	1.39
21	A	6002	LMT	O3'-C3'	-2.68	1.36	1.43
14	a	1113	CLA	C4D-CHA	2.68	1.47	1.38
14	B	1223	CLA	C4D-CHA	2.68	1.47	1.38
14	b	1224	CLA	MG-NC	2.68	2.12	2.06
14	G	1114	CLA	C1C-NC	-2.68	1.33	1.37
14	G	1101	CLA	C4B-NB	-2.68	1.34	1.37
14	A	1140	CLA	MG-NC	2.68	2.12	2.06
21	G	6001	LMT	O3'-C3'	-2.68	1.36	1.43
14	H	1218	CLA	C4D-CHA	2.68	1.47	1.38
14	b	1218	CLA	C4D-CHA	2.68	1.47	1.38
14	A	1107	CLA	C3D-C2D	2.68	1.46	1.39
14	a	1140	CLA	MG-NC	2.68	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1224	CLA	MG-NC	2.68	2.12	2.06
14	G	1101	CLA	C4D-CHA	2.68	1.47	1.38
21	a	6002	LMT	O3'-C3'	-2.68	1.36	1.43
14	G	1122	CLA	C3D-C2D	2.68	1.46	1.39
14	A	1137	CLA	C3D-C2D	2.68	1.46	1.39
14	H	1213	CLA	MG-NC	2.68	2.12	2.06
14	b	1222	CLA	MG-NC	2.68	2.12	2.06
14	b	1216	CLA	C4B-NB	-2.68	1.34	1.37
21	a	6002	LMT	O3B-C3B	-2.68	1.36	1.43
14	a	1130	CLA	C3D-C2D	2.68	1.46	1.39
15	B	1230	F6C	C4B-NB	-2.68	1.33	1.37
14	a	1012	CLA	MG-NC	2.68	2.12	2.06
14	G	1130	CLA	C3D-C2D	2.68	1.46	1.39
14	H	1235	CLA	C4D-CHA	2.68	1.47	1.38
14	a	1128	CLA	C4D-CHA	2.68	1.47	1.38
14	A	1102	CLA	C3D-C2D	2.68	1.46	1.39
15	H	1230	F6C	C4C-NC	-2.68	1.34	1.37
14	U	1501	CLA	MG-NC	2.68	2.12	2.06
14	b	1220	CLA	C1B-C2B	2.68	1.49	1.43
15	b	1207	F6C	C1A-C2A	2.68	1.51	1.45
14	x	1701	CLA	C4B-NB	-2.68	1.34	1.37
14	G	1110	CLA	C3D-C2D	2.68	1.46	1.39
14	G	1139	CLA	MG-NC	2.68	2.12	2.06
14	H	1232	CLA	C1C-NC	-2.68	1.33	1.37
14	H	1214	CLA	C4D-CHA	2.68	1.47	1.38
14	a	1119	CLA	C4D-CHA	2.68	1.47	1.38
14	A	1101	CLA	C4B-NB	-2.68	1.34	1.37
14	a	1109	CLA	C3D-C2D	2.68	1.46	1.39
14	A	1101	CLA	C4D-CHA	2.68	1.47	1.38
14	L	1501	CLA	MG-NC	2.68	2.12	2.06
14	A	1123	CLA	C3D-C2D	2.68	1.46	1.39
14	a	1110	CLA	C3D-C2D	2.68	1.46	1.39
14	B	1206	CLA	OBD-CAD	2.68	1.27	1.22
14	B	1209	CLA	C4D-CHA	2.68	1.47	1.38
14	a	1135	CLA	MG-NC	2.68	2.12	2.06
15	G	1121	F6C	C3B-C2B	2.68	1.45	1.39
14	a	1113	CLA	C4B-NB	-2.68	1.34	1.37
14	H	1220	CLA	C1B-C2B	2.67	1.49	1.43
21	G	6002	LMT	O3'-C3'	-2.67	1.36	1.43
14	G	1140	CLA	MG-NC	2.67	2.12	2.06
15	B	1207	F6C	C1A-C2A	2.67	1.51	1.45
14	B	1235	CLA	C4D-CHA	2.67	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1113	CLA	C4B-NB	-2.67	1.34	1.37
14	H	1204	CLA	C3D-C2D	2.67	1.46	1.39
14	A	1102	CLA	C1C-NC	-2.67	1.33	1.37
14	H	1206	CLA	C4D-CHA	2.67	1.47	1.38
14	b	1209	CLA	C4D-CHA	2.67	1.47	1.38
14	A	1119	CLA	C4D-CHA	2.67	1.47	1.38
14	a	1116	CLA	C4D-CHA	2.67	1.47	1.38
14	A	1116	CLA	C4D-CHA	2.67	1.47	1.38
14	b	1214	CLA	C4D-CHA	2.67	1.47	1.38
14	b	1209	CLA	C4B-NB	-2.67	1.34	1.37
14	G	1129	CLA	MG-NC	2.67	2.12	2.06
14	A	1130	CLA	C3D-C2D	2.67	1.46	1.39
14	b	1221	CLA	C4D-CHA	2.67	1.47	1.38
15	a	1121	F6C	C3B-C2B	2.67	1.45	1.39
14	b	1232	CLA	C1C-NC	-2.67	1.33	1.37
14	a	1132	CLA	C4D-CHA	2.67	1.47	1.38
14	A	1127	CLA	C4D-CHA	2.67	1.47	1.38
14	b	1204	CLA	C3D-C2D	2.67	1.46	1.39
14	B	1231	CLA	MG-NC	2.67	2.12	2.06
14	A	1135	CLA	MG-NC	2.67	2.12	2.06
14	B	1222	CLA	MG-NC	2.67	2.12	2.06
14	G	1131	CLA	C4D-CHA	2.66	1.47	1.38
14	H	1235	CLA	MG-NC	2.66	2.12	2.06
14	G	1126	CLA	C3D-C2D	2.66	1.46	1.39
14	B	1214	CLA	C4D-CHA	2.66	1.47	1.38
15	A	1121	F6C	C3B-C2B	2.66	1.45	1.39
14	H	1239	CLA	C4D-CHA	2.66	1.47	1.38
14	B	1208	CLA	C4D-CHA	2.66	1.47	1.38
14	G	1109	CLA	MG-NC	2.66	2.12	2.06
15	b	1230	F6C	C4B-NB	-2.66	1.33	1.37
14	B	1210	CLA	C4D-CHA	2.66	1.47	1.38
14	a	1109	CLA	C4D-CHA	2.66	1.47	1.38
14	b	1223	CLA	MG-NC	2.66	2.12	2.06
14	X	1701	CLA	C4B-NB	-2.66	1.34	1.37
14	b	1208	CLA	C4D-CHA	2.66	1.47	1.38
14	G	1105	CLA	C4D-CHA	2.66	1.47	1.38
14	A	1106	CLA	C4D-CHA	2.66	1.47	1.38
14	A	1128	CLA	C4D-CHA	2.66	1.47	1.38
14	a	1105	CLA	C4D-CHA	2.66	1.47	1.38
14	b	1210	CLA	C4D-CHA	2.66	1.47	1.38
14	a	1127	CLA	C4D-CHA	2.66	1.47	1.38
14	B	1221	CLA	C4D-CHA	2.66	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1231	CLA	C4D-CHA	2.66	1.47	1.38
15	B	1207	F6C	C3D-C2D	2.66	1.46	1.39
14	G	1135	CLA	MG-NC	2.66	2.12	2.06
14	G	1115	CLA	MG-NC	2.66	2.12	2.06
14	b	1235	CLA	MG-NC	2.66	2.12	2.06
14	G	1127	CLA	C4D-CHA	2.66	1.47	1.38
14	H	1209	CLA	C4D-CHA	2.65	1.47	1.38
14	K	1401	CLA	C1B-C2B	2.65	1.49	1.43
14	H	1209	CLA	C4B-NB	-2.65	1.34	1.37
14	G	1119	CLA	C4D-CHA	2.65	1.47	1.38
15	b	1207	F6C	C3D-C2D	2.65	1.46	1.39
21	A	6002	LMT	O3B-C3B	-2.65	1.36	1.43
14	B	1216	CLA	C4B-NB	-2.65	1.34	1.37
14	B	1220	CLA	C1B-C2B	2.65	1.49	1.43
14	B	1206	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1139	CLA	MG-NC	2.65	2.12	2.06
14	G	1132	CLA	C4D-CHA	2.65	1.47	1.38
14	H	1221	CLA	C4D-CHA	2.65	1.47	1.38
14	G	1106	CLA	C4D-CHA	2.65	1.47	1.38
14	A	1105	CLA	C4D-CHA	2.65	1.47	1.38
15	H	1207	F6C	C3D-C2D	2.65	1.46	1.39
14	H	1210	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1126	CLA	C3D-C2D	2.65	1.46	1.39
14	G	1120	CLA	C4D-CHA	2.65	1.47	1.38
14	B	1215	CLA	C4B-NB	-2.65	1.34	1.37
14	A	1120	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1115	CLA	MG-NC	2.65	2.12	2.06
14	a	1139	CLA	C4B-NB	-2.65	1.34	1.37
14	G	1125	CLA	C3D-C2D	2.65	1.46	1.39
14	B	1223	CLA	MG-NC	2.65	2.12	2.06
14	H	1205	CLA	C4D-CHA	2.65	1.47	1.38
14	a	1125	CLA	C3D-C2D	2.65	1.46	1.39
15	H	1207	F6C	C1A-C2A	2.65	1.51	1.45
14	A	1126	CLA	C3D-C2D	2.65	1.46	1.39
14	a	1109	CLA	MG-NC	2.65	2.12	2.06
14	b	1206	CLA	C4D-CHA	2.64	1.47	1.38
14	H	1203	CLA	C4D-CHA	2.64	1.47	1.38
14	H	1234	CLA	C4D-CHA	2.64	1.47	1.38
14	A	1132	CLA	C4D-CHA	2.64	1.47	1.38
14	A	1110	CLA	C3D-C2D	2.64	1.46	1.39
14	A	1125	CLA	C3D-C2D	2.64	1.46	1.39
14	a	1120	CLA	C4D-CHA	2.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	1022	CLA	C4D-CHA	2.64	1.47	1.38
14	B	1204	CLA	C3D-C2D	2.64	1.46	1.39
14	H	1223	CLA	MG-NC	2.64	2.12	2.06
14	b	1221	CLA	MG-NC	2.64	2.12	2.06
15	A	1121	F6C	CHB-C4A	-2.64	1.33	1.38
14	A	1131	CLA	C4D-CHA	2.64	1.47	1.38
14	B	1235	CLA	MG-NC	2.64	2.12	2.06
14	b	1235	CLA	C4D-CHA	2.64	1.47	1.38
14	H	1227	CLA	C4D-CHA	2.64	1.47	1.38
18	B	4017	BCR	C30-C25	-2.64	1.50	1.53
14	A	1109	CLA	C4D-CHA	2.64	1.47	1.38
14	A	1139	CLA	C4B-NB	-2.64	1.34	1.37
14	B	1203	CLA	C4D-CHA	2.64	1.47	1.38
14	a	1131	CLA	C4D-CHA	2.64	1.47	1.38
14	b	1203	CLA	C4D-CHA	2.64	1.47	1.38
14	G	1139	CLA	C4B-NB	-2.64	1.34	1.37
14	b	1215	CLA	C4B-NB	-2.64	1.34	1.37
14	b	1233	CLA	C1C-NC	-2.64	1.33	1.37
14	B	1227	CLA	C4D-CHA	2.63	1.47	1.38
14	H	1215	CLA	C4B-NB	-2.63	1.34	1.37
14	a	1106	CLA	C4D-CHA	2.63	1.47	1.38
15	a	1121	F6C	CHB-C4A	-2.63	1.33	1.38
14	B	1225	CLA	C3D-C2D	2.63	1.46	1.39
14	G	1012	CLA	MG-NC	2.63	2.12	2.06
14	a	1012	CLA	C4D-CHA	2.63	1.47	1.38
14	b	1234	CLA	C4D-CHA	2.63	1.47	1.38
14	B	1022	CLA	C4D-CHA	2.63	1.47	1.38
14	B	1217	CLA	C1B-C2B	2.63	1.49	1.43
14	a	1140	CLA	C4D-CHA	2.63	1.47	1.38
14	b	1239	CLA	C4D-CHA	2.63	1.47	1.38
14	G	1109	CLA	C4D-CHA	2.63	1.47	1.38
15	B	1230	F6C	C4C-NC	-2.63	1.34	1.37
14	a	1129	CLA	MG-NC	2.63	2.12	2.06
14	A	1114	CLA	MG-NC	2.63	2.12	2.06
14	H	1022	CLA	C4D-CHA	2.63	1.47	1.38
14	B	1234	CLA	C4D-CHA	2.63	1.47	1.38
14	G	1110	CLA	C4B-NB	-2.63	1.34	1.37
14	b	1205	CLA	C4D-CHA	2.63	1.47	1.38
14	H	1203	CLA	OBD-CAD	2.63	1.27	1.22
14	B	1205	CLA	C4D-CHA	2.63	1.47	1.38
14	b	1226	CLA	C4D-CHA	2.63	1.47	1.38
14	A	1109	CLA	MG-NC	2.63	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1233	CLA	C1C-NC	-2.63	1.33	1.37
14	b	1227	CLA	C4D-CHA	2.63	1.47	1.38
14	B	1210	CLA	MG-NC	2.63	2.12	2.06
14	a	1113	CLA	MG-NC	2.62	2.12	2.06
14	H	1225	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1208	CLA	MG-NC	2.62	2.12	2.06
14	b	1222	CLA	C4D-CHA	2.62	1.47	1.38
14	b	1212	CLA	MG-NC	2.62	2.12	2.06
15	G	1121	F6C	CHB-C4A	-2.62	1.33	1.38
14	A	1113	CLA	MG-NC	2.62	2.12	2.06
14	G	1118	CLA	C4D-CHA	2.62	1.47	1.38
14	H	1021	CLA	C3D-C2D	2.62	1.46	1.39
14	B	1219	CLA	C1C-NC	-2.62	1.33	1.37
14	B	1203	CLA	OBD-CAD	2.62	1.27	1.22
14	A	1110	CLA	C4D-CHA	2.62	1.47	1.38
14	B	1233	CLA	C1C-NC	-2.62	1.33	1.37
14	B	1234	CLA	C3D-C2D	2.62	1.46	1.39
14	G	1110	CLA	C4D-CHA	2.62	1.47	1.38
14	a	1120	CLA	C4B-NB	-2.62	1.34	1.37
14	b	1210	CLA	MG-NC	2.62	2.12	2.06
14	B	1209	CLA	C4B-NB	-2.62	1.34	1.37
14	b	1225	CLA	C4D-CHA	2.62	1.47	1.38
14	B	1236	CLA	C4B-NB	-2.62	1.34	1.37
14	G	1140	CLA	C4D-CHA	2.62	1.47	1.38
14	H	1221	CLA	MG-NC	2.62	2.12	2.06
14	b	1217	CLA	C1B-C2B	2.62	1.49	1.43
14	G	1124	CLA	C3D-C2D	2.62	1.46	1.39
14	H	1226	CLA	C4D-CHA	2.61	1.47	1.38
14	b	1234	CLA	C3D-C2D	2.61	1.46	1.39
14	H	1234	CLA	C3D-C2D	2.61	1.46	1.39
14	b	1209	CLA	MG-NC	2.61	2.12	2.06
14	G	1133	CLA	MG-NC	2.61	2.12	2.06
14	A	1118	CLA	C4D-CHA	2.61	1.47	1.38
14	a	1118	CLA	C4D-CHA	2.61	1.47	1.38
14	G	1132	CLA	C3D-C2D	2.61	1.46	1.39
14	a	1130	CLA	C4D-CHA	2.61	1.47	1.38
14	a	1114	CLA	MG-NC	2.61	2.12	2.06
14	H	1219	CLA	C1C-NC	-2.61	1.33	1.37
14	A	1120	CLA	C4B-NB	-2.61	1.34	1.37
14	b	1203	CLA	OBD-CAD	2.61	1.27	1.22
14	a	1110	CLA	MG-NC	2.61	2.12	2.06
14	A	1110	CLA	MG-NC	2.61	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1137	CLA	C4D-CHA	2.61	1.47	1.38
14	B	1225	CLA	C4D-CHA	2.61	1.47	1.38
14	B	1226	CLA	C4D-CHA	2.61	1.47	1.38
14	B	1221	CLA	MG-NC	2.61	2.12	2.06
14	B	1239	CLA	C4D-CHA	2.61	1.47	1.38
14	A	1132	CLA	C3D-C2D	2.61	1.46	1.39
14	G	1110	CLA	MG-NC	2.61	2.12	2.06
14	H	1225	CLA	C3D-C2D	2.61	1.46	1.39
14	B	1219	CLA	C4B-NB	-2.61	1.34	1.37
14	a	1110	CLA	C4D-CHA	2.60	1.47	1.38
14	a	1133	CLA	MG-NC	2.60	2.12	2.06
14	a	1107	CLA	C1B-C2B	2.60	1.49	1.43
14	A	1129	CLA	MG-NC	2.60	2.12	2.06
14	B	1208	CLA	MG-NC	2.60	2.12	2.06
14	b	1211	CLA	C4D-CHA	2.60	1.47	1.38
18	H	4017	BCR	C30-C25	-2.60	1.50	1.53
14	H	1220	CLA	MG-NC	2.60	2.12	2.06
14	A	1140	CLA	C4D-CHA	2.60	1.47	1.38
14	B	1211	CLA	C4D-CHA	2.60	1.47	1.38
14	a	1137	CLA	C4D-CHA	2.60	1.47	1.38
14	H	1236	CLA	C3D-C2D	2.60	1.46	1.39
14	A	1126	CLA	C4D-CHA	2.60	1.47	1.38
14	H	1212	CLA	MG-NC	2.60	2.12	2.06
14	W	1701	CLA	C1B-C2B	2.60	1.49	1.43
14	H	1211	CLA	C4D-CHA	2.60	1.47	1.38
14	b	1236	CLA	C3D-C2D	2.60	1.46	1.39
21	A	6002	LMT	O4'-C4B	-2.60	1.36	1.43
14	B	1202	CLA	C4D-CHA	2.59	1.47	1.38
14	G	1113	CLA	MG-NC	2.59	2.12	2.06
14	A	1012	CLA	C4D-CHA	2.59	1.47	1.38
14	B	1222	CLA	C4D-CHA	2.59	1.47	1.38
14	G	1126	CLA	C4D-CHA	2.59	1.47	1.38
14	A	1133	CLA	MG-NC	2.59	2.12	2.06
14	a	1132	CLA	C3D-C2D	2.59	1.46	1.39
14	A	1110	CLA	C4B-NB	-2.59	1.34	1.37
14	a	1124	CLA	C3D-C2D	2.59	1.46	1.39
14	H	1217	CLA	C1B-C2B	2.59	1.49	1.43
14	G	1125	CLA	C4D-CHA	2.59	1.47	1.38
14	H	1208	CLA	MG-NC	2.59	2.12	2.06
14	B	1236	CLA	C3D-C2D	2.59	1.46	1.39
14	B	1220	CLA	MG-NC	2.59	2.12	2.06
14	G	1132	CLA	MG-NC	2.59	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	1209	CLA	MG-NC	2.59	2.12	2.06
21	a	6002	LMT	O4'-C4B	-2.59	1.36	1.43
14	A	1130	CLA	C4D-CHA	2.59	1.47	1.38
14	b	1202	CLA	C4D-CHA	2.59	1.47	1.38
14	H	1210	CLA	MG-NC	2.59	2.12	2.06
21	G	6002	LMT	O4'-C4B	-2.59	1.36	1.43
14	G	1012	CLA	C4D-CHA	2.59	1.47	1.38
14	G	1137	CLA	C4D-CHA	2.59	1.47	1.38
14	b	1021	CLA	C3D-C2D	2.59	1.46	1.39
14	b	1225	CLA	C3D-C2D	2.59	1.46	1.39
14	G	1130	CLA	C4D-CHA	2.59	1.47	1.38
14	x	1701	CLA	C1B-C2B	2.59	1.49	1.43
14	H	1222	CLA	C4D-CHA	2.59	1.47	1.38
14	a	1126	CLA	C4D-CHA	2.58	1.47	1.38
14	B	1212	CLA	MG-NC	2.58	2.12	2.06
14	G	1107	CLA	C1B-C2B	2.58	1.49	1.43
14	U	1503	CLA	C4D-CHA	2.58	1.47	1.38
14	a	1139	CLA	C4D-CHA	2.58	1.47	1.38
14	B	1224	CLA	C4D-CHA	2.58	1.47	1.38
14	G	1114	CLA	MG-NC	2.58	2.12	2.06
14	A	1124	CLA	C3D-C2D	2.58	1.46	1.39
14	X	1701	CLA	C1B-C2B	2.58	1.49	1.43
14	H	1233	CLA	C1B-C2B	2.58	1.49	1.43
14	a	1103	CLA	C3D-C2D	2.58	1.46	1.39
14	a	1137	CLA	MG-NC	2.58	2.12	2.06
14	H	1202	CLA	C4D-CHA	2.58	1.47	1.38
14	A	1139	CLA	C4D-CHA	2.58	1.47	1.38
14	G	1120	CLA	C4B-NB	-2.58	1.34	1.37
14	b	1233	CLA	C1B-C2B	2.58	1.49	1.43
14	b	1201	CLA	MG-NC	2.58	2.12	2.06
14	L	1503	CLA	C4D-CHA	2.58	1.47	1.38
14	B	1021	CLA	C3D-C2D	2.57	1.46	1.39
15	A	1121	F6C	C3C-C2C	2.57	1.45	1.38
15	G	1121	F6C	C3C-C2C	2.57	1.45	1.38
14	A	1132	CLA	MG-NC	2.57	2.12	2.06
14	G	1139	CLA	C4D-CHA	2.57	1.47	1.38
14	b	1224	CLA	C4D-CHA	2.57	1.47	1.38
15	B	1238	F6C	C3C-C2C	2.57	1.45	1.38
14	H	1201	CLA	MG-NC	2.57	2.12	2.06
14	A	1125	CLA	C1B-C2B	2.57	1.49	1.43
15	H	1238	F6C	C3C-C2C	2.57	1.45	1.38
14	B	1209	CLA	MG-NC	2.57	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1138	CLA	MG-NC	2.57	2.12	2.06
14	a	1101	CLA	MG-NC	2.57	2.12	2.06
14	B	1201	CLA	MG-NC	2.57	2.12	2.06
14	A	1112	CLA	MG-NC	2.57	2.12	2.06
14	a	1129	CLA	C4D-CHA	2.57	1.47	1.38
14	A	1107	CLA	C1B-C2B	2.57	1.49	1.43
14	B	1239	CLA	MG-NC	2.57	2.12	2.06
14	G	1125	CLA	C1B-C2B	2.57	1.49	1.43
14	a	1125	CLA	C4D-CHA	2.57	1.47	1.38
14	A	1103	CLA	C3D-C2D	2.56	1.46	1.39
14	a	1103	CLA	C4D-CHA	2.56	1.47	1.38
14	l	1503	CLA	C4D-CHA	2.56	1.47	1.38
14	b	1219	CLA	C1C-NC	-2.56	1.33	1.37
14	G	1103	CLA	C3D-C2D	2.56	1.46	1.39
14	A	1124	CLA	C4D-CHA	2.56	1.47	1.38
14	b	1216	CLA	MG-NC	2.56	2.12	2.06
14	b	1220	CLA	MG-NC	2.56	2.12	2.06
14	H	1224	CLA	C4D-CHA	2.56	1.47	1.38
14	a	1124	CLA	C4D-CHA	2.56	1.47	1.38
14	B	1236	CLA	C4D-CHA	2.56	1.47	1.38
14	A	1137	CLA	MG-NC	2.56	2.12	2.06
14	G	1124	CLA	C4D-CHA	2.56	1.47	1.38
14	B	1233	CLA	C1B-C2B	2.56	1.49	1.43
14	G	1129	CLA	C4D-CHA	2.56	1.47	1.38
14	B	1202	CLA	C3D-C2D	2.55	1.46	1.39
14	a	1132	CLA	MG-NC	2.55	2.12	2.06
14	b	1236	CLA	C4D-CHA	2.55	1.47	1.38
14	H	1236	CLA	C4D-CHA	2.55	1.47	1.38
14	A	1114	CLA	C4B-NB	-2.55	1.34	1.37
14	H	1216	CLA	MG-NC	2.55	2.12	2.06
14	a	1131	CLA	MG-NC	2.55	2.12	2.06
14	H	1219	CLA	C4B-NB	-2.55	1.34	1.37
14	b	1202	CLA	C3D-C2D	2.55	1.45	1.39
14	G	1101	CLA	MG-NC	2.55	2.12	2.06
14	G	1106	CLA	MG-NC	2.55	2.12	2.06
14	A	1104	CLA	C4D-CHA	2.55	1.47	1.38
14	A	1125	CLA	C4D-CHA	2.55	1.47	1.38
14	G	1138	CLA	MG-NC	2.55	2.12	2.06
15	a	1121	F6C	C3C-C2C	2.55	1.45	1.38
14	H	1239	CLA	MG-NC	2.55	2.12	2.06
14	A	1131	CLA	MG-NC	2.55	2.12	2.06
15	b	1238	F6C	C3C-C2C	2.55	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1125	CLA	C1B-C2B	2.55	1.49	1.43
14	a	1112	CLA	MG-NC	2.55	2.12	2.06
14	U	1502	CLA	MG-NC	2.55	2.12	2.06
14	a	1111	CLA	MG-NC	2.55	2.12	2.06
14	A	1138	CLA	MG-NC	2.54	2.12	2.06
14	H	1228	CLA	MG-NC	2.54	2.12	2.06
14	b	1229	CLA	C4D-CHA	2.54	1.47	1.38
14	B	1227	CLA	C3D-C2D	2.54	1.45	1.39
14	A	1129	CLA	C4D-CHA	2.54	1.47	1.38
14	G	1112	CLA	MG-NC	2.54	2.12	2.06
14	a	1110	CLA	C4B-NB	-2.54	1.34	1.37
14	B	1216	CLA	MG-NC	2.54	2.12	2.06
14	B	1023	CLA	C4D-CHA	2.54	1.47	1.38
14	G	1104	CLA	C3D-C2D	2.54	1.45	1.39
14	b	1202	CLA	C4B-NB	-2.54	1.34	1.37
14	G	1103	CLA	C4D-CHA	2.54	1.47	1.38
14	B	1229	CLA	C4D-CHA	2.54	1.47	1.38
14	H	1202	CLA	C3D-C2D	2.54	1.45	1.39
14	b	1218	CLA	C1B-C2B	2.54	1.49	1.43
14	b	1228	CLA	MG-NC	2.53	2.12	2.06
14	B	1228	CLA	MG-NC	2.53	2.12	2.06
14	H	1229	CLA	C4D-CHA	2.53	1.47	1.38
14	l	1502	CLA	MG-NC	2.53	2.12	2.06
14	A	1101	CLA	MG-NC	2.53	2.12	2.06
18	b	4017	BCR	C30-C25	-2.53	1.50	1.53
14	G	1111	CLA	MG-NC	2.53	2.12	2.06
14	a	1120	CLA	MG-NC	2.53	2.12	2.06
14	a	1114	CLA	C4B-NB	-2.53	1.34	1.37
14	G	1137	CLA	MG-NC	2.53	2.12	2.06
14	H	1218	CLA	C1B-C2B	2.53	1.49	1.43
14	b	1023	CLA	C4D-CHA	2.53	1.47	1.38
14	B	1228	CLA	C4D-CHA	2.53	1.47	1.38
14	G	1131	CLA	MG-NC	2.53	2.12	2.06
14	G	1104	CLA	C4D-CHA	2.53	1.47	1.38
14	G	1114	CLA	C4B-NB	-2.53	1.34	1.37
14	l	1503	CLA	MG-NC	2.52	2.12	2.06
14	a	1104	CLA	C4D-CHA	2.52	1.47	1.38
14	A	1111	CLA	MG-NC	2.52	2.12	2.06
14	A	1120	CLA	MG-NC	2.52	2.12	2.06
14	b	1239	CLA	MG-NC	2.52	2.12	2.06
14	G	1105	CLA	MG-NC	2.52	2.12	2.06
14	A	1103	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1223	CLA	C3D-C2D	2.52	1.45	1.39
14	B	1211	CLA	MG-NC	2.52	2.12	2.06
14	H	1228	CLA	C4D-CHA	2.52	1.47	1.38
14	a	1112	CLA	C1B-C2B	2.52	1.49	1.43
14	A	1120	CLA	C1B-C2B	2.52	1.49	1.43
14	L	1502	CLA	MG-NC	2.52	2.12	2.06
14	H	1234	CLA	MG-NC	2.52	2.12	2.06
14	A	1112	CLA	C1B-C2B	2.52	1.49	1.43
14	a	1106	CLA	MG-NC	2.52	2.12	2.06
14	L	1503	CLA	MG-NC	2.52	2.12	2.06
14	H	1023	CLA	C4D-CHA	2.52	1.47	1.38
14	b	1211	CLA	MG-NC	2.52	2.12	2.06
14	A	1109	CLA	C1B-C2B	2.52	1.49	1.43
18	A	4011	BCR	C1-C6	-2.52	1.50	1.53
14	a	1136	CLA	MG-NC	2.52	2.12	2.06
14	H	1202	CLA	C4B-NB	-2.51	1.34	1.37
15	B	1237	F6C	C3C-C2C	2.51	1.45	1.38
14	a	1122	CLA	MG-NC	2.51	2.12	2.06
14	A	1106	CLA	C1B-C2B	2.51	1.49	1.43
14	a	1103	CLA	C1B-C2B	2.51	1.49	1.43
14	A	1122	CLA	MG-NC	2.51	2.12	2.06
14	b	1234	CLA	MG-NC	2.51	2.12	2.06
14	B	1234	CLA	MG-NC	2.51	2.12	2.06
14	b	1228	CLA	C4D-CHA	2.51	1.47	1.38
14	A	1139	CLA	C3D-C2D	2.51	1.45	1.39
14	G	1120	CLA	C1B-C2B	2.51	1.49	1.43
14	B	1218	CLA	C1B-C2B	2.51	1.49	1.43
14	H	1225	CLA	MG-NC	2.51	2.12	2.06
14	b	1231	CLA	C1B-C2B	2.51	1.49	1.43
14	b	1203	CLA	C3D-C2D	2.51	1.45	1.39
14	H	1227	CLA	C3D-C2D	2.51	1.45	1.39
14	A	1104	CLA	C3D-C2D	2.51	1.45	1.39
18	G	4011	BCR	C1-C6	-2.51	1.50	1.53
14	A	1106	CLA	MG-NC	2.51	2.12	2.06
14	U	1503	CLA	MG-NC	2.51	2.12	2.06
14	G	1129	CLA	C3D-C2D	2.51	1.45	1.39
14	a	1139	CLA	C3D-C2D	2.51	1.45	1.39
14	H	1203	CLA	C3D-C2D	2.50	1.45	1.39
14	a	1129	CLA	C3D-C2D	2.50	1.45	1.39
14	H	1211	CLA	MG-NC	2.50	2.12	2.06
14	a	1104	CLA	C3D-C2D	2.50	1.45	1.39
14	G	1122	CLA	MG-NC	2.50	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1120	CLA	C1B-C2B	2.50	1.49	1.43
14	B	1225	CLA	MG-NC	2.50	2.12	2.06
14	a	1135	CLA	C4D-CHA	2.50	1.47	1.38
14	B	1203	CLA	C3D-C2D	2.50	1.45	1.39
14	b	1226	CLA	MG-NC	2.50	2.12	2.06
14	A	1136	CLA	MG-NC	2.50	2.12	2.06
14	a	1109	CLA	C1B-C2B	2.50	1.49	1.43
14	b	1208	CLA	C1B-C2B	2.50	1.49	1.43
14	a	1122	CLA	C1B-C2B	2.50	1.49	1.43
14	G	1103	CLA	C1B-C2B	2.50	1.49	1.43
14	G	1112	CLA	C1B-C2B	2.50	1.49	1.43
14	H	1231	CLA	C1B-C2B	2.49	1.49	1.43
14	G	1120	CLA	MG-NC	2.49	2.12	2.06
14	G	1128	CLA	MG-NC	2.49	2.12	2.06
14	G	1135	CLA	C4D-CHA	2.49	1.47	1.38
14	a	1108	CLA	MG-NC	2.49	2.12	2.06
14	A	1108	CLA	MG-NC	2.49	2.12	2.06
14	G	1013	CLA	C4D-CHA	2.49	1.46	1.38
14	G	1139	CLA	C3D-C2D	2.49	1.45	1.39
14	A	1129	CLA	C3D-C2D	2.49	1.45	1.39
18	a	4011	BCR	C1-C6	-2.49	1.50	1.53
14	B	1208	CLA	C1B-C2B	2.49	1.49	1.43
14	b	1223	CLA	C3D-C2D	2.49	1.45	1.39
14	H	1021	CLA	C4D-CHA	2.49	1.46	1.38
14	a	1134	CLA	C4B-NB	-2.49	1.34	1.37
14	A	1105	CLA	MG-NC	2.49	2.12	2.06
14	A	1103	CLA	C1B-C2B	2.49	1.49	1.43
14	A	1122	CLA	C1B-C2B	2.49	1.49	1.43
14	A	1013	CLA	C4D-CHA	2.49	1.46	1.38
14	G	1106	CLA	C1B-C2B	2.49	1.49	1.43
14	B	1231	CLA	C1B-C2B	2.49	1.49	1.43
14	H	1223	CLA	C3D-C2D	2.49	1.45	1.39
14	b	1225	CLA	MG-NC	2.49	2.12	2.06
14	B	1226	CLA	MG-NC	2.49	2.12	2.06
14	k	1401	CLA	C1C-NC	-2.49	1.34	1.37
14	H	1226	CLA	MG-NC	2.48	2.12	2.06
14	G	1136	CLA	MG-NC	2.48	2.12	2.06
14	b	1227	CLA	C3D-C2D	2.48	1.45	1.39
14	a	1013	CLA	C4D-CHA	2.48	1.46	1.38
14	a	1134	CLA	C1D-C2D	2.48	1.50	1.45
14	H	1208	CLA	C1B-C2B	2.48	1.49	1.43
14	a	1105	CLA	MG-NC	2.48	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1202	CLA	C4B-NB	-2.48	1.34	1.37
14	B	1233	CLA	C4B-NB	-2.48	1.34	1.37
14	K	1401	CLA	C1C-NC	-2.48	1.34	1.37
14	l	1502	CLA	C4D-CHA	2.48	1.46	1.38
14	G	1104	CLA	C1B-C2B	2.48	1.48	1.43
21	G	6001	LMT	O2'-C2'	-2.48	1.36	1.43
14	B	1021	CLA	C4D-CHA	2.48	1.46	1.38
14	a	1128	CLA	MG-NC	2.48	2.12	2.06
14	A	1135	CLA	C4D-CHA	2.47	1.46	1.38
14	G	1134	CLA	C1D-C2D	2.47	1.50	1.45
14	b	1021	CLA	C4D-CHA	2.47	1.46	1.38
14	G	1122	CLA	C1B-C2B	2.47	1.48	1.43
14	B	1229	CLA	MG-NC	2.47	2.12	2.06
14	A	1128	CLA	MG-NC	2.47	2.12	2.06
15	H	1237	F6C	C3C-C2C	2.47	1.45	1.38
14	a	1104	CLA	C1B-C2B	2.47	1.48	1.43
14	L	1502	CLA	C4D-CHA	2.47	1.46	1.38
14	A	1105	CLA	C1B-C2B	2.47	1.48	1.43
14	A	1103	CLA	MG-NC	2.47	2.12	2.06
14	G	1109	CLA	C1B-C2B	2.46	1.48	1.43
15	b	1237	F6C	C3C-C2C	2.46	1.45	1.38
21	a	6002	LMT	O2'-C2'	-2.46	1.36	1.43
21	G	6002	LMT	O2'-C2'	-2.46	1.36	1.43
14	A	1134	CLA	C4B-NB	-2.46	1.34	1.37
14	U	1502	CLA	C4D-CHA	2.46	1.46	1.38
21	A	6001	LMT	O2'-C2'	-2.46	1.36	1.43
14	b	1219	CLA	C4B-NB	-2.46	1.34	1.37
14	a	1126	CLA	MG-NC	2.46	2.12	2.06
14	G	1108	CLA	MG-NC	2.46	2.12	2.06
14	H	1236	CLA	MG-NC	2.46	2.12	2.06
14	G	1101	CLA	C1B-C2B	2.46	1.48	1.43
14	a	1103	CLA	MG-NC	2.46	2.12	2.06
14	G	1134	CLA	C4B-NB	-2.45	1.34	1.37
14	A	1104	CLA	C1B-C2B	2.45	1.48	1.43
14	b	1229	CLA	MG-NC	2.45	2.12	2.06
14	A	1126	CLA	MG-NC	2.45	2.12	2.06
14	T	1401	CLA	C1C-NC	-2.45	1.34	1.37
14	a	1106	CLA	C1B-C2B	2.45	1.48	1.43
14	a	1101	CLA	C1B-C2B	2.45	1.48	1.43
14	B	1215	CLA	MG-NC	2.45	2.12	2.06
14	b	1217	CLA	C4B-NB	-2.45	1.34	1.37
21	A	6002	LMT	O2'-C2'	-2.45	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1105	CLA	C1B-C2B	2.45	1.48	1.43
14	A	1101	CLA	C1B-C2B	2.45	1.48	1.43
14	H	1229	CLA	MG-NC	2.45	2.12	2.06
14	A	1134	CLA	C1D-C2D	2.44	1.50	1.45
14	a	1105	CLA	C1B-C2B	2.44	1.48	1.43
21	G	6001	LMT	O1'-C1'	-2.44	1.36	1.40
21	a	6001	LMT	O2'-C2'	-2.44	1.36	1.43
14	H	1204	CLA	C4D-CHA	2.44	1.46	1.38
21	G	6001	LMT	O2B-C2B	-2.44	1.36	1.43
14	H	1215	CLA	MG-NC	2.43	2.12	2.06
14	G	1126	CLA	MG-NC	2.43	2.12	2.06
14	b	1233	CLA	C4B-NB	-2.43	1.34	1.37
14	b	1204	CLA	C4D-CHA	2.43	1.46	1.38
14	a	1134	CLA	C1B-C2B	2.43	1.48	1.43
14	K	1401	CLA	C4B-NB	-2.43	1.34	1.37
14	G	1103	CLA	MG-NC	2.43	2.12	2.06
14	B	1217	CLA	C4B-NB	-2.42	1.34	1.37
14	b	1236	CLA	MG-NC	2.42	2.12	2.06
14	B	1204	CLA	C4D-CHA	2.42	1.46	1.38
14	B	1236	CLA	MG-NC	2.42	2.12	2.06
14	l	1501	CLA	C1B-C2B	2.42	1.48	1.43
14	H	1212	CLA	C1B-C2B	2.42	1.48	1.43
14	k	1401	CLA	C4B-NB	-2.42	1.34	1.37
14	U	1503	CLA	C1B-C2B	2.42	1.48	1.43
14	G	1134	CLA	C1B-C2B	2.42	1.48	1.43
14	A	1134	CLA	C1C-NC	-2.42	1.34	1.37
14	U	1501	CLA	C1B-C2B	2.41	1.48	1.43
21	A	6001	LMT	O2B-C2B	-2.41	1.37	1.43
18	H	4004	BCR	C30-C25	-2.41	1.50	1.53
14	H	1217	CLA	C4B-NB	-2.41	1.34	1.37
14	a	1130	CLA	OBD-CAD	2.41	1.26	1.22
14	a	1134	CLA	C1C-NC	-2.41	1.34	1.37
21	a	6001	LMT	O1'-C1'	-2.41	1.36	1.40
14	H	1201	CLA	C1B-C2B	2.41	1.48	1.43
14	B	1228	CLA	C1B-C2B	2.41	1.48	1.43
14	T	1401	CLA	C4B-NB	-2.41	1.34	1.37
14	b	1215	CLA	MG-NC	2.41	2.12	2.06
14	B	1201	CLA	C1B-C2B	2.40	1.48	1.43
14	B	1212	CLA	C1B-C2B	2.40	1.48	1.43
14	L	1503	CLA	C1B-C2B	2.40	1.48	1.43
14	b	1219	CLA	C1B-C2B	2.40	1.48	1.43
14	G	1134	CLA	C1C-NC	-2.40	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1219	CLA	C1B-C2B	2.40	1.48	1.43
14	A	1117	CLA	MG-NC	2.40	2.12	2.06
14	L	1501	CLA	C1B-C2B	2.40	1.48	1.43
14	b	1205	CLA	MG-NC	2.40	2.12	2.06
21	G	6001	LMT	O3B-C3B	-2.40	1.37	1.43
14	l	1503	CLA	C1B-C2B	2.40	1.48	1.43
14	B	1205	CLA	MG-NC	2.39	2.12	2.06
14	H	1228	CLA	C1B-C2B	2.39	1.48	1.43
18	B	4004	BCR	C30-C25	-2.39	1.50	1.53
14	A	1130	CLA	OBD-CAD	2.39	1.26	1.22
14	G	1117	CLA	MG-NC	2.39	2.12	2.06
15	b	1230	F6C	C3C-C2C	2.39	1.45	1.38
21	a	6001	LMT	O2B-C2B	-2.39	1.37	1.43
14	b	1213	CLA	C1B-C2B	2.39	1.48	1.43
14	A	1118	CLA	C1B-C2B	2.39	1.48	1.43
20	i	5006	LMG	C37-C36	-2.39	1.33	1.50
14	b	1021	CLA	C1B-C2B	2.39	1.48	1.43
14	b	1212	CLA	C1B-C2B	2.39	1.48	1.43
14	G	1133	CLA	C1B-C2B	2.39	1.48	1.43
18	b	4004	BCR	C30-C25	-2.39	1.50	1.53
21	A	6001	LMT	O1'-C1'	-2.39	1.36	1.40
14	B	1021	CLA	C1B-C2B	2.39	1.48	1.43
14	A	1134	CLA	C1B-C2B	2.39	1.48	1.43
15	B	1230	F6C	C1A-C2A	2.39	1.50	1.45
14	H	1219	CLA	C1B-C2B	2.39	1.48	1.43
14	b	1228	CLA	C1B-C2B	2.38	1.48	1.43
21	a	6001	LMT	O3B-C3B	-2.38	1.37	1.43
14	b	1204	CLA	MG-NC	2.38	2.11	2.06
14	H	1211	CLA	C1B-C2B	2.38	1.48	1.43
20	I	5006	LMG	C37-C36	-2.38	1.33	1.50
21	A	6001	LMT	O3B-C3B	-2.38	1.37	1.43
14	H	1233	CLA	C4B-NB	-2.38	1.34	1.37
14	b	1201	CLA	C1B-C2B	2.38	1.48	1.43
20	R	5006	LMG	C37-C36	-2.38	1.33	1.50
15	H	1230	F6C	C3C-C2C	2.38	1.45	1.38
14	a	1117	CLA	MG-NC	2.38	2.11	2.06
14	b	1202	CLA	MG-NC	2.38	2.11	2.06
14	B	1222	CLA	C1B-C2B	2.38	1.48	1.43
15	H	1230	F6C	C1A-C2A	2.38	1.50	1.45
14	A	1133	CLA	C1B-C2B	2.37	1.48	1.43
14	B	1213	CLA	C1B-C2B	2.37	1.48	1.43
14	B	1211	CLA	C1B-C2B	2.37	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	1204	CLA	MG-NC	2.37	2.11	2.06
14	H	1205	CLA	MG-NC	2.37	2.11	2.06
14	H	1213	CLA	C1B-C2B	2.37	1.48	1.43
14	a	1133	CLA	C1B-C2B	2.37	1.48	1.43
15	b	1238	F6C	C3D-C2D	2.37	1.45	1.39
14	H	1021	CLA	C1B-C2B	2.37	1.48	1.43
14	b	1211	CLA	C1B-C2B	2.37	1.48	1.43
14	G	1130	CLA	OBD-CAD	2.37	1.26	1.22
14	G	1118	CLA	C1B-C2B	2.37	1.48	1.43
14	A	1115	CLA	C1B-C2B	2.36	1.48	1.43
14	G	1125	CLA	MG-NC	2.36	2.11	2.06
14	B	1202	CLA	MG-NC	2.36	2.11	2.06
14	a	1118	CLA	C1B-C2B	2.36	1.48	1.43
14	b	1203	CLA	MG-NC	2.36	2.11	2.06
14	B	1203	CLA	MG-NC	2.36	2.11	2.06
15	B	1238	F6C	C3D-C2D	2.36	1.45	1.39
15	B	1230	F6C	C3C-C2C	2.36	1.45	1.38
14	G	1139	CLA	C1B-C2B	2.36	1.48	1.43
14	G	1115	CLA	C1B-C2B	2.36	1.48	1.43
14	a	1115	CLA	C1B-C2B	2.36	1.48	1.43
14	G	1127	CLA	C1B-C2B	2.35	1.48	1.43
14	H	1202	CLA	MG-NC	2.35	2.11	2.06
14	A	1130	CLA	MG-NC	2.35	2.11	2.06
14	H	1204	CLA	MG-NC	2.35	2.11	2.06
15	G	1121	F6C	C1A-C2A	2.35	1.50	1.45
15	B	1207	F6C	C3C-C2C	2.35	1.45	1.38
14	G	1130	CLA	MG-NC	2.35	2.11	2.06
14	G	1124	CLA	MG-NC	2.35	2.11	2.06
14	H	1203	CLA	MG-NC	2.35	2.11	2.06
14	b	1222	CLA	C1B-C2B	2.35	1.48	1.43
15	H	1238	F6C	C3D-C2D	2.35	1.45	1.39
14	B	1023	CLA	C4C-C3C	2.35	1.49	1.45
14	G	1140	CLA	C4B-NB	-2.35	1.34	1.37
14	a	1130	CLA	MG-NC	2.35	2.11	2.06
14	A	1125	CLA	MG-NC	2.35	2.11	2.06
14	a	1125	CLA	MG-NC	2.34	2.11	2.06
14	H	1023	CLA	C4C-C3C	2.34	1.49	1.45
14	a	1137	CLA	C1B-C2B	2.34	1.48	1.43
15	a	1121	F6C	C1A-C2A	2.34	1.50	1.45
14	a	1139	CLA	C1B-C2B	2.34	1.48	1.43
14	K	1401	CLA	C1D-C2D	2.34	1.50	1.45
14	G	1137	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1117	CLA	C1B-C2B	2.34	1.48	1.43
14	H	1203	CLA	C1B-C2B	2.33	1.48	1.43
14	a	1117	CLA	C1B-C2B	2.33	1.48	1.43
14	A	1124	CLA	MG-NC	2.33	2.11	2.06
14	H	1222	CLA	C1B-C2B	2.33	1.48	1.43
14	a	1124	CLA	MG-NC	2.33	2.11	2.06
15	H	1207	F6C	C3C-C2C	2.33	1.45	1.38
15	A	1121	F6C	C1D-C2D	2.33	1.49	1.44
15	b	1230	F6C	C1A-C2A	2.33	1.50	1.45
15	a	1121	F6C	C4B-NB	-2.33	1.34	1.37
14	a	1127	CLA	C1B-C2B	2.32	1.48	1.43
15	b	1207	F6C	C3C-C2C	2.32	1.45	1.38
15	a	1121	F6C	C1D-C2D	2.32	1.49	1.44
14	b	1205	CLA	C1B-C2B	2.32	1.48	1.43
14	A	1137	CLA	C1B-C2B	2.32	1.48	1.43
14	b	1023	CLA	C4C-C3C	2.32	1.49	1.45
15	A	1121	F6C	C4B-NB	-2.32	1.34	1.37
14	A	1139	CLA	C1B-C2B	2.32	1.48	1.43
14	H	1205	CLA	C1B-C2B	2.32	1.48	1.43
14	B	1202	CLA	C1B-C2B	2.32	1.48	1.43
15	G	1121	F6C	C1D-C2D	2.32	1.49	1.44
15	A	1121	F6C	C1A-C2A	2.31	1.50	1.45
18	b	4009	BCR	C30-C25	-2.31	1.50	1.53
15	G	1121	F6C	C4B-NB	-2.31	1.34	1.37
14	b	1229	CLA	C1B-C2B	2.30	1.48	1.43
14	B	1221	CLA	C1B-C2B	2.30	1.48	1.43
14	A	1140	CLA	C4B-NB	-2.30	1.34	1.37
14	B	1203	CLA	C1B-C2B	2.30	1.48	1.43
14	A	1127	CLA	C1B-C2B	2.30	1.48	1.43
14	B	1205	CLA	C1B-C2B	2.30	1.48	1.43
14	k	1401	CLA	C1D-C2D	2.30	1.49	1.45
14	G	1108	CLA	C1B-C2B	2.30	1.48	1.43
14	G	1117	CLA	C1B-C2B	2.30	1.48	1.43
14	H	1229	CLA	C1B-C2B	2.30	1.48	1.43
21	a	6002	LMT	O2B-C2B	-2.30	1.37	1.43
14	B	1232	CLA	C1B-C2B	2.29	1.48	1.43
14	B	1219	CLA	C4C-C3C	2.29	1.48	1.45
14	a	1140	CLA	C4B-NB	-2.29	1.34	1.37
14	a	1134	CLA	C4C-C3C	2.29	1.48	1.45
14	b	1204	CLA	C1B-C2B	2.29	1.48	1.43
14	H	1204	CLA	C1B-C2B	2.29	1.48	1.43
18	B	4009	BCR	C30-C25	-2.29	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1108	CLA	C1B-C2B	2.29	1.48	1.43
21	A	6002	LMT	O1'-C1'	-2.29	1.36	1.40
14	b	1232	CLA	C1B-C2B	2.29	1.48	1.43
14	H	1232	CLA	C1B-C2B	2.29	1.48	1.43
14	H	1221	CLA	C1B-C2B	2.29	1.48	1.43
14	A	1134	CLA	C4C-C3C	2.29	1.48	1.45
13	a	1011	CL0	CMA-C3A	-2.28	1.49	1.53
14	b	1219	CLA	C4C-C3C	2.28	1.48	1.45
21	G	6002	LMT	O1'-C1'	-2.28	1.36	1.40
14	G	1140	CLA	C3B-C4B	2.28	1.49	1.42
14	G	1134	CLA	C4C-C3C	2.28	1.48	1.45
14	H	1219	CLA	C4C-C3C	2.28	1.48	1.45
14	H	1202	CLA	C1B-C2B	2.28	1.48	1.43
14	B	1229	CLA	C1B-C2B	2.28	1.48	1.43
14	b	1202	CLA	C1B-C2B	2.28	1.48	1.43
14	b	1203	CLA	C1B-C2B	2.28	1.48	1.43
14	b	1221	CLA	C1B-C2B	2.28	1.48	1.43
14	a	1108	CLA	C1B-C2B	2.28	1.48	1.43
14	T	1401	CLA	C1D-C2D	2.28	1.49	1.45
14	A	1111	CLA	C1B-C2B	2.27	1.48	1.43
14	B	1204	CLA	C1B-C2B	2.27	1.48	1.43
18	H	4009	BCR	C30-C25	-2.27	1.50	1.53
14	a	1118	CLA	C4B-NB	-2.27	1.34	1.37
14	A	1140	CLA	C3B-C4B	2.27	1.49	1.42
14	B	1233	CLA	C1D-C2D	2.26	1.49	1.45
14	G	1110	CLA	C1B-C2B	2.26	1.48	1.43
14	A	1110	CLA	C1B-C2B	2.26	1.48	1.43
14	H	1209	CLA	C1B-C2B	2.26	1.48	1.43
14	H	1235	CLA	C1B-C2B	2.26	1.48	1.43
14	a	1140	CLA	C3B-C4B	2.26	1.49	1.42
14	B	1209	CLA	C1B-C2B	2.26	1.48	1.43
14	H	1227	CLA	C1B-C2B	2.26	1.48	1.43
14	G	1114	CLA	C1D-C2D	2.26	1.49	1.45
14	a	1110	CLA	C1B-C2B	2.26	1.48	1.43
14	A	1102	CLA	C1B-C2B	2.26	1.48	1.43
18	m	4021	BCR	C1-C6	-2.26	1.50	1.53
14	B	1223	CLA	C1B-C2B	2.26	1.48	1.43
13	A	1011	CL0	CMA-C3A	-2.26	1.49	1.53
14	b	1206	CLA	MG-NC	2.25	2.11	2.06
14	A	1118	CLA	C4B-NB	-2.25	1.34	1.37
14	H	1206	CLA	MG-NC	2.25	2.11	2.06
14	a	1119	CLA	MG-NC	2.25	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	6002	LMT	O2B-C2B	-2.25	1.37	1.43
14	b	1235	CLA	C1B-C2B	2.25	1.48	1.43
14	B	1206	CLA	MG-NC	2.25	2.11	2.06
14	b	1023	CLA	C1B-C2B	2.25	1.48	1.43
13	G	1011	CL0	CMA-C3A	-2.24	1.49	1.53
14	G	1102	CLA	C1B-C2B	2.24	1.48	1.43
14	a	1111	CLA	C1B-C2B	2.24	1.48	1.43
14	H	1210	CLA	C1B-C2B	2.24	1.48	1.43
14	b	1210	CLA	C1B-C2B	2.24	1.48	1.43
21	G	6002	LMT	O2B-C2B	-2.24	1.37	1.43
14	G	1118	CLA	C4B-NB	-2.24	1.34	1.37
15	H	1207	F6C	C4D-CHA	2.24	1.48	1.42
18	M	4021	BCR	C1-C6	-2.24	1.50	1.53
14	B	1236	CLA	C3B-C4B	2.23	1.49	1.42
14	b	1223	CLA	C1B-C2B	2.23	1.48	1.43
15	B	1230	F6C	CHB-C4A	-2.23	1.34	1.38
14	B	1210	CLA	C1B-C2B	2.23	1.48	1.43
14	A	1114	CLA	C1D-C2D	2.23	1.49	1.45
18	V	4021	BCR	C1-C6	-2.23	1.50	1.53
14	a	1114	CLA	C1D-C2D	2.23	1.49	1.45
14	H	1023	CLA	C1B-C2B	2.23	1.48	1.43
14	B	1235	CLA	C1B-C2B	2.23	1.48	1.43
14	H	1236	CLA	C3B-C4B	2.23	1.49	1.42
14	b	1236	CLA	C3B-C4B	2.23	1.49	1.42
14	G	1135	CLA	C1B-C2B	2.23	1.48	1.43
14	B	1023	CLA	C1B-C2B	2.23	1.48	1.43
14	B	1227	CLA	C1B-C2B	2.22	1.48	1.43
14	A	1119	CLA	C4C-C3C	2.22	1.48	1.45
21	a	6002	LMT	O1'-C1'	-2.22	1.36	1.40
14	b	1227	CLA	C1B-C2B	2.22	1.48	1.43
14	G	1111	CLA	C1B-C2B	2.22	1.48	1.43
14	H	1223	CLA	C1B-C2B	2.22	1.48	1.43
14	A	1119	CLA	MG-NC	2.22	2.11	2.06
14	G	1123	CLA	C1B-C2B	2.22	1.48	1.43
15	b	1230	F6C	CHB-C4A	-2.22	1.34	1.38
14	b	1209	CLA	C1B-C2B	2.22	1.48	1.43
14	A	1132	CLA	C1B-C2B	2.22	1.48	1.43
14	A	1135	CLA	C1B-C2B	2.22	1.48	1.43
14	G	1119	CLA	MG-NC	2.21	2.11	2.06
14	G	1132	CLA	C1B-C2B	2.21	1.48	1.43
14	a	1102	CLA	C1B-C2B	2.21	1.48	1.43
15	b	1237	F6C	CHB-C4A	-2.21	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	1207	F6C	C4D-CHA	2.21	1.48	1.42
14	a	1132	CLA	C1B-C2B	2.21	1.48	1.43
14	a	1118	CLA	C3B-C4B	2.21	1.49	1.42
14	G	1113	CLA	C3B-C4B	2.20	1.49	1.42
15	b	1207	F6C	C4D-CHA	2.20	1.48	1.42
14	a	1113	CLA	C3B-C4B	2.20	1.49	1.42
14	G	1118	CLA	C3B-C4B	2.20	1.49	1.42
14	H	1233	CLA	C1D-C2D	2.20	1.49	1.45
18	R	4020	BCR	C30-C25	-2.19	1.51	1.53
15	H	1230	F6C	CHB-C4A	-2.19	1.34	1.38
14	a	1135	CLA	C1B-C2B	2.19	1.48	1.43
14	A	1123	CLA	C1B-C2B	2.19	1.48	1.43
14	A	1135	CLA	C3D-C2D	2.19	1.45	1.39
14	A	1113	CLA	C3B-C4B	2.19	1.49	1.42
14	G	1119	CLA	C4C-C3C	2.19	1.48	1.45
18	i	4020	BCR	C30-C25	-2.19	1.51	1.53
14	a	1114	CLA	C1B-C2B	2.19	1.48	1.43
14	b	1233	CLA	C1D-C2D	2.19	1.49	1.45
14	G	1135	CLA	C3D-C2D	2.19	1.44	1.39
15	B	1237	F6C	CHB-C4A	-2.18	1.34	1.38
18	I	4020	BCR	C30-C25	-2.18	1.51	1.53
14	b	1023	CLA	MG-NC	2.18	2.11	2.06
14	a	1135	CLA	C3D-C2D	2.18	1.44	1.39
14	A	1140	CLA	C1B-C2B	2.18	1.48	1.43
14	G	1114	CLA	C1B-C2B	2.18	1.48	1.43
14	a	1119	CLA	C4C-C3C	2.18	1.48	1.45
14	a	1123	CLA	C1B-C2B	2.18	1.48	1.43
14	A	1138	CLA	C1B-C2B	2.18	1.48	1.43
14	A	1114	CLA	C1B-C2B	2.17	1.48	1.43
14	a	1138	CLA	C1B-C2B	2.17	1.48	1.43
14	a	1140	CLA	C1B-C2B	2.17	1.48	1.43
14	a	1131	CLA	C1B-C2B	2.16	1.48	1.43
14	G	1116	CLA	C1B-C2B	2.16	1.48	1.43
18	b	4014	BCR	C1-C6	-2.16	1.51	1.53
13	a	1011	CL0	CBD-CGD	-2.16	1.49	1.52
14	A	1118	CLA	C3B-C4B	2.16	1.49	1.42
14	T	1401	CLA	C4C-C3C	2.16	1.48	1.45
15	B	1230	F6C	C2B-C1B	2.16	1.49	1.44
15	H	1230	F6C	C2B-C1B	2.16	1.49	1.44
14	H	1023	CLA	MG-NC	2.16	2.11	2.06
14	G	1140	CLA	C1B-C2B	2.16	1.48	1.43
14	A	1114	CLA	C4C-C3C	2.16	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1114	CLA	C4C-C3C	2.16	1.48	1.45
14	G	1131	CLA	C1B-C2B	2.15	1.48	1.43
14	A	1113	CLA	C1B-C2B	2.15	1.48	1.43
14	b	1209	CLA	C1D-C2D	2.15	1.49	1.45
15	b	1230	F6C	C2B-C1B	2.15	1.49	1.44
14	k	1401	CLA	C4C-C3C	2.15	1.48	1.45
14	G	1114	CLA	C4C-C3C	2.15	1.48	1.45
15	b	1207	F6C	CMB-C2B	2.15	1.50	1.45
14	A	1116	CLA	C1B-C2B	2.15	1.48	1.43
14	b	1239	CLA	C1B-C2B	2.15	1.48	1.43
14	a	1113	CLA	C1B-C2B	2.14	1.48	1.43
14	G	1013	CLA	MG-NC	2.14	2.11	2.06
15	b	1230	F6C	CMB-C2B	2.14	1.50	1.45
14	G	1138	CLA	C1B-C2B	2.14	1.48	1.43
14	K	1401	CLA	C4C-C3C	2.14	1.48	1.45
14	a	1013	CLA	MG-NC	2.14	2.11	2.06
14	H	1209	CLA	C1D-C2D	2.14	1.49	1.45
18	H	4014	BCR	C30-C25	-2.13	1.51	1.53
14	b	1228	CLA	C1D-C2D	2.13	1.49	1.45
14	B	1239	CLA	C1B-C2B	2.13	1.48	1.43
14	a	1116	CLA	C1B-C2B	2.13	1.48	1.43
14	H	1236	CLA	C1B-C2B	2.13	1.48	1.43
18	H	4014	BCR	C1-C6	-2.13	1.51	1.53
18	B	4014	BCR	C1-C6	-2.13	1.51	1.53
15	H	1237	F6C	CHB-C4A	-2.13	1.34	1.38
14	b	1216	CLA	C1B-C2B	2.13	1.48	1.43
14	G	1113	CLA	C1B-C2B	2.13	1.48	1.43
15	B	1207	F6C	CMB-C2B	2.13	1.50	1.45
14	b	1021	CLA	C3A-C2A	-2.13	1.48	1.54
15	B	1230	F6C	CMB-C2B	2.12	1.50	1.45
14	H	1021	CLA	C3A-C2A	-2.12	1.48	1.54
18	B	4014	BCR	C30-C25	-2.12	1.51	1.53
14	A	1013	CLA	MG-NC	2.12	2.11	2.06
18	R	4020	BCR	C1-C6	-2.12	1.51	1.53
14	H	1239	CLA	C1B-C2B	2.12	1.48	1.43
14	H	1216	CLA	C1B-C2B	2.12	1.48	1.43
14	b	1022	CLA	C1B-C2B	2.12	1.48	1.43
14	B	1023	CLA	MG-NC	2.12	2.11	2.06
14	A	1013	CLA	CHB-C4A	-2.12	1.32	1.37
14	B	1209	CLA	C1D-C2D	2.12	1.49	1.45
13	G	1011	CL0	CBD-CGD	-2.12	1.49	1.52
18	I	4020	BCR	C1-C6	-2.11	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	1207	F6C	CMB-C2B	2.11	1.50	1.45
14	A	1131	CLA	C1B-C2B	2.11	1.48	1.43
14	H	1022	CLA	C1B-C2B	2.11	1.48	1.43
14	B	1021	CLA	C3A-C2A	-2.11	1.48	1.54
13	A	1011	CL0	CBD-CGD	-2.11	1.49	1.52
14	l	1502	CLA	C1D-C2D	2.11	1.49	1.45
14	B	1228	CLA	C1D-C2D	2.11	1.49	1.45
14	U	1502	CLA	C1D-C2D	2.10	1.49	1.45
14	a	1013	CLA	CHB-C4A	-2.10	1.32	1.37
14	B	1234	CLA	C1B-C2B	2.10	1.48	1.43
14	H	1228	CLA	C1D-C2D	2.10	1.49	1.45
15	H	1230	F6C	CMB-C2B	2.10	1.50	1.45
14	G	1139	CLA	C3B-C4B	2.10	1.48	1.42
14	L	1502	CLA	C1D-C2D	2.10	1.49	1.45
14	a	1108	CLA	C1D-C2D	2.10	1.49	1.45
14	A	1104	CLA	MG-NC	2.09	2.11	2.06
18	i	4020	BCR	C1-C6	-2.09	1.51	1.53
14	a	1104	CLA	MG-NC	2.09	2.11	2.06
14	b	1236	CLA	C1B-C2B	2.09	1.48	1.43
14	b	1224	CLA	C1B-C2B	2.09	1.48	1.43
14	B	1021	CLA	MG-NC	2.09	2.11	2.06
14	H	1234	CLA	C1B-C2B	2.09	1.48	1.43
14	B	1224	CLA	C1B-C2B	2.09	1.48	1.43
14	b	1214	CLA	C1D-C2D	2.09	1.49	1.45
14	H	1224	CLA	C1B-C2B	2.09	1.48	1.43
14	A	1108	CLA	C1D-C2D	2.08	1.49	1.45
14	b	1219	CLA	C1D-C2D	2.08	1.49	1.45
14	H	1216	CLA	C1D-C2D	2.08	1.49	1.45
14	B	1216	CLA	C3B-C4B	2.08	1.48	1.42
14	B	1228	CLA	C4C-C3C	2.08	1.48	1.45
14	G	1013	CLA	CHB-C4A	-2.08	1.32	1.37
14	A	1139	CLA	C3B-C4B	2.08	1.48	1.42
14	G	1108	CLA	C1D-C2D	2.08	1.49	1.45
14	b	1216	CLA	C3B-C4B	2.08	1.48	1.42
15	b	1230	F6C	C4A-C3A	2.08	1.49	1.45
14	B	1022	CLA	C1B-C2B	2.08	1.48	1.43
14	B	1236	CLA	C1B-C2B	2.08	1.48	1.43
14	a	1013	CLA	C3B-C4B	2.07	1.48	1.42
14	G	1104	CLA	MG-NC	2.07	2.11	2.06
14	B	1216	CLA	C1B-C2B	2.07	1.48	1.43
14	b	1228	CLA	C4C-C3C	2.07	1.48	1.45
14	b	1234	CLA	C1B-C2B	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	1139	CLA	C3B-C4B	2.07	1.48	1.42
14	B	1214	CLA	C1D-C2D	2.06	1.49	1.45
14	G	1013	CLA	C3B-C4B	2.06	1.48	1.42
14	H	1021	CLA	MG-NC	2.06	2.11	2.06
14	b	1227	CLA	C4C-C3C	2.06	1.48	1.45
14	b	1021	CLA	MG-NC	2.05	2.11	2.06
18	b	4014	BCR	C30-C25	-2.05	1.51	1.53
14	H	1216	CLA	C3B-C4B	2.05	1.48	1.42
14	G	1105	CLA	C1D-C2D	2.05	1.49	1.45
14	A	1119	CLA	C1D-C2D	2.05	1.49	1.45
14	B	1214	CLA	C1B-C2B	2.05	1.47	1.43
14	B	1219	CLA	C1D-C2D	2.05	1.49	1.45
18	A	4008	BCR	C30-C25	-2.05	1.51	1.53
14	a	1119	CLA	C1D-C2D	2.05	1.49	1.45
14	H	1219	CLA	C3B-C4B	2.05	1.48	1.42
14	A	1119	CLA	C1B-C2B	2.05	1.47	1.43
14	G	1129	CLA	C1B-C2B	2.05	1.47	1.43
14	A	1013	CLA	C3B-C4B	2.05	1.48	1.42
14	b	1214	CLA	C1B-C2B	2.05	1.47	1.43
14	B	1227	CLA	C4C-C3C	2.05	1.48	1.45
14	H	1219	CLA	C1D-C2D	2.05	1.49	1.45
15	B	1230	F6C	C4A-C3A	2.05	1.49	1.45
18	U	4022	BCR	C1-C6	-2.04	1.51	1.53
14	a	1105	CLA	C1D-C2D	2.04	1.49	1.45
14	a	1119	CLA	C1B-C2B	2.04	1.47	1.43
15	H	1230	F6C	C1D-C2D	2.04	1.48	1.44
14	b	1219	CLA	C3B-C4B	2.04	1.48	1.42
14	H	1227	CLA	C4C-C3C	2.04	1.48	1.45
15	B	1230	F6C	C1D-C2D	2.04	1.48	1.44
14	A	1129	CLA	C1B-C2B	2.04	1.47	1.43
15	b	1230	F6C	C1D-C2D	2.04	1.48	1.44
18	a	4007	BCR	C30-C25	-2.03	1.51	1.53
14	H	1228	CLA	C4C-C3C	2.03	1.48	1.45
14	H	1209	CLA	C3B-C4B	2.03	1.48	1.42
14	H	1214	CLA	C1D-C2D	2.03	1.49	1.45
14	b	1210	CLA	C4C-C3C	2.03	1.48	1.45
14	H	1214	CLA	C1B-C2B	2.03	1.47	1.43
14	a	1129	CLA	C1B-C2B	2.03	1.47	1.43
15	H	1230	F6C	C4A-C3A	2.03	1.49	1.45
18	G	4007	BCR	C30-C25	-2.03	1.51	1.53
14	K	1401	CLA	C3B-C4B	2.03	1.48	1.42
14	b	1216	CLA	C1D-C2D	2.03	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1119	CLA	C1B-C2B	2.03	1.47	1.43
14	k	1401	CLA	C3B-C4B	2.03	1.48	1.42
14	B	1211	CLA	C1D-C2D	2.03	1.49	1.45
14	G	1124	CLA	CHB-C4A	-2.03	1.32	1.37
18	l	4022	BCR	C1-C6	-2.02	1.51	1.53
14	H	1210	CLA	C1D-C2D	2.02	1.49	1.45
15	b	1237	F6C	CMB-C2B	2.02	1.49	1.45
14	B	1229	CLA	C1D-C2D	2.02	1.49	1.45
14	B	1210	CLA	C4C-C3C	2.02	1.48	1.45
14	H	1210	CLA	C4C-C3C	2.02	1.48	1.45
18	H	4005	BCR	C1-C6	-2.02	1.51	1.53
14	B	1219	CLA	C3B-C4B	2.02	1.48	1.42
14	b	1202	CLA	C3B-C4B	2.02	1.48	1.42
14	T	1401	CLA	C3B-C4B	2.02	1.48	1.42
18	A	4007	BCR	C30-C25	-2.02	1.51	1.53
14	A	1105	CLA	C1D-C2D	2.02	1.49	1.45
14	A	1136	CLA	C3B-C4B	2.02	1.48	1.42
14	G	1105	CLA	C4C-C3C	2.02	1.48	1.45
14	H	1211	CLA	C1D-C2D	2.02	1.49	1.45
14	b	1210	CLA	C1D-C2D	2.01	1.49	1.45
14	G	1119	CLA	C1D-C2D	2.01	1.49	1.45
14	H	1229	CLA	C1D-C2D	2.01	1.49	1.45
18	G	4008	BCR	C30-C25	-2.01	1.51	1.53
14	G	1136	CLA	C3B-C4B	2.01	1.48	1.42
14	b	1209	CLA	C3B-C4B	2.01	1.48	1.42
14	a	1105	CLA	C4C-C3C	2.01	1.48	1.45
14	B	1216	CLA	C1D-C2D	2.01	1.49	1.45
14	b	1233	CLA	C4C-C3C	2.01	1.48	1.45
18	A	4003	BCR	C30-C25	-2.01	1.51	1.53
14	H	1233	CLA	C4C-C3C	2.01	1.48	1.45
14	b	1211	CLA	C1D-C2D	2.01	1.49	1.45
14	G	1101	CLA	C3B-C4B	2.01	1.48	1.42
14	A	1126	CLA	CHB-C4A	-2.00	1.32	1.37
14	G	1124	CLA	C1B-C2B	2.00	1.47	1.43
14	a	1133	CLA	C1D-C2D	2.00	1.49	1.45

All (8492) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4010	BCR	C16-C17-C18	26.23	164.06	127.28
18	b	4010	BCR	C16-C17-C18	26.18	164.00	127.28
18	B	4010	BCR	C16-C17-C18	26.16	163.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4017	BCR	C20-C21-C22	24.75	161.99	127.28
18	B	4017	BCR	C20-C21-C22	24.75	161.99	127.28
18	U	4019	BCR	C16-C17-C18	24.74	161.98	127.28
18	l	4019	BCR	C16-C17-C18	24.74	161.98	127.28
18	L	4019	BCR	C16-C17-C18	24.73	161.96	127.28
18	b	4017	BCR	C20-C21-C22	24.68	161.89	127.28
18	R	4020	BCR	C20-C21-C22	24.59	161.76	127.28
18	i	4020	BCR	C20-C21-C22	24.58	161.75	127.28
18	I	4020	BCR	C20-C21-C22	24.55	161.71	127.28
18	B	4016	BCR	C16-C17-C18	23.76	160.60	127.28
18	b	4016	BCR	C16-C17-C18	23.74	160.57	127.28
18	H	4016	BCR	C16-C17-C18	23.70	160.51	127.28
18	I	4018	BCR	C16-C17-C18	23.26	159.90	127.28
18	i	4018	BCR	C16-C17-C18	23.23	159.86	127.28
18	R	4018	BCR	C16-C17-C18	23.19	159.80	127.28
18	b	4013	BCR	C16-C17-C18	23.01	159.55	127.28
18	H	4013	BCR	C16-C17-C18	23.00	159.54	127.28
18	B	4013	BCR	C16-C17-C18	22.97	159.50	127.28
18	a	4007	BCR	C20-C21-C22	22.94	159.45	127.28
18	G	4007	BCR	C20-C21-C22	22.92	159.42	127.28
18	A	4007	BCR	C20-C21-C22	22.92	159.42	127.28
18	A	4001	BCR	C20-C21-C22	22.65	159.04	127.28
18	G	4001	BCR	C20-C21-C22	22.63	159.01	127.28
18	a	4001	BCR	C20-C21-C22	22.61	158.99	127.28
18	B	4006	BCR	C20-C21-C22	22.59	158.97	127.28
18	b	4006	BCR	C20-C21-C22	22.54	158.89	127.28
18	H	4006	BCR	C20-C21-C22	22.53	158.88	127.28
18	b	4016	BCR	C20-C21-C22	22.39	158.68	127.28
18	B	4016	BCR	C20-C21-C22	22.38	158.67	127.28
18	H	4016	BCR	C20-C21-C22	22.37	158.65	127.28
18	A	4003	BCR	C20-C21-C22	22.29	158.53	127.28
18	G	4003	BCR	C20-C21-C22	22.26	158.50	127.28
18	a	4003	BCR	C20-C21-C22	22.23	158.46	127.28
18	M	4021	BCR	C20-C21-C22	22.21	158.42	127.28
18	V	4021	BCR	C20-C21-C22	22.19	158.40	127.28
18	m	4021	BCR	C20-C21-C22	22.15	158.35	127.28
18	A	4001	BCR	C16-C17-C18	22.13	158.31	127.28
18	G	4001	BCR	C16-C17-C18	22.11	158.28	127.28
18	G	4008	BCR	C20-C21-C22	22.09	158.26	127.28
18	a	4008	BCR	C20-C21-C22	22.08	158.25	127.28
18	A	4008	BCR	C20-C21-C22	22.06	158.22	127.28
18	a	4001	BCR	C16-C17-C18	22.06	158.21	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4013	BCR	C20-C21-C22	21.98	158.11	127.28
18	H	4013	BCR	C20-C21-C22	21.97	158.09	127.28
18	b	4013	BCR	C20-C21-C22	21.97	158.09	127.28
18	B	4009	BCR	C16-C17-C18	21.89	157.98	127.28
18	b	4010	BCR	C20-C21-C22	21.87	157.95	127.28
18	b	4009	BCR	C16-C17-C18	21.87	157.95	127.28
18	H	4010	BCR	C20-C21-C22	21.85	157.91	127.28
18	B	4010	BCR	C20-C21-C22	21.84	157.91	127.28
18	H	4009	BCR	C16-C17-C18	21.83	157.90	127.28
18	I	4020	BCR	C16-C17-C18	21.82	157.88	127.28
18	i	4020	BCR	C16-C17-C18	21.82	157.88	127.28
18	R	4020	BCR	C16-C17-C18	21.81	157.86	127.28
18	A	4002	BCR	C15-C16-C17	21.60	167.71	123.52
18	G	4002	BCR	C15-C16-C17	21.59	167.69	123.52
18	a	4002	BCR	C15-C16-C17	21.59	167.69	123.52
18	H	4014	BCR	C15-C16-C17	21.56	167.63	123.52
18	b	4014	BCR	C15-C16-C17	21.55	167.62	123.52
18	B	4014	BCR	C15-C16-C17	21.54	167.60	123.52
18	V	4021	BCR	C16-C17-C18	21.54	157.49	127.28
18	M	4021	BCR	C16-C17-C18	21.52	157.46	127.28
18	m	4021	BCR	C16-C17-C18	21.51	157.45	127.28
18	G	4002	BCR	C20-C21-C22	21.43	157.34	127.28
18	a	4002	BCR	C20-C21-C22	21.41	157.31	127.28
18	A	4002	BCR	C20-C21-C22	21.40	157.29	127.28
18	U	4019	BCR	C20-C21-C22	21.40	157.29	127.28
18	l	4019	BCR	C20-C21-C22	21.39	157.27	127.28
18	H	4005	BCR	C16-C17-C18	21.38	157.26	127.28
18	L	4019	BCR	C20-C21-C22	21.37	157.25	127.28
18	b	4005	BCR	C16-C17-C18	21.36	157.23	127.28
18	B	4005	BCR	C16-C17-C18	21.36	157.23	127.28
18	B	4014	BCR	C20-C21-C22	21.28	157.13	127.28
18	b	4014	BCR	C20-C21-C22	21.27	157.11	127.28
18	H	4014	BCR	C20-C21-C22	21.25	157.08	127.28
18	b	4006	BCR	C16-C17-C18	21.09	156.86	127.28
18	H	4006	BCR	C16-C17-C18	21.09	156.85	127.28
18	H	4009	BCR	C20-C21-C22	21.07	156.83	127.28
18	B	4009	BCR	C20-C21-C22	21.05	156.81	127.28
18	b	4009	BCR	C20-C21-C22	21.05	156.80	127.28
18	a	4011	BCR	C16-C17-C18	21.04	156.78	127.28
18	A	4011	BCR	C16-C17-C18	21.03	156.78	127.28
18	B	4006	BCR	C16-C17-C18	21.03	156.77	127.28
18	G	4011	BCR	C16-C17-C18	21.00	156.73	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4007	BCR	C16-C17-C18	20.95	156.66	127.28
18	G	4007	BCR	C16-C17-C18	20.92	156.62	127.28
18	A	4007	BCR	C16-C17-C18	20.92	156.62	127.28
18	b	4017	BCR	C16-C17-C18	20.90	156.59	127.28
18	B	4017	BCR	C16-C17-C18	20.88	156.56	127.28
18	H	4017	BCR	C16-C17-C18	20.84	156.51	127.28
18	G	4003	BCR	C16-C17-C18	20.81	156.47	127.28
18	A	4003	BCR	C16-C17-C18	20.79	156.44	127.28
18	a	4003	BCR	C16-C17-C18	20.79	156.44	127.28
18	b	4005	BCR	C20-C21-C22	20.77	156.40	127.28
18	B	4005	BCR	C20-C21-C22	20.76	156.40	127.28
18	H	4005	BCR	C20-C21-C22	20.74	156.36	127.28
18	L	4022	BCR	C20-C21-C22	20.64	156.22	127.28
18	l	4022	BCR	C20-C21-C22	20.64	156.22	127.28
18	U	4022	BCR	C20-C21-C22	20.60	156.17	127.28
18	H	4005	BCR	C15-C16-C17	20.55	165.57	123.52
18	b	4005	BCR	C15-C16-C17	20.54	165.54	123.52
18	B	4005	BCR	C15-C16-C17	20.53	165.53	123.52
18	G	4008	BCR	C15-C16-C17	20.47	165.41	123.52
18	A	4008	BCR	C15-C16-C17	20.47	165.40	123.52
18	a	4008	BCR	C15-C16-C17	20.43	165.31	123.52
18	R	4018	BCR	C20-C21-C22	20.42	155.92	127.28
18	i	4018	BCR	C20-C21-C22	20.41	155.90	127.28
14	a	1111	CLA	C4-C3-C5	-20.37	79.87	115.23
14	A	1111	CLA	C4-C3-C5	-20.37	79.87	115.23
18	l	4022	BCR	C15-C16-C17	20.37	165.20	123.52
18	I	4018	BCR	C20-C21-C22	20.37	155.84	127.28
14	G	1111	CLA	C4-C3-C5	-20.35	79.91	115.23
18	L	4022	BCR	C15-C16-C17	20.34	165.14	123.52
18	U	4022	BCR	C15-C16-C17	20.33	165.11	123.52
18	B	4004	BCR	C15-C16-C17	20.32	165.10	123.52
18	b	4004	BCR	C15-C16-C17	20.31	165.09	123.52
18	H	4004	BCR	C15-C16-C17	20.31	165.08	123.52
18	G	4003	BCR	C15-C16-C17	20.10	164.65	123.52
18	a	4003	BCR	C15-C16-C17	20.10	164.65	123.52
18	A	4003	BCR	C15-C16-C17	20.10	164.64	123.52
18	I	4020	BCR	C15-C16-C17	20.03	164.51	123.52
18	i	4020	BCR	C15-C16-C17	20.02	164.49	123.52
18	R	4020	BCR	C15-C16-C17	20.00	164.44	123.52
18	l	4022	BCR	C16-C17-C18	19.93	155.22	127.28
18	L	4022	BCR	C16-C17-C18	19.87	155.15	127.28
18	U	4022	BCR	C16-C17-C18	19.87	155.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	4011	BCR	C20-C21-C22	19.83	155.09	127.28
18	a	4011	BCR	C20-C21-C22	19.81	155.06	127.28
18	A	4011	BCR	C20-C21-C22	19.81	155.06	127.28
18	L	4019	BCR	C15-C16-C17	19.79	164.01	123.52
18	l	4019	BCR	C15-C16-C17	19.79	164.00	123.52
18	U	4019	BCR	C15-C16-C17	19.78	163.99	123.52
18	H	4006	BCR	C15-C16-C17	19.75	163.93	123.52
18	b	4006	BCR	C15-C16-C17	19.75	163.93	123.52
18	a	4011	BCR	C15-C16-C17	19.75	163.92	123.52
18	A	4011	BCR	C15-C16-C17	19.74	163.91	123.52
18	B	4006	BCR	C15-C16-C17	19.73	163.89	123.52
18	G	4011	BCR	C15-C16-C17	19.73	163.89	123.52
18	M	4021	BCR	C15-C16-C17	19.64	163.70	123.52
18	V	4021	BCR	C15-C16-C17	19.62	163.67	123.52
18	m	4021	BCR	C15-C16-C17	19.62	163.65	123.52
18	B	4017	BCR	C15-C16-C17	19.56	163.54	123.52
18	b	4009	BCR	C15-C16-C17	19.55	163.53	123.52
18	B	4009	BCR	C15-C16-C17	19.55	163.53	123.52
18	H	4009	BCR	C15-C16-C17	19.54	163.50	123.52
18	b	4017	BCR	C15-C16-C17	19.54	163.50	123.52
18	H	4017	BCR	C15-C16-C17	19.54	163.49	123.52
18	H	4004	BCR	C20-C21-C22	19.44	154.54	127.28
18	B	4004	BCR	C20-C21-C22	19.43	154.53	127.28
18	b	4004	BCR	C20-C21-C22	19.43	154.53	127.28
18	G	4008	BCR	C16-C17-C18	19.39	154.47	127.28
18	A	4008	BCR	C16-C17-C18	19.36	154.42	127.28
18	B	4004	BCR	C16-C17-C18	19.34	154.40	127.28
18	H	4004	BCR	C16-C17-C18	19.31	154.35	127.28
18	b	4004	BCR	C16-C17-C18	19.30	154.35	127.28
18	a	4008	BCR	C16-C17-C18	19.30	154.35	127.28
18	A	4007	BCR	C15-C16-C17	19.25	162.91	123.52
18	G	4007	BCR	C15-C16-C17	19.25	162.90	123.52
18	a	4007	BCR	C15-C16-C17	19.25	162.90	123.52
18	V	4021	BCR	C10-C11-C12	18.95	178.11	123.20
18	M	4021	BCR	C10-C11-C12	18.93	178.06	123.20
18	m	4021	BCR	C10-C11-C12	18.93	178.04	123.20
18	B	4010	BCR	C10-C11-C12	18.80	177.69	123.20
18	G	4003	BCR	C10-C11-C12	18.80	177.67	123.20
18	H	4010	BCR	C10-C11-C12	18.80	177.66	123.20
18	a	4003	BCR	C10-C11-C12	18.79	177.65	123.20
18	A	4003	BCR	C10-C11-C12	18.78	177.62	123.20
18	b	4010	BCR	C10-C11-C12	18.78	177.60	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4001	BCR	C10-C11-C12	18.77	177.58	123.20
18	G	4001	BCR	C10-C11-C12	18.75	177.52	123.20
18	a	4001	BCR	C10-C11-C12	18.75	177.52	123.20
18	a	4007	BCR	C10-C11-C12	18.70	177.38	123.20
18	A	4007	BCR	C10-C11-C12	18.70	177.37	123.20
18	G	4007	BCR	C10-C11-C12	18.67	177.29	123.20
18	U	4022	BCR	C10-C11-C12	18.66	177.26	123.20
18	l	4022	BCR	C10-C11-C12	18.65	177.24	123.20
18	L	4022	BCR	C10-C11-C12	18.65	177.24	123.20
18	b	4014	BCR	C16-C17-C18	18.62	153.39	127.28
18	R	4018	BCR	C10-C11-C12	18.62	177.14	123.20
18	H	4014	BCR	C16-C17-C18	18.61	153.38	127.28
18	B	4014	BCR	C16-C17-C18	18.61	153.37	127.28
18	H	4016	BCR	C10-C11-C12	18.60	177.10	123.20
18	b	4016	BCR	C10-C11-C12	18.59	177.08	123.20
18	B	4016	BCR	C10-C11-C12	18.59	177.08	123.20
18	i	4018	BCR	C10-C11-C12	18.59	177.07	123.20
18	H	4004	BCR	C10-C11-C12	18.59	177.05	123.20
18	b	4004	BCR	C10-C11-C12	18.58	177.05	123.20
18	B	4004	BCR	C10-C11-C12	18.58	177.03	123.20
18	I	4018	BCR	C10-C11-C12	18.58	177.02	123.20
18	A	4008	BCR	C10-C11-C12	18.50	176.81	123.20
18	a	4008	BCR	C10-C11-C12	18.50	176.79	123.20
18	G	4008	BCR	C10-C11-C12	18.49	176.78	123.20
18	U	4019	BCR	C10-C11-C12	18.48	176.73	123.20
18	l	4019	BCR	C10-C11-C12	18.47	176.72	123.20
18	L	4019	BCR	C10-C11-C12	18.45	176.65	123.20
18	B	4017	BCR	C10-C11-C12	18.43	176.60	123.20
18	H	4017	BCR	C10-C11-C12	18.42	176.57	123.20
18	b	4017	BCR	C10-C11-C12	18.42	176.57	123.20
18	I	4018	BCR	C15-C16-C17	18.31	160.99	123.52
18	b	4014	BCR	C10-C11-C12	18.30	176.23	123.20
18	B	4014	BCR	C10-C11-C12	18.30	176.23	123.20
18	H	4014	BCR	C10-C11-C12	18.30	176.23	123.20
18	R	4018	BCR	C15-C16-C17	18.29	160.94	123.52
18	i	4018	BCR	C15-C16-C17	18.27	160.91	123.52
18	H	4009	BCR	C10-C11-C12	18.25	176.08	123.20
18	B	4009	BCR	C10-C11-C12	18.24	176.06	123.20
18	b	4009	BCR	C10-C11-C12	18.24	176.04	123.20
18	R	4020	BCR	C10-C11-C12	18.19	175.90	123.20
18	B	4005	BCR	C10-C11-C12	18.18	175.88	123.20
18	i	4020	BCR	C10-C11-C12	18.18	175.88	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	I	4020	BCR	C10-C11-C12	18.18	175.86	123.20
18	A	4001	BCR	C15-C16-C17	18.17	160.70	123.52
18	H	4005	BCR	C10-C11-C12	18.16	175.83	123.20
18	a	4001	BCR	C15-C16-C17	18.15	160.66	123.52
18	b	4005	BCR	C10-C11-C12	18.15	175.79	123.20
18	G	4001	BCR	C15-C16-C17	18.14	160.64	123.52
18	H	4006	BCR	C10-C11-C12	18.09	175.62	123.20
18	B	4006	BCR	C10-C11-C12	18.08	175.60	123.20
18	b	4006	BCR	C10-C11-C12	18.08	175.58	123.20
18	H	4013	BCR	C10-C11-C12	17.91	175.08	123.20
18	B	4013	BCR	C10-C11-C12	17.89	175.05	123.20
18	b	4013	BCR	C10-C11-C12	17.89	175.02	123.20
18	b	4013	BCR	C15-C16-C17	17.78	159.90	123.52
18	H	4013	BCR	C15-C16-C17	17.77	159.87	123.52
18	B	4013	BCR	C15-C16-C17	17.74	159.81	123.52
18	H	4016	BCR	C15-C16-C17	17.58	159.49	123.52
18	G	4002	BCR	C10-C11-C12	17.58	174.14	123.20
18	a	4002	BCR	C10-C11-C12	17.58	174.14	123.20
18	A	4002	BCR	C10-C11-C12	17.57	174.10	123.20
18	b	4016	BCR	C15-C16-C17	17.56	159.44	123.52
18	B	4016	BCR	C15-C16-C17	17.55	159.43	123.52
18	A	4002	BCR	C16-C17-C18	17.34	151.59	127.28
18	G	4011	BCR	C10-C11-C12	17.33	173.40	123.20
18	G	4002	BCR	C16-C17-C18	17.32	151.57	127.28
18	A	4011	BCR	C10-C11-C12	17.32	173.38	123.20
18	a	4011	BCR	C10-C11-C12	17.31	173.36	123.20
18	a	4002	BCR	C16-C17-C18	17.30	151.55	127.28
14	G	1111	CLA	C5-C3-C2	17.26	159.91	121.17
14	a	1111	CLA	C5-C3-C2	17.26	159.91	121.17
14	A	1111	CLA	C5-C3-C2	17.24	159.87	121.17
14	A	1111	CLA	C4-C3-C2	-16.97	80.04	123.63
14	G	1111	CLA	C4-C3-C2	-16.97	80.04	123.63
14	a	1111	CLA	C4-C3-C2	-16.96	80.07	123.63
18	L	4019	BCR	C16-C15-C14	16.59	157.46	123.52
18	l	4019	BCR	C16-C15-C14	16.57	157.43	123.52
18	U	4019	BCR	C16-C15-C14	16.56	157.41	123.52
18	H	4010	BCR	C15-C16-C17	15.84	155.94	123.52
18	B	4010	BCR	C15-C16-C17	15.82	155.88	123.52
18	b	4010	BCR	C15-C16-C17	15.80	155.85	123.52
18	V	4021	BCR	C16-C15-C14	15.25	154.73	123.52
18	M	4021	BCR	C16-C15-C14	15.24	154.69	123.52
18	m	4021	BCR	C16-C15-C14	15.23	154.69	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4004	BCR	C21-C20-C19	15.07	166.85	123.20
18	b	4004	BCR	C21-C20-C19	15.07	166.85	123.20
18	G	4011	BCR	C11-C10-C9	15.07	148.41	127.28
18	a	4011	BCR	C11-C10-C9	15.06	148.40	127.28
18	B	4004	BCR	C21-C20-C19	15.05	166.81	123.20
18	A	4011	BCR	C11-C10-C9	15.02	148.35	127.28
18	H	4013	BCR	C11-C10-C9	14.65	147.82	127.28
18	i	4018	BCR	C16-C15-C14	14.63	153.46	123.52
18	R	4018	BCR	C16-C15-C14	14.63	153.46	123.52
18	b	4013	BCR	C11-C10-C9	14.63	147.79	127.28
18	B	4013	BCR	C11-C10-C9	14.62	147.79	127.28
18	I	4018	BCR	C16-C15-C14	14.58	153.36	123.52
18	B	4013	BCR	C16-C15-C14	14.55	153.29	123.52
18	B	4017	BCR	C11-C10-C9	14.55	147.68	127.28
18	H	4017	BCR	C11-C10-C9	14.54	147.68	127.28
18	H	4013	BCR	C16-C15-C14	14.52	153.22	123.52
18	b	4013	BCR	C16-C15-C14	14.51	153.21	123.52
18	b	4017	BCR	C11-C10-C9	14.51	147.62	127.28
18	G	4001	BCR	C16-C15-C14	14.46	153.10	123.52
18	a	4001	BCR	C16-C15-C14	14.44	153.07	123.52
18	A	4001	BCR	C16-C15-C14	14.43	153.05	123.52
18	b	4006	BCR	C11-C10-C9	14.41	147.48	127.28
18	H	4006	BCR	C11-C10-C9	14.40	147.48	127.28
18	B	4006	BCR	C11-C10-C9	14.40	147.47	127.28
18	L	4022	BCR	C21-C20-C19	14.36	164.82	123.20
18	l	4022	BCR	C21-C20-C19	14.36	164.81	123.20
18	U	4022	BCR	C21-C20-C19	14.34	164.76	123.20
18	B	4016	BCR	C16-C15-C14	14.33	152.84	123.52
18	b	4016	BCR	C16-C15-C14	14.32	152.81	123.52
18	H	4016	BCR	C16-C15-C14	14.31	152.81	123.52
18	B	4014	BCR	C21-C20-C19	14.29	164.60	123.20
18	b	4014	BCR	C21-C20-C19	14.29	164.59	123.20
18	H	4014	BCR	C21-C20-C19	14.26	164.53	123.20
18	G	4011	BCR	C21-C20-C19	14.20	164.35	123.20
18	A	4011	BCR	C21-C20-C19	14.20	164.35	123.20
18	a	4011	BCR	C21-C20-C19	14.18	164.30	123.20
18	b	4010	BCR	C21-C20-C19	13.94	163.58	123.20
18	B	4010	BCR	C21-C20-C19	13.92	163.53	123.20
18	H	4010	BCR	C21-C20-C19	13.92	163.52	123.20
18	a	4002	BCR	C21-C20-C19	13.91	163.50	123.20
18	G	4002	BCR	C21-C20-C19	13.90	163.49	123.20
18	A	4002	BCR	C21-C20-C19	13.90	163.49	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4008	BCR	C21-C20-C19	13.87	163.39	123.20
18	a	4008	BCR	C21-C20-C19	13.87	163.39	123.20
18	G	4008	BCR	C21-C20-C19	13.87	163.38	123.20
18	B	4005	BCR	C11-C10-C9	13.71	146.51	127.28
18	U	4019	BCR	C11-C10-C9	13.70	146.49	127.28
18	H	4004	BCR	C11-C10-C9	13.70	146.49	127.28
18	l	4019	BCR	C11-C10-C9	13.70	146.49	127.28
18	b	4004	BCR	C11-C10-C9	13.69	146.48	127.28
18	H	4005	BCR	C11-C10-C9	13.68	146.47	127.28
18	B	4004	BCR	C11-C10-C9	13.67	146.45	127.28
18	b	4005	BCR	C11-C10-C9	13.66	146.43	127.28
18	b	4005	BCR	C21-C20-C19	13.65	162.76	123.20
18	L	4019	BCR	C11-C10-C9	13.65	146.43	127.28
18	H	4005	BCR	C21-C20-C19	13.65	162.76	123.20
18	B	4005	BCR	C21-C20-C19	13.64	162.71	123.20
18	B	4013	BCR	C21-C20-C19	13.58	162.56	123.20
18	b	4013	BCR	C21-C20-C19	13.57	162.53	123.20
18	H	4013	BCR	C21-C20-C19	13.57	162.51	123.20
18	i	4020	BCR	C21-C20-C19	13.55	162.45	123.20
18	H	4016	BCR	C11-C10-C9	13.55	146.28	127.28
18	R	4020	BCR	C21-C20-C19	13.54	162.42	123.20
18	I	4020	BCR	C21-C20-C19	13.53	162.41	123.20
18	B	4016	BCR	C11-C10-C9	13.51	146.23	127.28
18	b	4016	BCR	C11-C10-C9	13.51	146.23	127.28
18	I	4020	BCR	C11-C10-C9	13.46	146.15	127.28
18	H	4009	BCR	C21-C20-C19	13.44	162.15	123.20
18	G	4001	BCR	C21-C20-C19	13.44	162.15	123.20
18	A	4001	BCR	C21-C20-C19	13.44	162.14	123.20
18	B	4009	BCR	C21-C20-C19	13.44	162.13	123.20
18	R	4020	BCR	C11-C10-C9	13.44	146.12	127.28
18	i	4020	BCR	C11-C10-C9	13.43	146.12	127.28
18	a	4001	BCR	C21-C20-C19	13.43	162.10	123.20
18	b	4009	BCR	C21-C20-C19	13.41	162.07	123.20
18	M	4021	BCR	C21-C20-C19	13.39	162.00	123.20
18	V	4021	BCR	C21-C20-C19	13.37	161.93	123.20
18	b	4017	BCR	C21-C20-C19	13.36	161.92	123.20
18	m	4021	BCR	C21-C20-C19	13.36	161.92	123.20
18	H	4017	BCR	C21-C20-C19	13.36	161.90	123.20
18	B	4017	BCR	C21-C20-C19	13.35	161.90	123.20
18	H	4016	BCR	C21-C20-C19	13.35	161.88	123.20
18	B	4016	BCR	C21-C20-C19	13.35	161.88	123.20
18	b	4016	BCR	C21-C20-C19	13.34	161.86	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b	4010	BCR	C16-C15-C14	13.18	150.48	123.52
18	B	4010	BCR	C16-C15-C14	13.17	150.46	123.52
18	H	4010	BCR	C16-C15-C14	13.16	150.44	123.52
18	B	4009	BCR	C16-C15-C14	13.15	150.43	123.52
18	H	4009	BCR	C16-C15-C14	13.15	150.43	123.52
18	b	4009	BCR	C16-C15-C14	13.15	150.42	123.52
18	G	4003	BCR	C11-C10-C9	13.14	145.71	127.28
18	A	4003	BCR	C11-C10-C9	13.11	145.67	127.28
18	a	4003	BCR	C11-C10-C9	13.10	145.65	127.28
18	a	4007	BCR	C21-C20-C19	13.10	161.14	123.20
18	l	4022	BCR	C11-C10-C9	13.10	145.64	127.28
18	A	4007	BCR	C21-C20-C19	13.09	161.14	123.20
18	U	4022	BCR	C11-C10-C9	13.09	145.64	127.28
18	G	4007	BCR	C21-C20-C19	13.09	161.13	123.20
18	L	4022	BCR	C11-C10-C9	13.08	145.62	127.28
18	B	4006	BCR	C21-C20-C19	13.04	160.99	123.20
18	b	4006	BCR	C21-C20-C19	13.02	160.92	123.20
18	H	4006	BCR	C21-C20-C19	13.01	160.89	123.20
18	L	4019	BCR	C21-C20-C19	13.01	160.88	123.20
18	l	4019	BCR	C21-C20-C19	12.99	160.84	123.20
18	U	4019	BCR	C21-C20-C19	12.99	160.84	123.20
13	G	1011	CL0	C1B-CHB-C4A	12.99	129.68	121.32
13	A	1011	CL0	C1B-CHB-C4A	12.98	129.67	121.32
13	a	1011	CL0	C1B-CHB-C4A	12.97	129.66	121.32
18	B	4004	BCR	C16-C15-C14	12.90	149.91	123.52
18	b	4004	BCR	C16-C15-C14	12.89	149.89	123.52
18	H	4004	BCR	C16-C15-C14	12.89	149.88	123.52
18	A	4003	BCR	C21-C20-C19	12.83	160.38	123.20
18	a	4003	BCR	C21-C20-C19	12.82	160.35	123.20
18	G	4003	BCR	C21-C20-C19	12.82	160.34	123.20
18	b	4006	BCR	C16-C15-C14	12.75	149.61	123.52
18	B	4006	BCR	C16-C15-C14	12.75	149.61	123.52
18	H	4006	BCR	C16-C15-C14	12.74	149.59	123.52
18	A	4007	BCR	C16-C15-C14	12.67	149.45	123.52
18	G	4007	BCR	C16-C15-C14	12.67	149.44	123.52
18	a	4007	BCR	C16-C15-C14	12.66	149.41	123.52
18	R	4018	BCR	C21-C20-C19	12.58	159.64	123.20
18	i	4018	BCR	C21-C20-C19	12.56	159.60	123.20
18	I	4018	BCR	C21-C20-C19	12.55	159.56	123.20
18	B	4014	BCR	C11-C10-C9	12.50	144.81	127.28
18	V	4021	BCR	C11-C10-C9	12.48	144.79	127.28
18	b	4014	BCR	C11-C10-C9	12.48	144.78	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4014	BCR	C11-C10-C9	12.47	144.76	127.28
18	M	4021	BCR	C11-C10-C9	12.46	144.75	127.28
18	A	4003	BCR	C16-C15-C14	12.46	149.00	123.52
18	m	4021	BCR	C11-C10-C9	12.46	144.75	127.28
18	B	4017	BCR	C16-C15-C14	12.45	148.99	123.52
18	a	4003	BCR	C16-C15-C14	12.44	148.98	123.52
18	H	4017	BCR	C16-C15-C14	12.44	148.97	123.52
18	b	4017	BCR	C16-C15-C14	12.44	148.97	123.52
18	G	4003	BCR	C16-C15-C14	12.43	148.95	123.52
18	G	4011	BCR	C16-C15-C14	12.41	148.91	123.52
18	a	4011	BCR	C16-C15-C14	12.40	148.90	123.52
18	A	4011	BCR	C16-C15-C14	12.40	148.88	123.52
18	a	4007	BCR	C11-C10-C9	12.28	144.50	127.28
18	A	4007	BCR	C11-C10-C9	12.26	144.47	127.28
18	G	4007	BCR	C11-C10-C9	12.24	144.44	127.28
18	a	4008	BCR	C11-C10-C9	12.20	144.39	127.28
18	a	4002	BCR	C16-C15-C14	12.18	148.44	123.52
18	G	4002	BCR	C16-C15-C14	12.17	148.41	123.52
18	G	4008	BCR	C11-C10-C9	12.16	144.34	127.28
18	A	4002	BCR	C16-C15-C14	12.16	148.40	123.52
18	A	4008	BCR	C11-C10-C9	12.14	144.30	127.28
18	l	4022	BCR	C16-C15-C14	11.99	148.06	123.52
18	U	4022	BCR	C16-C15-C14	11.99	148.05	123.52
18	L	4022	BCR	C16-C15-C14	11.98	148.02	123.52
18	A	4001	BCR	C11-C10-C9	11.95	144.03	127.28
18	a	4001	BCR	C11-C10-C9	11.94	144.03	127.28
18	G	4001	BCR	C11-C10-C9	11.94	144.02	127.28
18	I	4020	BCR	C16-C15-C14	11.92	147.90	123.52
18	i	4020	BCR	C16-C15-C14	11.91	147.88	123.52
18	R	4020	BCR	C16-C15-C14	11.90	147.86	123.52
18	A	4008	BCR	C16-C15-C14	11.86	147.78	123.52
18	G	4008	BCR	C16-C15-C14	11.84	147.75	123.52
18	a	4008	BCR	C16-C15-C14	11.84	147.75	123.52
18	B	4010	BCR	C11-C10-C9	11.66	143.63	127.28
18	b	4010	BCR	C11-C10-C9	11.63	143.59	127.28
18	H	4010	BCR	C11-C10-C9	11.61	143.56	127.28
15	H	1230	F6C	CAA-C2A-C3A	-11.61	106.13	127.87
15	b	1230	F6C	CAA-C2A-C3A	-11.60	106.15	127.87
15	B	1230	F6C	CAA-C2A-C3A	-11.57	106.19	127.87
18	B	4005	BCR	C16-C15-C14	11.51	147.06	123.52
18	H	4005	BCR	C16-C15-C14	11.50	147.05	123.52
18	b	4005	BCR	C16-C15-C14	11.49	147.03	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4013	BCR	C11-C12-C13	11.45	157.76	126.36
18	H	4013	BCR	C11-C12-C13	11.45	157.75	126.36
18	b	4013	BCR	C11-C12-C13	11.44	157.72	126.36
18	H	4014	BCR	C11-C12-C13	11.38	157.56	126.36
18	B	4014	BCR	C11-C12-C13	11.37	157.55	126.36
18	b	4014	BCR	C11-C12-C13	11.37	157.54	126.36
18	A	4008	BCR	C11-C12-C13	11.35	157.49	126.36
18	a	4008	BCR	C11-C12-C13	11.34	157.46	126.36
18	H	4006	BCR	C11-C12-C13	11.33	157.42	126.36
18	G	4008	BCR	C11-C12-C13	11.32	157.41	126.36
15	H	1238	F6C	CAA-C2A-C3A	-11.32	106.67	127.87
18	B	4006	BCR	C11-C12-C13	11.32	157.39	126.36
18	b	4006	BCR	C11-C12-C13	11.31	157.38	126.36
15	b	1238	F6C	CAA-C2A-C3A	-11.31	106.69	127.87
15	B	1238	F6C	CAA-C2A-C3A	-11.29	106.73	127.87
15	H	1237	F6C	C3B-C2B-C1B	-11.28	100.64	106.46
18	B	4005	BCR	C11-C12-C13	11.22	157.12	126.36
18	H	4005	BCR	C11-C12-C13	11.21	157.11	126.36
18	b	4005	BCR	C11-C12-C13	11.21	157.10	126.36
18	G	4011	BCR	C11-C12-C13	11.20	157.08	126.36
15	b	1237	F6C	C3B-C2B-C1B	-11.20	100.68	106.46
15	B	1237	F6C	C3B-C2B-C1B	-11.20	100.68	106.46
18	A	4011	BCR	C11-C12-C13	11.18	157.03	126.36
18	a	4011	BCR	C11-C12-C13	11.17	156.99	126.36
15	b	1238	F6C	C3B-C2B-C1B	-11.17	100.70	106.46
15	H	1238	F6C	C3B-C2B-C1B	-11.15	100.70	106.46
15	B	1238	F6C	C3B-C2B-C1B	-11.13	100.72	106.46
18	i	4020	BCR	C11-C12-C13	11.13	156.87	126.36
18	R	4020	BCR	C11-C12-C13	11.12	156.86	126.36
18	I	4020	BCR	C11-C12-C13	11.10	156.81	126.36
18	H	4014	BCR	C16-C15-C14	11.01	146.04	123.52
18	b	4014	BCR	C16-C15-C14	10.99	146.01	123.52
18	H	4004	BCR	C11-C12-C13	10.98	156.48	126.36
18	B	4014	BCR	C16-C15-C14	10.97	145.97	123.52
18	L	4022	BCR	C11-C12-C13	10.97	156.44	126.36
18	B	4004	BCR	C11-C12-C13	10.96	156.41	126.36
18	b	4004	BCR	C11-C12-C13	10.96	156.41	126.36
18	l	4022	BCR	C11-C12-C13	10.95	156.40	126.36
18	U	4022	BCR	C11-C12-C13	10.95	156.39	126.36
18	a	4007	BCR	C11-C12-C13	10.94	156.37	126.36
18	a	4002	BCR	C11-C12-C13	10.94	156.35	126.36
18	A	4007	BCR	C11-C12-C13	10.93	156.33	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4009	BCR	C11-C10-C9	10.92	142.59	127.28
18	b	4009	BCR	C11-C10-C9	10.92	142.59	127.28
18	G	4007	BCR	C11-C12-C13	10.92	156.30	126.36
18	A	4002	BCR	C11-C12-C13	10.91	156.28	126.36
18	B	4009	BCR	C11-C10-C9	10.91	142.58	127.28
18	G	4002	BCR	C11-C12-C13	10.91	156.27	126.36
18	A	4001	BCR	C11-C12-C13	10.90	156.25	126.36
18	a	4001	BCR	C11-C12-C13	10.90	156.25	126.36
18	G	4001	BCR	C11-C12-C13	10.89	156.22	126.36
18	H	4010	BCR	C11-C12-C13	10.72	155.76	126.36
18	B	4010	BCR	C11-C12-C13	10.72	155.75	126.36
18	b	4010	BCR	C11-C12-C13	10.71	155.73	126.36
18	i	4018	BCR	C11-C10-C9	10.68	142.26	127.28
18	R	4018	BCR	C11-C10-C9	10.67	142.25	127.28
15	B	1207	F6C	CAA-C2A-C3A	-10.65	107.93	127.87
15	H	1207	F6C	CAA-C2A-C3A	-10.65	107.93	127.87
15	b	1237	F6C	CAA-C2A-C3A	-10.64	107.94	127.87
15	H	1237	F6C	CAA-C2A-C3A	-10.63	107.95	127.87
15	B	1237	F6C	CAA-C2A-C3A	-10.63	107.96	127.87
18	I	4018	BCR	C11-C10-C9	10.63	142.19	127.28
15	b	1207	F6C	CAA-C2A-C3A	-10.62	107.97	127.87
15	B	1207	F6C	C3B-C2B-C1B	-10.59	101.00	106.46
18	H	4016	BCR	C11-C12-C13	10.58	155.38	126.36
18	b	4016	BCR	C11-C12-C13	10.56	155.33	126.36
18	B	4016	BCR	C11-C12-C13	10.56	155.32	126.36
15	b	1207	F6C	C3B-C2B-C1B	-10.55	101.02	106.46
15	H	1207	F6C	C3B-C2B-C1B	-10.51	101.04	106.46
18	A	4003	BCR	C11-C12-C13	10.49	155.13	126.36
18	a	4003	BCR	C11-C12-C13	10.48	155.09	126.36
18	G	4003	BCR	C11-C12-C13	10.46	155.06	126.36
18	L	4019	BCR	C11-C12-C13	10.44	154.98	126.36
18	l	4019	BCR	C11-C12-C13	10.43	154.95	126.36
18	U	4019	BCR	C11-C12-C13	10.42	154.93	126.36
15	G	1121	F6C	CAA-C2A-C3A	-10.29	108.59	127.87
15	A	1121	F6C	CAA-C2A-C3A	-10.29	108.59	127.87
15	a	1121	F6C	CAA-C2A-C3A	-10.29	108.60	127.87
18	V	4021	BCR	C11-C12-C13	10.15	154.20	126.36
18	M	4021	BCR	C11-C12-C13	10.15	154.19	126.36
18	m	4021	BCR	C11-C12-C13	10.14	154.16	126.36
15	B	1230	F6C	C3B-C2B-C1B	-9.94	101.33	106.46
15	H	1230	F6C	C3B-C2B-C1B	-9.93	101.33	106.46
15	b	1230	F6C	C3B-C2B-C1B	-9.93	101.34	106.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	4018	BCR	C11-C12-C13	9.83	153.32	126.36
18	i	4018	BCR	C11-C12-C13	9.81	153.25	126.36
18	I	4018	BCR	C11-C12-C13	9.81	153.25	126.36
18	H	4009	BCR	C11-C12-C13	9.70	152.96	126.36
18	b	4009	BCR	C11-C12-C13	9.70	152.96	126.36
18	B	4009	BCR	C11-C12-C13	9.69	152.94	126.36
13	G	1011	CL0	O2D-CGD-CBD	9.55	121.44	110.95
13	A	1011	CL0	O2D-CGD-CBD	9.54	121.43	110.95
13	a	1011	CL0	O2D-CGD-CBD	9.52	121.41	110.95
18	B	4017	BCR	C11-C12-C13	9.34	151.96	126.36
18	H	4017	BCR	C11-C12-C13	9.33	151.95	126.36
18	b	4017	BCR	C11-C12-C13	9.32	151.93	126.36
15	G	1121	F6C	C3B-C2B-C1B	-9.19	101.72	106.46
15	A	1121	F6C	C3B-C2B-C1B	-9.14	101.74	106.46
15	a	1121	F6C	C3B-C2B-C1B	-9.14	101.75	106.46
18	H	4013	BCR	C20-C19-C18	9.07	151.22	126.36
18	b	4013	BCR	C20-C19-C18	9.05	151.17	126.36
18	B	4013	BCR	C20-C19-C18	9.04	151.16	126.36
14	a	1135	CLA	CMD-C2D-C1D	8.96	140.51	124.73
14	A	1135	CLA	CMD-C2D-C1D	8.95	140.49	124.73
14	G	1135	CLA	CMD-C2D-C1D	8.94	140.47	124.73
18	I	4020	BCR	C20-C19-C18	8.81	150.51	126.36
18	R	4020	BCR	C20-C19-C18	8.79	150.48	126.36
18	i	4020	BCR	C20-C19-C18	8.78	150.44	126.36
15	B	1238	F6C	CMD-C2D-C1D	8.75	138.71	125.03
15	b	1238	F6C	CMD-C2D-C1D	8.74	138.70	125.03
15	H	1238	F6C	CMD-C2D-C1D	8.74	138.69	125.03
15	G	1121	F6C	CMD-C2D-C1D	8.54	138.38	125.03
15	A	1121	F6C	CMD-C2D-C1D	8.52	138.35	125.03
15	a	1121	F6C	CMD-C2D-C1D	8.51	138.34	125.03
18	a	4003	BCR	C20-C19-C18	8.51	149.70	126.36
18	G	4003	BCR	C20-C19-C18	8.50	149.67	126.36
18	A	4003	BCR	C20-C19-C18	8.50	149.67	126.36
15	B	1230	F6C	C1D-ND-C4D	-8.48	102.81	106.68
15	B	1207	F6C	CMD-C2D-C1D	8.47	138.26	125.03
15	b	1230	F6C	C1D-ND-C4D	-8.46	102.82	106.68
15	b	1207	F6C	CMD-C2D-C1D	8.45	138.25	125.03
14	B	1227	CLA	CMD-C2D-C1D	8.45	139.61	124.73
15	H	1207	F6C	CMD-C2D-C1D	8.44	138.23	125.03
14	b	1227	CLA	CMD-C2D-C1D	8.42	139.56	124.73
14	H	1227	CLA	CMD-C2D-C1D	8.41	139.54	124.73
15	H	1230	F6C	C1D-ND-C4D	-8.39	102.85	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4006	BCR	C20-C19-C18	8.37	149.32	126.36
15	B	1237	F6C	CMD-C2D-C1D	8.36	138.09	125.03
18	B	4006	BCR	C20-C19-C18	8.36	149.28	126.36
15	H	1237	F6C	CMD-C2D-C1D	8.35	138.09	125.03
18	b	4006	BCR	C20-C19-C18	8.35	149.27	126.36
14	H	1232	CLA	CMD-C2D-C1D	8.35	139.43	124.73
14	B	1232	CLA	CMD-C2D-C1D	8.35	139.43	124.73
15	b	1237	F6C	CMD-C2D-C1D	8.34	138.07	125.03
14	b	1232	CLA	CMD-C2D-C1D	8.34	139.41	124.73
14	H	1209	CLA	CMD-C2D-C1D	8.30	139.35	124.73
14	a	1130	CLA	CMD-C2D-C1D	8.29	139.32	124.73
14	B	1209	CLA	CMD-C2D-C1D	8.28	139.31	124.73
14	b	1209	CLA	CMD-C2D-C1D	8.28	139.31	124.73
14	A	1130	CLA	CMD-C2D-C1D	8.28	139.30	124.73
14	G	1130	CLA	CMD-C2D-C1D	8.27	139.29	124.73
14	G	1124	CLA	CMD-C2D-C1D	8.27	139.29	124.73
14	A	1124	CLA	CMD-C2D-C1D	8.27	139.29	124.73
14	A	1132	CLA	CMD-C2D-C1D	8.27	139.28	124.73
14	a	1114	CLA	CMD-C2D-C1D	8.26	139.28	124.73
14	G	1132	CLA	CMD-C2D-C1D	8.26	139.27	124.73
14	A	1114	CLA	CMD-C2D-C1D	8.25	139.26	124.73
14	a	1124	CLA	CMD-C2D-C1D	8.25	139.26	124.73
14	a	1132	CLA	CMD-C2D-C1D	8.25	139.25	124.73
14	B	1223	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	G	1114	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	K	1401	CLA	CMD-C2D-C1D	8.24	139.24	124.73
14	H	1223	CLA	CMD-C2D-C1D	8.23	139.22	124.73
14	k	1401	CLA	CMD-C2D-C1D	8.22	139.21	124.73
15	b	1230	F6C	CMD-C2D-C1D	8.22	137.88	125.03
14	T	1401	CLA	CMD-C2D-C1D	8.22	139.20	124.73
14	b	1223	CLA	CMD-C2D-C1D	8.22	139.20	124.73
15	H	1230	F6C	CMD-C2D-C1D	8.21	137.87	125.03
15	B	1230	F6C	CMD-C2D-C1D	8.21	137.86	125.03
14	G	1139	CLA	CMD-C2D-C1D	8.20	139.18	124.73
14	G	1104	CLA	CMD-C2D-C1D	8.20	139.16	124.73
14	H	1228	CLA	CMD-C2D-C1D	8.19	139.16	124.73
14	A	1139	CLA	CMD-C2D-C1D	8.19	139.16	124.73
14	A	1131	CLA	CMD-C2D-C1D	8.19	139.16	124.73
14	H	1213	CLA	CMD-C2D-C1D	8.19	139.15	124.73
14	a	1139	CLA	CMD-C2D-C1D	8.19	139.15	124.73
14	A	1103	CLA	CMD-C2D-C1D	8.19	139.15	124.73
14	a	1116	CLA	CMD-C2D-C1D	8.19	139.15	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1103	CLA	CMD-C2D-C1D	8.18	139.14	124.73
14	B	1213	CLA	CMD-C2D-C1D	8.18	139.14	124.73
14	A	1116	CLA	CMD-C2D-C1D	8.18	139.14	124.73
14	B	1228	CLA	CMD-C2D-C1D	8.18	139.14	124.73
14	H	1203	CLA	CMD-C2D-C1D	8.18	139.12	124.73
14	G	1103	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	a	1104	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	A	1104	CLA	CMD-C2D-C1D	8.17	139.12	124.73
14	G	1131	CLA	CMD-C2D-C1D	8.17	139.11	124.73
18	A	4007	BCR	C20-C19-C18	8.17	148.75	126.36
14	b	1213	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	b	1228	CLA	CMD-C2D-C1D	8.17	139.11	124.73
14	A	1105	CLA	CMD-C2D-C1D	8.16	139.10	124.73
14	A	1109	CLA	CMD-C2D-C1D	8.16	139.10	124.73
18	G	4007	BCR	C20-C19-C18	8.16	148.74	126.36
14	A	1115	CLA	CMD-C2D-C1D	8.16	139.10	124.73
18	L	4019	BCR	C20-C19-C18	8.16	148.74	126.36
14	G	1115	CLA	CMD-C2D-C1D	8.16	139.10	124.73
14	a	1131	CLA	CMD-C2D-C1D	8.16	139.09	124.73
18	G	4002	BCR	C11-C10-C9	8.16	138.72	127.28
14	a	1105	CLA	CMD-C2D-C1D	8.15	139.09	124.73
14	b	1203	CLA	CMD-C2D-C1D	8.15	139.09	124.73
18	a	4007	BCR	C20-C19-C18	8.15	148.72	126.36
14	G	1105	CLA	CMD-C2D-C1D	8.15	139.08	124.73
18	U	4019	BCR	C20-C19-C18	8.15	148.71	126.36
18	l	4019	BCR	C20-C19-C18	8.14	148.69	126.36
14	B	1211	CLA	CMD-C2D-C1D	8.14	139.07	124.73
14	G	1109	CLA	CMD-C2D-C1D	8.14	139.06	124.73
14	a	1109	CLA	CMD-C2D-C1D	8.14	139.06	124.73
14	b	1211	CLA	CMD-C2D-C1D	8.14	139.06	124.73
18	H	4017	BCR	C20-C19-C18	8.14	148.68	126.36
18	A	4002	BCR	C11-C10-C9	8.14	138.69	127.28
18	b	4017	BCR	C20-C19-C18	8.13	148.66	126.36
18	a	4002	BCR	C11-C10-C9	8.13	138.68	127.28
14	B	1203	CLA	CMD-C2D-C1D	8.13	139.05	124.73
14	H	1211	CLA	CMD-C2D-C1D	8.13	139.04	124.73
18	B	4017	BCR	C20-C19-C18	8.13	148.65	126.36
18	R	4018	BCR	C20-C19-C18	8.13	148.65	126.36
14	a	1115	CLA	CMD-C2D-C1D	8.12	139.03	124.73
14	G	1116	CLA	CMD-C2D-C1D	8.12	139.03	124.73
14	B	1201	CLA	CMD-C2D-C1D	8.11	139.01	124.73
18	I	4018	BCR	C20-C19-C18	8.11	148.60	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	i	4018	BCR	C20-C19-C18	8.10	148.58	126.36
14	A	1133	CLA	CMD-C2D-C1D	8.10	138.99	124.73
14	H	1201	CLA	CMD-C2D-C1D	8.10	138.99	124.73
14	a	1133	CLA	CMD-C2D-C1D	8.10	138.98	124.73
18	l	4019	BCR	C24-C23-C22	-8.09	114.26	126.23
14	b	1201	CLA	CMD-C2D-C1D	8.09	138.97	124.73
14	G	1133	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	B	1229	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	a	1134	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	U	1502	CLA	CMD-C2D-C1D	8.08	138.96	124.73
14	A	1134	CLA	CMD-C2D-C1D	8.08	138.95	124.73
18	U	4019	BCR	C24-C23-C22	-8.08	114.28	126.23
14	A	1101	CLA	CMD-C2D-C1D	8.07	138.95	124.73
14	G	1101	CLA	CMD-C2D-C1D	8.07	138.94	124.73
14	a	1101	CLA	CMD-C2D-C1D	8.07	138.94	124.73
18	L	4019	BCR	C24-C23-C22	-8.06	114.31	126.23
14	G	1134	CLA	CMD-C2D-C1D	8.06	138.93	124.73
14	H	1229	CLA	CMD-C2D-C1D	8.06	138.92	124.73
14	b	1229	CLA	CMD-C2D-C1D	8.06	138.92	124.73
14	b	1210	CLA	CMD-C2D-C1D	8.05	138.91	124.73
14	L	1502	CLA	CMD-C2D-C1D	8.05	138.91	124.73
14	B	1210	CLA	CMD-C2D-C1D	8.05	138.91	124.73
14	a	1137	CLA	CMD-C2D-C1D	8.05	138.90	124.73
14	H	1210	CLA	CMD-C2D-C1D	8.04	138.90	124.73
14	l	1502	CLA	CMD-C2D-C1D	8.03	138.88	124.73
14	G	1137	CLA	CMD-C2D-C1D	8.02	138.86	124.73
14	G	1111	CLA	CMD-C2D-C1D	8.02	138.84	124.73
14	G	1112	CLA	CMD-C2D-C1D	8.00	138.82	124.73
14	a	1112	CLA	CMD-C2D-C1D	8.00	138.82	124.73
14	A	1137	CLA	CMD-C2D-C1D	8.00	138.82	124.73
14	A	1136	CLA	CMD-C2D-C1D	8.00	138.81	124.73
14	A	1112	CLA	CMD-C2D-C1D	8.00	138.81	124.73
14	a	1111	CLA	CMD-C2D-C1D	7.99	138.80	124.73
14	G	1110	CLA	CMD-C2D-C1D	7.98	138.78	124.73
14	a	1122	CLA	CMD-C2D-C1D	7.98	138.77	124.73
14	A	1111	CLA	CMD-C2D-C1D	7.97	138.76	124.73
14	A	1122	CLA	CMD-C2D-C1D	7.97	138.76	124.73
14	G	1122	CLA	CMD-C2D-C1D	7.97	138.75	124.73
14	a	1110	CLA	CMD-C2D-C1D	7.97	138.75	124.73
14	a	1136	CLA	CMD-C2D-C1D	7.97	138.75	124.73
14	B	1233	CLA	CMD-C2D-C1D	7.96	138.75	124.73
14	A	1110	CLA	CMD-C2D-C1D	7.96	138.74	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1233	CLA	CMD-C2D-C1D	7.96	138.74	124.73
14	G	1136	CLA	CMD-C2D-C1D	7.95	138.73	124.73
14	b	1233	CLA	CMD-C2D-C1D	7.95	138.72	124.73
14	B	1214	CLA	CMD-C2D-C1D	7.94	138.70	124.73
14	H	1214	CLA	CMD-C2D-C1D	7.92	138.68	124.73
14	B	1202	CLA	CMD-C2D-C1D	7.92	138.68	124.73
14	b	1202	CLA	CMD-C2D-C1D	7.92	138.67	124.73
14	b	1214	CLA	CMD-C2D-C1D	7.92	138.67	124.73
14	H	1202	CLA	CMD-C2D-C1D	7.91	138.67	124.73
14	A	1113	CLA	CMD-C2D-C1D	7.90	138.64	124.73
14	a	1113	CLA	CMD-C2D-C1D	7.90	138.63	124.73
14	G	1113	CLA	CMD-C2D-C1D	7.90	138.63	124.73
15	H	1237	F6C	C1D-ND-C4D	-7.89	103.08	106.68
14	G	1117	CLA	CMD-C2D-C1D	7.88	138.60	124.73
14	A	1117	CLA	CMD-C2D-C1D	7.87	138.59	124.73
14	a	1108	CLA	CMD-C2D-C1D	7.87	138.58	124.73
14	b	1217	CLA	CMD-C2D-C1D	7.87	138.58	124.73
14	G	1129	CLA	CMD-C2D-C1D	7.86	138.57	124.73
14	B	1217	CLA	CMD-C2D-C1D	7.86	138.57	124.73
14	a	1129	CLA	CMD-C2D-C1D	7.86	138.57	124.73
14	A	1137	CLA	O2D-CGD-CBD	7.86	124.97	111.23
14	a	1117	CLA	CMD-C2D-C1D	7.86	138.56	124.73
14	G	1108	CLA	CMD-C2D-C1D	7.85	138.55	124.73
14	H	1217	CLA	CMD-C2D-C1D	7.85	138.55	124.73
14	A	1108	CLA	CMD-C2D-C1D	7.85	138.55	124.73
18	H	4016	BCR	C20-C19-C18	7.85	147.88	126.36
14	G	1137	CLA	O2D-CGD-CBD	7.85	124.95	111.23
14	A	1129	CLA	CMD-C2D-C1D	7.85	138.54	124.73
18	B	4016	BCR	C20-C19-C18	7.84	147.87	126.36
14	a	1137	CLA	O2D-CGD-CBD	7.84	124.93	111.23
18	b	4016	BCR	C20-C19-C18	7.84	147.85	126.36
14	H	1219	CLA	CMD-C2D-C1D	7.83	138.51	124.73
14	a	1106	CLA	CMD-C2D-C1D	7.82	138.50	124.73
14	b	1219	CLA	CMD-C2D-C1D	7.82	138.49	124.73
14	H	1239	CLA	CMD-C2D-C1D	7.82	138.49	124.73
14	b	1239	CLA	CMD-C2D-C1D	7.81	138.49	124.73
14	G	1106	CLA	CMD-C2D-C1D	7.81	138.48	124.73
14	B	1219	CLA	CMD-C2D-C1D	7.81	138.48	124.73
14	A	1106	CLA	CMD-C2D-C1D	7.80	138.47	124.73
14	B	1239	CLA	CMD-C2D-C1D	7.79	138.44	124.73
14	B	1236	CLA	CMD-C2D-C1D	7.77	138.42	124.73
15	B	1237	F6C	C1D-ND-C4D	-7.77	103.13	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1236	CLA	CMD-C2D-C1D	7.77	138.41	124.73
14	b	1236	CLA	CMD-C2D-C1D	7.76	138.39	124.73
14	A	1102	CLA	CMD-C2D-C1D	7.76	138.39	124.73
14	a	1102	CLA	CMD-C2D-C1D	7.75	138.38	124.73
14	G	1102	CLA	CMD-C2D-C1D	7.74	138.37	124.73
14	a	1119	CLA	CMD-C2D-C1D	7.73	138.34	124.73
18	m	4021	BCR	C20-C19-C18	7.73	147.55	126.36
18	V	4021	BCR	C20-C19-C18	7.71	147.51	126.36
14	A	1119	CLA	CMD-C2D-C1D	7.71	138.31	124.73
18	M	4021	BCR	C20-C19-C18	7.71	147.49	126.36
15	b	1237	F6C	C1D-ND-C4D	-7.70	103.17	106.68
14	G	1119	CLA	CMD-C2D-C1D	7.70	138.28	124.73
14	X	1701	CLA	CMD-C2D-C1D	7.69	138.28	124.73
14	b	1216	CLA	CMD-C2D-C1D	7.69	138.27	124.73
14	x	1701	CLA	CMD-C2D-C1D	7.68	138.25	124.73
14	W	1701	CLA	CMD-C2D-C1D	7.67	138.24	124.73
14	H	1216	CLA	CMD-C2D-C1D	7.67	138.23	124.73
14	G	1126	CLA	CMD-C2D-C1D	7.66	138.22	124.73
15	b	1238	F6C	C1D-ND-C4D	-7.66	103.19	106.68
14	A	1126	CLA	CMD-C2D-C1D	7.66	138.21	124.73
14	b	1208	CLA	CMD-C2D-C1D	7.65	138.20	124.73
14	B	1216	CLA	CMD-C2D-C1D	7.65	138.20	124.73
18	H	4005	BCR	C20-C19-C18	7.64	147.32	126.36
18	l	4022	BCR	C7-C8-C9	-7.64	114.93	126.23
14	B	1208	CLA	CMD-C2D-C1D	7.64	138.18	124.73
15	B	1238	F6C	C1D-ND-C4D	-7.64	103.19	106.68
18	b	4005	BCR	C20-C19-C18	7.64	147.30	126.36
15	H	1238	F6C	C1D-ND-C4D	-7.63	103.20	106.68
14	H	1208	CLA	CMD-C2D-C1D	7.63	138.16	124.73
18	B	4005	BCR	C20-C19-C18	7.62	147.26	126.36
14	A	1132	CLA	O2D-CGD-CBD	7.62	124.54	111.23
14	a	1126	CLA	CMD-C2D-C1D	7.62	138.14	124.73
18	U	4022	BCR	C7-C8-C9	-7.61	114.97	126.23
14	B	1234	CLA	CMD-C2D-C1D	7.61	138.14	124.73
14	A	1118	CLA	CMD-C2D-C1D	7.61	138.12	124.73
14	H	1234	CLA	CMD-C2D-C1D	7.61	138.12	124.73
14	a	1118	CLA	CMD-C2D-C1D	7.60	138.12	124.73
14	a	1140	CLA	CMD-C2D-C1D	7.60	138.12	124.73
14	A	1140	CLA	CMD-C2D-C1D	7.60	138.11	124.73
14	G	1118	CLA	CMD-C2D-C1D	7.60	138.11	124.73
18	L	4022	BCR	C7-C8-C9	-7.59	115.00	126.23
14	G	1140	CLA	CMD-C2D-C1D	7.59	138.10	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1234	CLA	CMD-C2D-C1D	7.59	138.09	124.73
14	b	1220	CLA	CMD-C2D-C1D	7.58	138.08	124.73
14	H	1231	CLA	CMD-C2D-C1D	7.58	138.07	124.73
14	a	1132	CLA	O2D-CGD-CBD	7.58	124.47	111.23
14	B	1231	CLA	CMD-C2D-C1D	7.57	138.07	124.73
14	H	1220	CLA	CMD-C2D-C1D	7.57	138.06	124.73
14	G	1132	CLA	O2D-CGD-CBD	7.57	124.47	111.23
14	U	1503	CLA	CMD-C2D-C1D	7.57	138.05	124.73
14	B	1220	CLA	CMD-C2D-C1D	7.57	138.05	124.73
14	L	1503	CLA	CMD-C2D-C1D	7.56	138.04	124.73
14	b	1231	CLA	CMD-C2D-C1D	7.56	138.04	124.73
18	G	4001	BCR	C20-C19-C18	7.56	147.09	126.36
18	A	4001	BCR	C20-C19-C18	7.56	147.08	126.36
14	H	1210	CLA	O2D-CGD-CBD	7.55	124.44	111.23
14	l	1503	CLA	CMD-C2D-C1D	7.55	138.03	124.73
18	a	4001	BCR	C20-C19-C18	7.55	147.06	126.36
14	B	1210	CLA	O2D-CGD-CBD	7.55	124.43	111.23
14	a	1107	CLA	CMD-C2D-C1D	7.55	138.02	124.73
14	G	1107	CLA	CMD-C2D-C1D	7.55	138.02	124.73
14	B	1215	CLA	CMD-C2D-C1D	7.54	138.01	124.73
14	H	1215	CLA	CMD-C2D-C1D	7.54	138.01	124.73
14	b	1215	CLA	CMD-C2D-C1D	7.54	138.00	124.73
14	A	1107	CLA	CMD-C2D-C1D	7.53	138.00	124.73
14	b	1210	CLA	O2D-CGD-CBD	7.53	124.40	111.23
14	H	1235	CLA	CMD-C2D-C1D	7.53	137.99	124.73
14	B	1023	CLA	C4A-NA-C1A	7.53	110.11	106.68
14	B	1235	CLA	CMD-C2D-C1D	7.53	137.98	124.73
14	b	1235	CLA	CMD-C2D-C1D	7.52	137.97	124.73
14	A	1138	CLA	CMD-C2D-C1D	7.51	137.96	124.73
14	G	1138	CLA	CMD-C2D-C1D	7.51	137.95	124.73
14	A	1012	CLA	CMD-C2D-C1D	7.50	137.93	124.73
14	a	1138	CLA	CMD-C2D-C1D	7.49	137.93	124.73
14	H	1023	CLA	C4A-NA-C1A	7.47	110.09	106.68
14	G	1012	CLA	CMD-C2D-C1D	7.47	137.89	124.73
14	a	1012	CLA	CMD-C2D-C1D	7.46	137.87	124.73
14	H	1204	CLA	CMD-C2D-C1D	7.43	137.82	124.73
14	b	1204	CLA	CMD-C2D-C1D	7.43	137.82	124.73
14	B	1204	CLA	CMD-C2D-C1D	7.39	137.75	124.73
14	b	1023	CLA	C4A-NA-C1A	7.39	110.05	106.68
15	G	1121	F6C	C1D-ND-C4D	-7.30	103.35	106.68
14	a	1117	CLA	O2D-CGD-CBD	7.27	123.93	111.23
14	A	1117	CLA	O2D-CGD-CBD	7.26	123.92	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	4009	BCR	C20-C19-C18	7.26	146.26	126.36
18	H	4009	BCR	C20-C19-C18	7.25	146.24	126.36
14	G	1117	CLA	O2D-CGD-CBD	7.24	123.89	111.23
18	b	4009	BCR	C20-C19-C18	7.23	146.19	126.36
15	a	1121	F6C	C1D-ND-C4D	-7.22	103.38	106.68
14	G	1120	CLA	CMD-C2D-C1D	7.22	137.44	124.73
14	G	1123	CLA	CMD-C2D-C1D	7.22	137.44	124.73
14	a	1123	CLA	CMD-C2D-C1D	7.21	137.42	124.73
14	A	1123	CLA	CMD-C2D-C1D	7.21	137.42	124.73
15	G	1121	F6C	CAA-C2A-C1A	-7.20	107.89	128.01
15	A	1121	F6C	C1D-ND-C4D	-7.20	103.39	106.68
15	a	1121	F6C	CAA-C2A-C1A	-7.19	107.93	128.01
15	A	1121	F6C	CAA-C2A-C1A	-7.19	107.94	128.01
14	a	1120	CLA	CMD-C2D-C1D	7.18	137.38	124.73
14	A	1120	CLA	CMD-C2D-C1D	7.17	137.35	124.73
14	B	1224	CLA	CMD-C2D-C1D	7.08	137.19	124.73
14	b	1224	CLA	CMD-C2D-C1D	7.07	137.18	124.73
14	H	1224	CLA	CMD-C2D-C1D	7.05	137.15	124.73
18	b	4017	BCR	C7-C8-C9	-7.05	115.81	126.23
18	H	4017	BCR	C7-C8-C9	-7.03	115.84	126.23
14	A	1125	CLA	CMD-C2D-C1D	7.02	137.09	124.73
14	b	1222	CLA	CMD-C2D-C1D	7.01	137.07	124.73
14	H	1222	CLA	CMD-C2D-C1D	7.01	137.07	124.73
14	B	1222	CLA	CMD-C2D-C1D	7.00	137.06	124.73
14	a	1125	CLA	CMD-C2D-C1D	7.00	137.06	124.73
18	B	4017	BCR	C7-C8-C9	-6.99	115.89	126.23
14	G	1125	CLA	CMD-C2D-C1D	6.99	137.04	124.73
14	H	1239	CLA	C2C-C1C-NC	6.96	117.29	109.98
14	b	1239	CLA	C2C-C1C-NC	6.96	117.29	109.98
14	B	1226	CLA	CMD-C2D-C1D	6.95	136.97	124.73
14	b	1226	CLA	CMD-C2D-C1D	6.95	136.97	124.73
14	B	1239	CLA	C2C-C1C-NC	6.95	117.28	109.98
14	H	1226	CLA	CMD-C2D-C1D	6.95	136.96	124.73
14	H	1206	CLA	CMD-C2D-C1D	6.94	136.96	124.73
15	H	1207	F6C	O2D-CGD-CBD	6.93	123.35	111.23
14	A	1013	CLA	C4A-NA-C1A	6.93	109.84	106.68
14	b	1206	CLA	CMD-C2D-C1D	6.93	136.93	124.73
15	b	1230	F6C	O2D-CGD-CBD	6.92	123.33	111.23
15	b	1207	F6C	O2D-CGD-CBD	6.92	123.33	111.23
15	H	1230	F6C	O2D-CGD-CBD	6.92	123.33	111.23
15	B	1230	F6C	O2D-CGD-CBD	6.92	123.33	111.23
15	B	1207	F6C	O2D-CGD-CBD	6.92	123.32	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1206	CLA	CMD-C2D-C1D	6.91	136.90	124.73
14	a	1013	CLA	C4A-NA-C1A	6.90	109.83	106.68
14	b	1205	CLA	O2D-CGD-CBD	6.87	123.24	111.23
14	H	1022	CLA	CMD-C2D-C1D	6.86	136.81	124.73
14	B	1022	CLA	CMD-C2D-C1D	6.86	136.80	124.73
14	B	1205	CLA	O2D-CGD-CBD	6.85	123.21	111.23
14	b	1021	CLA	C4A-NA-C1A	6.85	109.80	106.68
14	b	1022	CLA	CMD-C2D-C1D	6.85	136.78	124.73
14	G	1013	CLA	C4A-NA-C1A	6.85	109.80	106.68
14	B	1021	CLA	C4A-NA-C1A	6.84	109.80	106.68
14	H	1205	CLA	O2D-CGD-CBD	6.83	123.17	111.23
14	b	1212	CLA	CMD-C2D-C1D	6.82	136.74	124.73
18	b	4004	BCR	C24-C23-C22	-6.82	116.15	126.23
18	H	4004	BCR	C24-C23-C22	-6.81	116.15	126.23
18	B	4004	BCR	C24-C23-C22	-6.80	116.18	126.23
14	B	1205	CLA	C4A-NA-C1A	6.79	109.78	106.68
14	b	1205	CLA	C4A-NA-C1A	6.77	109.77	106.68
14	H	1212	CLA	CMD-C2D-C1D	6.77	136.65	124.73
14	B	1212	CLA	CMD-C2D-C1D	6.77	136.65	124.73
14	H	1023	CLA	CMD-C2D-C1D	6.77	136.64	124.73
14	B	1225	CLA	CMD-C2D-C1D	6.75	136.62	124.73
14	H	1205	CLA	C4A-NA-C1A	6.75	109.76	106.68
14	B	1023	CLA	CMD-C2D-C1D	6.74	136.60	124.73
14	b	1023	CLA	CMD-C2D-C1D	6.73	136.58	124.73
14	H	1225	CLA	CMD-C2D-C1D	6.73	136.58	124.73
14	B	1221	CLA	CMD-C2D-C1D	6.72	136.57	124.73
14	b	1225	CLA	CMD-C2D-C1D	6.72	136.56	124.73
14	a	1129	CLA	O2D-CGD-CBD	6.71	122.96	111.23
14	H	1021	CLA	C4A-NA-C1A	6.71	109.74	106.68
14	G	1129	CLA	O2D-CGD-CBD	6.70	122.94	111.23
14	b	1221	CLA	CMD-C2D-C1D	6.70	136.52	124.73
14	A	1129	CLA	O2D-CGD-CBD	6.69	122.93	111.23
14	H	1221	CLA	CMD-C2D-C1D	6.69	136.51	124.73
18	G	4008	BCR	C20-C19-C18	6.68	144.69	126.36
18	a	4008	BCR	C20-C19-C18	6.68	144.69	126.36
18	A	4008	BCR	C20-C19-C18	6.68	144.69	126.36
14	A	1119	CLA	C2C-C1C-NC	6.61	116.92	109.98
14	a	1119	CLA	C2C-C1C-NC	6.60	116.92	109.98
14	a	1106	CLA	O2D-CGD-CBD	6.59	122.76	111.23
14	A	1106	CLA	O2D-CGD-CBD	6.59	122.76	111.23
14	A	1128	CLA	CMD-C2D-C1D	6.59	136.33	124.73
14	G	1128	CLA	CMD-C2D-C1D	6.59	136.33	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	b	4010	BCR	C20-C19-C18	6.58	144.41	126.36
14	a	1128	CLA	CMD-C2D-C1D	6.57	136.30	124.73
18	B	4010	BCR	C20-C19-C18	6.57	144.38	126.36
14	G	1119	CLA	C2C-C1C-NC	6.57	116.88	109.98
18	H	4010	BCR	C20-C19-C18	6.57	144.37	126.36
14	G	1106	CLA	O2D-CGD-CBD	6.56	122.69	111.23
15	B	1238	F6C	CAA-C2A-C1A	-6.54	109.73	128.01
14	G	1115	CLA	O2D-CGD-CBD	6.54	122.66	111.23
15	H	1238	F6C	CAA-C2A-C1A	-6.54	109.75	128.01
15	b	1238	F6C	CAA-C2A-C1A	-6.53	109.76	128.01
14	a	1115	CLA	O2D-CGD-CBD	6.53	122.65	111.23
14	A	1115	CLA	O2D-CGD-CBD	6.53	122.64	111.23
14	a	1125	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	G	1013	CLA	C2D-C1D-ND	6.47	116.53	110.13
14	H	1201	CLA	O2D-CGD-CBD	6.46	122.53	111.23
14	A	1013	CLA	C2D-C1D-ND	6.46	116.52	110.13
14	A	1128	CLA	C2C-C1C-NC	6.46	116.76	109.98
14	B	1223	CLA	O2D-CGD-CBD	6.45	122.51	111.23
18	b	4014	BCR	C20-C19-C18	6.45	144.06	126.36
14	a	1013	CLA	C2D-C1D-ND	6.45	116.51	110.13
14	b	1201	CLA	O2D-CGD-CBD	6.45	122.50	111.23
18	B	4014	BCR	C20-C19-C18	6.45	144.04	126.36
14	B	1201	CLA	O2D-CGD-CBD	6.45	122.50	111.23
18	a	4002	BCR	C20-C19-C18	6.44	144.03	126.36
18	H	4014	BCR	C20-C19-C18	6.44	144.03	126.36
14	G	1125	CLA	C4A-NA-C1A	6.44	109.62	106.68
14	H	1223	CLA	O2D-CGD-CBD	6.44	122.49	111.23
18	A	4002	BCR	C20-C19-C18	6.44	144.02	126.36
14	b	1223	CLA	O2D-CGD-CBD	6.44	122.48	111.23
14	a	1128	CLA	C2C-C1C-NC	6.44	116.74	109.98
18	G	4002	BCR	C20-C19-C18	6.43	143.99	126.36
14	a	1012	CLA	C2C-C1C-NC	6.43	116.73	109.98
14	A	1127	CLA	CMD-C2D-C1D	6.41	136.02	124.73
14	G	1127	CLA	CMD-C2D-C1D	6.41	136.02	124.73
14	G	1012	CLA	C2C-C1C-NC	6.41	116.71	109.98
14	a	1114	CLA	C2C-C1C-NC	6.41	116.71	109.98
14	a	1127	CLA	CMD-C2D-C1D	6.41	136.01	124.73
14	A	1114	CLA	C2C-C1C-NC	6.41	116.71	109.98
14	G	1128	CLA	C2C-C1C-NC	6.40	116.71	109.98
14	L	1501	CLA	CMD-C2D-C1D	6.40	136.00	124.73
14	A	1125	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	l	1501	CLA	CMD-C2D-C1D	6.40	136.00	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1222	CLA	O2D-CGD-CBD	6.39	122.41	111.23
14	B	1222	CLA	O2D-CGD-CBD	6.39	122.41	111.23
14	G	1114	CLA	C2C-C1C-NC	6.39	116.69	109.98
14	U	1501	CLA	CMD-C2D-C1D	6.39	135.98	124.73
14	H	1222	CLA	O2D-CGD-CBD	6.39	122.39	111.23
15	B	1207	F6C	C2C-C1C-NC	6.39	116.95	110.33
15	H	1207	F6C	C2C-C1C-NC	6.38	116.94	110.33
14	A	1012	CLA	C2C-C1C-NC	6.38	116.68	109.98
14	b	1213	CLA	O2D-CGD-CBD	6.37	122.37	111.23
15	b	1207	F6C	C2C-C1C-NC	6.37	116.93	110.33
14	L	1502	CLA	O2D-CGD-CBD	6.37	122.36	111.23
14	G	1138	CLA	O2D-CGD-CBD	6.36	122.35	111.23
14	a	1138	CLA	O2D-CGD-CBD	6.36	122.35	111.23
14	G	1118	CLA	C2C-C1C-NC	6.34	116.64	109.98
14	A	1118	CLA	C2C-C1C-NC	6.34	116.64	109.98
14	l	1502	CLA	O2D-CGD-CBD	6.34	122.31	111.23
14	A	1138	CLA	O2D-CGD-CBD	6.34	122.31	111.23
13	A	1011	CL0	CBC-CAC-C3C	-6.33	103.81	112.87
14	B	1213	CLA	O2D-CGD-CBD	6.33	122.29	111.23
14	H	1213	CLA	O2D-CGD-CBD	6.32	122.29	111.23
14	U	1502	CLA	O2D-CGD-CBD	6.32	122.29	111.23
14	H	1201	CLA	C4A-NA-C1A	6.32	109.56	106.68
14	a	1118	CLA	C2C-C1C-NC	6.32	116.62	109.98
14	a	1133	CLA	C2C-C1C-NC	6.32	116.62	109.98
14	B	1023	CLA	CAC-C3C-C4C	6.32	133.01	124.79
14	G	1135	CLA	C2C-C1C-NC	6.32	116.62	109.98
14	a	1135	CLA	C2C-C1C-NC	6.32	116.61	109.98
14	A	1135	CLA	C2C-C1C-NC	6.32	116.61	109.98
13	G	1011	CL0	CBC-CAC-C3C	-6.31	103.84	112.87
14	G	1133	CLA	C2C-C1C-NC	6.30	116.59	109.98
14	H	1023	CLA	CAC-C3C-C4C	6.29	132.98	124.79
14	b	1023	CLA	CAC-C3C-C4C	6.28	132.97	124.79
14	A	1133	CLA	C2C-C1C-NC	6.28	116.58	109.98
13	a	1011	CL0	CBC-CAC-C3C	-6.28	103.88	112.87
14	b	1220	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	H	1206	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	G	1137	CLA	C2C-C1C-NC	6.28	116.58	109.98
14	H	1205	CLA	CMD-C2D-C1D	6.28	135.78	124.73
14	H	1220	CLA	C2C-C1C-NC	6.27	116.57	109.98
14	H	1220	CLA	C4A-NA-C1A	6.26	109.54	106.68
14	b	1205	CLA	CMD-C2D-C1D	6.26	135.76	124.73
14	a	1104	CLA	C1C-C2C-C3C	-6.26	100.39	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1226	CLA	C2C-C1C-NC	6.26	116.56	109.98
14	H	1021	CLA	CMD-C2D-C1D	6.26	135.75	124.73
14	G	1104	CLA	C1C-C2C-C3C	-6.26	100.40	106.98
14	B	1206	CLA	C2C-C1C-NC	6.26	116.55	109.98
14	B	1220	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	B	1205	CLA	CMD-C2D-C1D	6.25	135.74	124.73
18	U	4019	BCR	C15-C14-C13	-6.25	118.51	127.28
18	L	4019	BCR	C15-C14-C13	-6.25	118.51	127.28
14	H	1224	CLA	O2D-CGD-CBD	6.25	122.15	111.23
14	A	1104	CLA	C1C-C2C-C3C	-6.25	100.41	106.98
14	B	1224	CLA	O2D-CGD-CBD	6.25	122.15	111.23
14	b	1206	CLA	C2C-C1C-NC	6.25	116.54	109.98
14	b	1226	CLA	C2C-C1C-NC	6.25	116.54	109.98
14	H	1226	CLA	C2C-C1C-NC	6.24	116.54	109.98
18	l	4019	BCR	C15-C14-C13	-6.24	118.52	127.28
14	B	1021	CLA	CMD-C2D-C1D	6.24	135.72	124.73
14	b	1021	CLA	CMD-C2D-C1D	6.24	135.72	124.73
14	a	1128	CLA	O2D-CGD-CBD	6.24	122.13	111.23
14	G	1128	CLA	O2D-CGD-CBD	6.23	122.13	111.23
14	b	1220	CLA	C4A-NA-C1A	6.23	109.52	106.68
18	R	4018	BCR	C3-C4-C5	-6.23	102.95	114.06
14	a	1137	CLA	C2C-C1C-NC	6.22	116.52	109.98
14	b	1224	CLA	O2D-CGD-CBD	6.22	122.10	111.23
14	A	1137	CLA	C2C-C1C-NC	6.21	116.50	109.98
14	A	1128	CLA	O2D-CGD-CBD	6.21	122.08	111.23
18	i	4018	BCR	C3-C4-C5	-6.20	102.99	114.06
18	B	4014	BCR	C24-C23-C22	-6.20	117.06	126.23
18	A	4011	BCR	C20-C19-C18	6.20	143.37	126.36
14	b	1214	CLA	C2C-C1C-NC	6.20	116.50	109.98
14	B	1220	CLA	C2C-C1C-NC	6.20	116.50	109.98
18	I	4018	BCR	C3-C4-C5	-6.20	103.00	114.06
18	G	4011	BCR	C20-C19-C18	6.19	143.34	126.36
14	l	1503	CLA	C4A-NA-C1A	6.19	109.50	106.68
18	b	4014	BCR	C24-C23-C22	-6.19	117.08	126.23
18	H	4005	BCR	C24-C23-C22	-6.18	117.09	126.23
18	a	4011	BCR	C20-C19-C18	6.18	143.31	126.36
14	G	1123	CLA	C2C-C1C-NC	6.18	116.47	109.98
14	A	1123	CLA	C2C-C1C-NC	6.18	116.47	109.98
14	A	1106	CLA	C4A-NA-C1A	6.17	109.50	106.68
14	H	1234	CLA	C2D-C1D-ND	6.17	116.24	110.13
18	H	4014	BCR	C24-C23-C22	-6.17	117.10	126.23
14	H	1214	CLA	C2C-C1C-NC	6.17	116.46	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1201	CLA	C4A-NA-C1A	6.17	109.49	106.68
15	H	1207	F6C	C1D-ND-C4D	-6.16	103.87	106.68
18	G	4011	BCR	C7-C8-C9	-6.16	117.12	126.23
14	B	1234	CLA	C2D-C1D-ND	6.16	116.22	110.13
14	G	1106	CLA	C4A-NA-C1A	6.15	109.49	106.68
18	A	4011	BCR	C7-C8-C9	-6.15	117.13	126.23
14	b	1201	CLA	C4A-NA-C1A	6.15	109.48	106.68
14	b	1234	CLA	C2D-C1D-ND	6.15	116.21	110.13
18	B	4005	BCR	C24-C23-C22	-6.15	117.14	126.23
15	B	1207	F6C	C1D-ND-C4D	-6.14	103.88	106.68
14	G	1104	CLA	C4A-NA-C1A	6.14	109.48	106.68
18	b	4005	BCR	C24-C23-C22	-6.14	117.16	126.23
14	a	1123	CLA	C2C-C1C-NC	6.13	116.42	109.98
14	G	1127	CLA	C4A-NA-C1A	6.13	109.47	106.68
18	a	4011	BCR	C7-C8-C9	-6.13	117.17	126.23
14	B	1214	CLA	C2C-C1C-NC	6.12	116.41	109.98
14	a	1119	CLA	C4A-NA-C1A	6.12	109.47	106.68
14	A	1104	CLA	C4A-NA-C1A	6.11	109.47	106.68
14	A	1126	CLA	C3B-C2B-C1B	-6.11	99.97	107.17
14	a	1104	CLA	C4A-NA-C1A	6.10	109.46	106.68
14	l	1501	CLA	C2C-C1C-NC	6.10	116.39	109.98
14	U	1503	CLA	C4A-NA-C1A	6.10	109.46	106.68
18	b	4004	BCR	C20-C19-C18	6.09	143.07	126.36
14	b	1235	CLA	O2D-CGD-CBD	6.09	121.88	111.23
14	a	1117	CLA	C2C-C1C-NC	6.09	116.38	109.98
14	G	1126	CLA	C3B-C2B-C1B	-6.09	99.99	107.17
14	A	1127	CLA	C2C-C1C-NC	6.09	116.37	109.98
14	a	1127	CLA	C4A-NA-C1A	6.08	109.45	106.68
14	K	1401	CLA	C2C-C1C-NC	6.08	116.37	109.98
14	H	1239	CLA	C1C-C2C-C3C	-6.08	100.58	106.98
14	A	1117	CLA	C2C-C1C-NC	6.08	116.37	109.98
18	B	4004	BCR	C20-C19-C18	6.08	143.03	126.36
14	H	1235	CLA	O2D-CGD-CBD	6.08	121.86	111.23
14	A	1127	CLA	C4A-NA-C1A	6.08	109.45	106.68
14	b	1217	CLA	C2C-C1C-NC	6.08	116.36	109.98
14	L	1501	CLA	C2C-C1C-NC	6.08	116.36	109.98
14	B	1204	CLA	O2D-CGD-CBD	6.07	121.85	111.23
14	B	1235	CLA	O2D-CGD-CBD	6.07	121.85	111.23
14	B	1227	CLA	C2C-C1C-NC	6.07	116.36	109.98
18	H	4004	BCR	C20-C19-C18	6.07	143.01	126.36
14	H	1204	CLA	O2D-CGD-CBD	6.07	121.84	111.23
14	B	1233	CLA	C2C-C1C-NC	6.07	116.36	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1013	CLA	CMD-C2D-C1D	6.07	135.41	124.73
14	a	1013	CLA	CMD-C2D-C1D	6.07	135.41	124.73
15	b	1207	F6C	C1D-ND-C4D	-6.07	103.91	106.68
14	H	1233	CLA	C2C-C1C-NC	6.07	116.35	109.98
14	U	1501	CLA	C2C-C1C-NC	6.07	116.35	109.98
14	A	1013	CLA	CMD-C2D-C1D	6.06	135.41	124.73
14	a	1127	CLA	C2C-C1C-NC	6.06	116.35	109.98
14	T	1401	CLA	C2C-C1C-NC	6.06	116.35	109.98
14	a	1106	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	L	1503	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	B	1217	CLA	C2C-C1C-NC	6.05	116.34	109.98
14	b	1204	CLA	O2D-CGD-CBD	6.05	121.81	111.23
14	B	1239	CLA	C1C-C2C-C3C	-6.05	100.62	106.98
14	b	1233	CLA	C2C-C1C-NC	6.05	116.34	109.98
14	b	1239	CLA	C1C-C2C-C3C	-6.05	100.62	106.98
14	G	1119	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	G	1117	CLA	C2C-C1C-NC	6.05	116.33	109.98
14	H	1227	CLA	C2C-C1C-NC	6.04	116.33	109.98
14	a	1126	CLA	C3B-C2B-C1B	-6.04	100.05	107.17
14	a	1131	CLA	O2D-CGD-CBD	6.04	121.78	111.23
14	H	1202	CLA	O2A-CGA-O1A	-6.04	108.53	123.63
14	b	1227	CLA	C2C-C1C-NC	6.04	116.32	109.98
14	a	1114	CLA	O2D-CGD-CBD	6.03	121.77	111.23
14	H	1217	CLA	C2C-C1C-NC	6.03	116.32	109.98
14	A	1114	CLA	O2D-CGD-CBD	6.03	121.77	111.23
14	b	1202	CLA	O2A-CGA-O1A	-6.03	108.55	123.63
14	A	1102	CLA	O2D-CGD-CBD	6.03	121.77	111.23
14	B	1202	CLA	O2A-CGA-O1A	-6.02	108.56	123.63
14	G	1127	CLA	C2C-C1C-NC	6.02	116.31	109.98
14	a	1134	CLA	C2C-C1C-NC	6.02	116.31	109.98
14	A	1131	CLA	O2D-CGD-CBD	6.01	121.74	111.23
14	G	1114	CLA	O2D-CGD-CBD	6.01	121.74	111.23
14	G	1102	CLA	O2D-CGD-CBD	6.01	121.73	111.23
14	G	1131	CLA	O2D-CGD-CBD	6.01	121.73	111.23
14	A	1134	CLA	C2C-C1C-NC	6.01	116.29	109.98
14	k	1401	CLA	C2C-C1C-NC	6.00	116.29	109.98
14	a	1102	CLA	O2D-CGD-CBD	6.00	121.72	111.23
14	B	1219	CLA	O2D-CGD-CBD	6.00	121.72	111.23
14	a	1112	CLA	C2C-C1C-NC	6.00	116.28	109.98
14	A	1119	CLA	C4A-NA-C1A	5.99	109.41	106.68
14	G	1120	CLA	C2D-C1D-ND	5.99	116.05	110.13
14	b	1219	CLA	O2D-CGD-CBD	5.98	121.69	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1120	CLA	C4A-NA-C1A	5.98	109.41	106.68
14	l	1501	CLA	C4A-NA-C1A	5.98	109.41	106.68
14	H	1022	CLA	O2D-CGD-CBD	5.97	121.67	111.23
14	a	1120	CLA	C2D-C1D-ND	5.97	116.04	110.13
14	G	1134	CLA	C2C-C1C-NC	5.97	116.25	109.98
14	a	1120	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	B	1202	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	G	1126	CLA	O2D-CGD-CBD	5.97	121.66	111.23
14	B	1022	CLA	O2D-CGD-CBD	5.97	121.66	111.23
14	B	1228	CLA	C2C-C1C-NC	5.96	116.25	109.98
14	b	1234	CLA	C3D-C2D-C1D	-5.96	97.69	105.83
14	H	1219	CLA	O2D-CGD-CBD	5.96	121.65	111.23
14	a	1101	CLA	O2D-CGD-CBD	5.96	121.65	111.23
14	G	1120	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	H	1202	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	b	1202	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	A	1104	CLA	C2D-C1D-ND	5.96	116.03	110.13
14	G	1109	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	a	1126	CLA	O2D-CGD-CBD	5.96	121.65	111.23
14	b	1022	CLA	O2D-CGD-CBD	5.96	121.64	111.23
14	U	1501	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	G	1112	CLA	C2C-C1C-NC	5.96	116.24	109.98
14	A	1105	CLA	C2C-C1C-NC	5.96	116.24	109.98
14	G	1104	CLA	C2D-C1D-ND	5.96	116.02	110.13
14	H	1234	CLA	C3D-C2D-C1D	-5.95	97.71	105.83
14	B	1234	CLA	C3D-C2D-C1D	-5.95	97.71	105.83
14	a	1118	CLA	O2D-CGD-CBD	5.95	121.64	111.23
14	G	1105	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	a	1105	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	A	1112	CLA	C2C-C1C-NC	5.95	116.23	109.98
14	G	1140	CLA	O2D-CGD-CBD	5.95	121.63	111.23
14	A	1101	CLA	O2D-CGD-CBD	5.95	121.62	111.23
14	A	1120	CLA	C2D-C1D-ND	5.95	116.01	110.13
14	A	1140	CLA	O2D-CGD-CBD	5.94	121.62	111.23
14	H	1228	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	A	1117	CLA	C4A-NA-C1A	5.94	109.39	106.68
14	A	1126	CLA	O2D-CGD-CBD	5.94	121.62	111.23
14	a	1140	CLA	O2D-CGD-CBD	5.94	121.62	111.23
14	G	1107	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	B	1216	CLA	C2C-C1C-NC	5.94	116.22	109.98
14	G	1118	CLA	O2D-CGD-CBD	5.93	121.60	111.23
14	a	1104	CLA	C2D-C1D-ND	5.93	115.99	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1118	CLA	O2D-CGD-CBD	5.93	121.59	111.23
14	B	1218	CLA	C2D-C1D-ND	5.92	115.99	110.13
14	H	1218	CLA	C2D-C1D-ND	5.92	115.99	110.13
14	L	1501	CLA	C4A-NA-C1A	5.92	109.38	106.68
14	A	1107	CLA	C2C-C1C-NC	5.92	116.19	109.98
14	G	1101	CLA	O2D-CGD-CBD	5.91	121.56	111.23
14	B	1203	CLA	C3D-C2D-C1D	-5.91	97.76	105.83
14	b	1228	CLA	C2C-C1C-NC	5.91	116.19	109.98
15	B	1230	F6C	CAA-C2A-C1A	-5.90	111.52	128.01
14	H	1239	CLA	O2D-CGD-CBD	5.90	121.55	111.23
14	H	1203	CLA	C3D-C2D-C1D	-5.90	97.78	105.83
14	b	1216	CLA	C2C-C1C-NC	5.90	116.18	109.98
14	B	1239	CLA	O2D-CGD-CBD	5.90	121.55	111.23
15	H	1230	F6C	CAA-C2A-C1A	-5.90	111.53	128.01
14	H	1216	CLA	C2C-C1C-NC	5.90	116.18	109.98
14	b	1203	CLA	C3D-C2D-C1D	-5.90	97.78	105.83
14	b	1212	CLA	C2D-C1D-ND	5.90	115.96	110.13
14	G	1117	CLA	C4A-NA-C1A	5.89	109.37	106.68
14	b	1218	CLA	C2D-C1D-ND	5.89	115.96	110.13
14	b	1214	CLA	O2D-CGD-CBD	5.89	121.53	111.23
15	b	1230	F6C	CAA-C2A-C1A	-5.89	111.55	128.01
14	b	1023	CLA	C3B-C2B-C1B	-5.89	100.23	107.17
14	H	1214	CLA	O2D-CGD-CBD	5.89	121.53	111.23
14	b	1239	CLA	O2D-CGD-CBD	5.89	121.52	111.23
14	A	1109	CLA	C4A-NA-C1A	5.88	109.36	106.68
14	H	1023	CLA	C3B-C2B-C1B	-5.88	100.23	107.17
14	b	1236	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	B	1023	CLA	C3B-C2B-C1B	-5.88	100.24	107.17
14	a	1107	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	G	1103	CLA	C2C-C1C-NC	5.88	116.16	109.98
14	H	1215	CLA	C2C-C1C-NC	5.88	116.16	109.98
18	l	4022	BCR	C20-C19-C18	5.88	142.48	126.36
18	L	4022	BCR	C20-C19-C18	5.87	142.47	126.36
18	U	4022	BCR	C20-C19-C18	5.87	142.47	126.36
14	b	1215	CLA	C1C-C2C-C3C	-5.87	100.81	106.98
14	B	1214	CLA	O2D-CGD-CBD	5.87	121.49	111.23
14	B	1209	CLA	O2D-CGD-CBD	5.87	121.49	111.23
14	b	1215	CLA	C2C-C1C-NC	5.87	116.14	109.98
14	H	1209	CLA	O2D-CGD-CBD	5.86	121.48	111.23
14	H	1215	CLA	C1C-C2C-C3C	-5.86	100.81	106.98
14	B	1215	CLA	C1C-C2C-C3C	-5.86	100.81	106.98
14	A	1103	CLA	C2C-C1C-NC	5.86	116.14	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1012	CLA	C1C-C2C-C3C	-5.86	100.82	106.98
14	b	1209	CLA	O2D-CGD-CBD	5.86	121.47	111.23
14	B	1215	CLA	C2C-C1C-NC	5.86	116.13	109.98
14	B	1236	CLA	O2D-CGD-CBD	5.86	121.47	111.23
14	H	1236	CLA	C2C-C1C-NC	5.86	116.13	109.98
14	A	1114	CLA	C1C-C2C-C3C	-5.85	100.82	106.98
14	H	1236	CLA	O2D-CGD-CBD	5.85	121.46	111.23
14	A	1012	CLA	C1C-C2C-C3C	-5.85	100.82	106.98
14	a	1109	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	G	1012	CLA	C1C-C2C-C3C	-5.84	100.83	106.98
14	b	1236	CLA	O2D-CGD-CBD	5.84	121.44	111.23
14	B	1236	CLA	C2C-C1C-NC	5.84	116.12	109.98
14	H	1212	CLA	C2D-C1D-ND	5.84	115.90	110.13
14	b	1202	CLA	O2D-CGD-CBD	5.84	121.44	111.23
14	a	1128	CLA	C4A-NA-C1A	5.83	109.34	106.68
14	H	1201	CLA	C2C-C1C-NC	5.83	116.11	109.98
14	A	1134	CLA	O2D-CGD-CBD	5.83	121.43	111.23
14	A	1103	CLA	O2D-CGD-CBD	5.83	121.42	111.23
14	a	1103	CLA	C2C-C1C-NC	5.83	116.11	109.98
14	B	1212	CLA	C2D-C1D-ND	5.83	115.89	110.13
14	H	1227	CLA	O2D-CGD-CBD	5.83	121.42	111.23
14	a	1109	CLA	C2C-C1C-NC	5.83	116.10	109.98
14	a	1138	CLA	C3B-C2B-C1B	-5.83	100.30	107.17
14	b	1204	CLA	C2C-C1C-NC	5.82	116.10	109.98
14	B	1202	CLA	O2D-CGD-CBD	5.82	121.41	111.23
14	H	1202	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	G	1103	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	b	1227	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	a	1124	CLA	C3B-C2B-C1B	-5.82	100.31	107.17
14	G	1114	CLA	C1C-C2C-C3C	-5.82	100.86	106.98
14	a	1103	CLA	O2D-CGD-CBD	5.82	121.40	111.23
14	G	1128	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	G	1124	CLA	C3B-C2B-C1B	-5.81	100.31	107.17
14	a	1134	CLA	O2D-CGD-CBD	5.81	121.39	111.23
14	A	1104	CLA	C1D-ND-C4D	-5.81	102.23	106.31
14	A	1128	CLA	C4A-NA-C1A	5.81	109.33	106.68
14	G	1134	CLA	O2D-CGD-CBD	5.81	121.39	111.23
14	B	1227	CLA	O2D-CGD-CBD	5.81	121.39	111.23
14	G	1109	CLA	C2C-C1C-NC	5.81	116.08	109.98
14	a	1114	CLA	C1C-C2C-C3C	-5.81	100.87	106.98
14	a	1136	CLA	O2D-CGD-CBD	5.81	121.38	111.23
14	A	1124	CLA	C3B-C2B-C1B	-5.81	100.33	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1125	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
14	A	1125	CLA	C3D-C2D-C1D	-5.80	97.91	105.83
14	G	1104	CLA	C1D-ND-C4D	-5.80	102.24	106.31
14	B	1204	CLA	C2C-C1C-NC	5.80	116.07	109.98
14	H	1223	CLA	C2C-C1C-NC	5.80	116.07	109.98
14	G	1131	CLA	C2C-C1C-NC	5.80	116.07	109.98
14	a	1117	CLA	C4A-NA-C1A	5.79	109.32	106.68
14	b	1221	CLA	C4A-NA-C1A	5.79	109.32	106.68
14	B	1218	CLA	C2C-C1C-NC	5.79	116.06	109.98
14	a	1125	CLA	C3D-C2D-C1D	-5.78	97.94	105.83
14	B	1232	CLA	C2C-C1C-NC	5.78	116.06	109.98
14	a	1137	CLA	C3B-C2B-C1B	-5.78	100.36	107.17
14	H	1204	CLA	C2C-C1C-NC	5.78	116.05	109.98
14	H	1221	CLA	C4A-NA-C1A	5.78	109.31	106.68
14	A	1109	CLA	C2C-C1C-NC	5.78	116.05	109.98
14	B	1201	CLA	C2C-C1C-NC	5.78	116.05	109.98
14	b	1232	CLA	C2C-C1C-NC	5.78	116.05	109.98
14	a	1111	CLA	O2D-CGD-CBD	5.77	121.33	111.23
14	b	1201	CLA	C2C-C1C-NC	5.77	116.05	109.98
14	A	1136	CLA	O2D-CGD-CBD	5.77	121.31	111.23
14	G	1133	CLA	C1C-C2C-C3C	-5.77	100.91	106.98
14	A	1138	CLA	C3B-C2B-C1B	-5.77	100.37	107.17
14	G	1136	CLA	O2D-CGD-CBD	5.77	121.31	111.23
14	G	1138	CLA	C3B-C2B-C1B	-5.77	100.37	107.17
14	H	1218	CLA	C2C-C1C-NC	5.77	116.04	109.98
14	G	1111	CLA	O2D-CGD-CBD	5.76	121.31	111.23
14	A	1137	CLA	C3B-C2B-C1B	-5.76	100.38	107.17
14	H	1232	CLA	C2C-C1C-NC	5.76	116.03	109.98
14	G	1125	CLA	O2D-CGD-CBD	5.76	121.30	111.23
14	A	1125	CLA	O2D-CGD-CBD	5.76	121.30	111.23
15	a	1121	F6C	C2C-C1C-NC	5.76	116.30	110.33
14	G	1132	CLA	C3B-C2B-C1B	-5.76	100.38	107.17
14	B	1223	CLA	C2C-C1C-NC	5.76	116.03	109.98
15	G	1121	F6C	C2C-C1C-NC	5.75	116.29	110.33
14	A	1111	CLA	O2D-CGD-CBD	5.75	121.29	111.23
14	b	1223	CLA	C2C-C1C-NC	5.75	116.02	109.98
14	H	1223	CLA	C3D-C2D-C1D	-5.75	97.98	105.83
14	G	1137	CLA	C3B-C2B-C1B	-5.75	100.39	107.17
14	A	1116	CLA	O2D-CGD-CBD	5.75	121.28	111.23
14	U	1503	CLA	C2C-C1C-NC	5.75	116.02	109.98
14	B	1231	CLA	C2C-C1C-NC	5.75	116.02	109.98
14	G	1103	CLA	C4A-NA-C1A	5.75	109.30	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1221	CLA	C4A-NA-C1A	5.75	109.30	106.68
14	A	1132	CLA	C3B-C2B-C1B	-5.75	100.40	107.17
14	A	1103	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	G	1106	CLA	C3B-C2B-C1B	-5.74	100.40	107.17
14	a	1132	CLA	C3B-C2B-C1B	-5.74	100.40	107.17
14	b	1218	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	b	1226	CLA	O2D-CGD-CBD	5.74	121.26	111.23
14	G	1120	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
14	a	1113	CLA	O2D-CGD-CBD	5.74	121.26	111.23
14	G	1129	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	A	1131	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	A	1129	CLA	C2C-C1C-NC	5.74	116.01	109.98
14	H	1226	CLA	O2D-CGD-CBD	5.74	121.26	111.23
14	G	1113	CLA	O2D-CGD-CBD	5.74	121.26	111.23
14	b	1217	CLA	C1C-C2C-C3C	-5.73	100.95	106.98
14	a	1125	CLA	O2D-CGD-CBD	5.73	121.25	111.23
15	A	1121	F6C	C2C-C1C-NC	5.73	116.27	110.33
14	a	1133	CLA	C1C-C2C-C3C	-5.73	100.95	106.98
14	B	1226	CLA	O2D-CGD-CBD	5.73	121.25	111.23
14	H	1023	CLA	C2D-C1D-ND	5.73	115.80	110.13
14	a	1130	CLA	C2C-C1C-NC	5.73	116.00	109.98
14	A	1122	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	b	1023	CLA	C2D-C1D-ND	5.72	115.79	110.13
14	A	1106	CLA	C3B-C2B-C1B	-5.72	100.42	107.17
14	B	1223	CLA	C3D-C2D-C1D	-5.72	98.02	105.83
14	B	1205	CLA	O2A-CGA-O1A	-5.72	109.32	123.63
14	a	1133	CLA	C4A-NA-C1A	5.72	109.29	106.68
14	b	1205	CLA	O2A-CGA-O1A	-5.72	109.33	123.63
14	a	1104	CLA	C1D-ND-C4D	-5.72	102.30	106.31
14	B	1023	CLA	C2C-C1C-NC	5.72	115.99	109.98
14	H	1205	CLA	O2A-CGA-O1A	-5.72	109.33	123.63
14	A	1113	CLA	O2D-CGD-CBD	5.71	121.22	111.23
14	G	1116	CLA	O2D-CGD-CBD	5.71	121.22	111.23
14	b	1235	CLA	C2C-C1C-NC	5.71	115.98	109.98
18	R	4018	BCR	C7-C8-C9	-5.71	117.78	126.23
14	H	1212	CLA	C4A-NA-C1A	5.71	109.28	106.68
14	H	1231	CLA	C2C-C1C-NC	5.71	115.98	109.98
14	B	1235	CLA	C2C-C1C-NC	5.71	115.98	109.98
14	A	1133	CLA	C1C-C2C-C3C	-5.71	100.98	106.98
14	a	1120	CLA	C3D-C2D-C1D	-5.71	98.04	105.83
14	a	1116	CLA	O2D-CGD-CBD	5.71	121.20	111.23
14	B	1217	CLA	C1C-C2C-C3C	-5.70	100.98	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1223	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
14	A	1120	CLA	C3D-C2D-C1D	-5.70	98.05	105.83
14	a	1106	CLA	C3B-C2B-C1B	-5.70	100.45	107.17
14	G	1133	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	H	1235	CLA	O2A-CGA-O1A	-5.70	109.37	123.63
14	L	1503	CLA	C2C-C1C-NC	5.70	115.97	109.98
18	m	4021	BCR	C7-C8-C9	-5.70	117.81	126.23
14	a	1125	CLA	C2D-C1D-ND	5.70	115.77	110.13
14	H	1203	CLA	C2D-C1D-ND	5.70	115.76	110.13
14	H	1217	CLA	C1C-C2C-C3C	-5.70	100.99	106.98
14	a	1129	CLA	C2C-C1C-NC	5.69	115.96	109.98
14	b	1231	CLA	C2C-C1C-NC	5.69	115.96	109.98
14	B	1023	CLA	C2D-C1D-ND	5.69	115.76	110.13
14	A	1133	CLA	C4A-NA-C1A	5.69	109.28	106.68
14	b	1203	CLA	C2D-C1D-ND	5.69	115.76	110.13
14	H	1235	CLA	C2C-C1C-NC	5.69	115.96	109.98
14	a	1103	CLA	C4A-NA-C1A	5.69	109.28	106.68
14	A	1130	CLA	C2C-C1C-NC	5.69	115.96	109.98
18	M	4021	BCR	C7-C8-C9	-5.69	117.82	126.23
14	H	1214	CLA	C1C-C2C-C3C	-5.69	101.00	106.98
18	V	4021	BCR	C7-C8-C9	-5.69	117.82	126.23
14	U	1503	CLA	O2D-CGD-CBD	5.69	121.17	111.23
14	b	1214	CLA	C1C-C2C-C3C	-5.69	101.00	106.98
14	A	1125	CLA	C2D-C1D-ND	5.69	115.75	110.13
14	l	1503	CLA	C2C-C1C-NC	5.69	115.95	109.98
14	B	1235	CLA	O2A-CGA-O1A	-5.68	109.41	123.63
14	G	1130	CLA	C2C-C1C-NC	5.68	115.95	109.98
14	a	1131	CLA	C2C-C1C-NC	5.68	115.95	109.98
14	G	1125	CLA	C2D-C1D-ND	5.68	115.75	110.13
14	H	1221	CLA	O2D-CGD-CBD	5.68	121.16	111.23
14	H	1204	CLA	C3B-C2B-C1B	-5.68	100.47	107.17
14	b	1235	CLA	O2A-CGA-O1A	-5.68	109.42	123.63
14	b	1231	CLA	O2D-CGD-CBD	5.68	121.16	111.23
14	B	1231	CLA	O2D-CGD-CBD	5.68	121.16	111.23
14	B	1204	CLA	C3B-C2B-C1B	-5.68	100.47	107.17
14	b	1208	CLA	O2D-CGD-CBD	5.68	121.16	111.23
14	B	1214	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
14	H	1231	CLA	O2D-CGD-CBD	5.67	121.15	111.23
18	i	4018	BCR	C7-C8-C9	-5.67	117.84	126.23
14	B	1221	CLA	O2D-CGD-CBD	5.67	121.14	111.23
14	b	1204	CLA	C3B-C2B-C1B	-5.67	100.48	107.17
18	V	4021	BCR	C24-C23-C22	-5.67	117.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1102	CLA	C3B-C2B-C1B	-5.67	100.49	107.17
14	l	1503	CLA	O2D-CGD-CBD	5.67	121.14	111.23
18	M	4021	BCR	C24-C23-C22	-5.67	117.85	126.23
14	H	1023	CLA	C2C-C1C-NC	5.67	115.93	109.98
14	G	1133	CLA	O2D-CGD-CBD	5.66	121.13	111.23
14	b	1023	CLA	C2C-C1C-NC	5.66	115.93	109.98
14	L	1503	CLA	O2D-CGD-CBD	5.66	121.13	111.23
14	G	1131	CLA	C1C-C2C-C3C	-5.66	101.02	106.98
14	B	1216	CLA	O2D-CGD-CBD	5.66	121.13	111.23
14	b	1216	CLA	O2D-CGD-CBD	5.66	121.13	111.23
18	I	4018	BCR	C7-C8-C9	-5.66	117.86	126.23
18	H	4005	BCR	C7-C8-C9	-5.66	117.86	126.23
14	A	1136	CLA	C2C-C1C-NC	5.66	115.92	109.98
14	G	1122	CLA	C2C-C1C-NC	5.66	115.92	109.98
14	H	1216	CLA	O2D-CGD-CBD	5.66	121.12	111.23
14	a	1136	CLA	O2A-CGA-O1A	-5.65	109.48	123.63
14	a	1115	CLA	C2C-C1C-NC	5.65	115.92	109.98
14	A	1132	CLA	C2C-C1C-NC	5.65	115.92	109.98
14	B	1203	CLA	C2D-C1D-ND	5.65	115.72	110.13
14	A	1136	CLA	O2A-CGA-O1A	-5.65	109.49	123.63
14	H	1208	CLA	O2D-CGD-CBD	5.65	121.11	111.23
14	G	1136	CLA	C2C-C1C-NC	5.65	115.92	109.98
14	b	1203	CLA	C2C-C1C-NC	5.65	115.92	109.98
14	b	1221	CLA	O2D-CGD-CBD	5.65	121.11	111.23
18	b	4005	BCR	C7-C8-C9	-5.65	117.88	126.23
14	A	1115	CLA	C2C-C1C-NC	5.65	115.91	109.98
18	H	4010	BCR	C24-C23-C22	-5.65	117.88	126.23
18	b	4010	BCR	C24-C23-C22	-5.65	117.88	126.23
15	B	1237	F6C	C1A-C2A-C3A	-5.64	101.03	106.97
14	G	1013	CLA	C1D-ND-C4D	-5.64	102.36	106.31
15	H	1237	F6C	C1A-C2A-C3A	-5.64	101.03	106.97
14	H	1208	CLA	C2C-C1C-NC	5.64	115.90	109.98
14	G	1122	CLA	C4A-NA-C1A	5.64	109.25	106.68
14	G	1136	CLA	O2A-CGA-O1A	-5.63	109.53	123.63
14	G	1115	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	a	1120	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	b	1224	CLA	C2C-C1C-NC	5.63	115.90	109.98
14	a	1133	CLA	O2D-CGD-CBD	5.63	121.08	111.23
14	A	1133	CLA	O2D-CGD-CBD	5.63	121.08	111.23
18	B	4010	BCR	C24-C23-C22	-5.63	117.91	126.23
14	a	1102	CLA	C3B-C2B-C1B	-5.63	100.53	107.17
14	G	1132	CLA	C2C-C1C-NC	5.63	115.89	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1224	CLA	C2C-C1C-NC	5.63	115.89	109.98
14	a	1132	CLA	C2C-C1C-NC	5.62	115.89	109.98
14	B	1208	CLA	O2D-CGD-CBD	5.62	121.06	111.23
18	m	4021	BCR	C24-C23-C22	-5.62	117.92	126.23
14	A	1108	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
14	b	1212	CLA	C4A-NA-C1A	5.62	109.24	106.68
14	a	1105	CLA	O2D-CGD-CBD	5.62	121.05	111.23
14	G	1137	CLA	C1C-C2C-C3C	-5.62	101.07	106.98
14	B	1217	CLA	C4A-NA-C1A	5.62	109.24	106.68
14	H	1222	CLA	C3B-C2B-C1B	-5.62	100.55	107.17
15	b	1237	F6C	C1A-C2A-C3A	-5.61	101.06	106.97
18	B	4005	BCR	C7-C8-C9	-5.61	117.93	126.23
14	b	1222	CLA	C3B-C2B-C1B	-5.61	100.55	107.17
14	a	1136	CLA	C2C-C1C-NC	5.61	115.88	109.98
14	B	1224	CLA	C2C-C1C-NC	5.61	115.88	109.98
14	B	1208	CLA	C2C-C1C-NC	5.61	115.88	109.98
14	A	1105	CLA	O2D-CGD-CBD	5.61	121.03	111.23
14	H	1217	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	G	1112	CLA	O2D-CGD-CBD	5.61	121.03	111.23
14	G	1120	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	a	1139	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	A	1120	CLA	C2C-C1C-NC	5.61	115.87	109.98
14	G	1102	CLA	C3B-C2B-C1B	-5.61	100.56	107.17
14	B	1229	CLA	C3B-C2B-C1B	-5.60	100.56	107.17
14	A	1104	CLA	C2C-C1C-NC	5.60	115.87	109.98
14	B	1222	CLA	C4A-NA-C1A	5.60	109.23	106.68
14	a	1104	CLA	C3D-C2D-C1D	-5.60	98.19	105.83
14	A	1102	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	B	1222	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
14	A	1131	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	B	1203	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	H	1203	CLA	C2C-C1C-NC	5.60	115.86	109.98
14	B	1226	CLA	C1C-C2C-C3C	-5.60	101.09	106.98
14	b	1226	CLA	C1C-C2C-C3C	-5.59	101.10	106.98
14	a	1112	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
14	G	1108	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
14	a	1122	CLA	C4A-NA-C1A	5.59	109.23	106.68
14	G	1105	CLA	O2D-CGD-CBD	5.59	121.00	111.23
14	a	1104	CLA	C2C-C1C-NC	5.59	115.85	109.98
14	A	1104	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
14	G	1102	CLA	C2C-C1C-NC	5.59	115.85	109.98
14	B	1212	CLA	C4A-NA-C1A	5.59	109.23	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1224	CLA	C3B-C2B-C1B	-5.59	100.58	107.17
14	A	1013	CLA	C1D-ND-C4D	-5.59	102.39	106.31
14	B	1224	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
14	H	1226	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	a	1108	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
14	a	1013	CLA	C1D-ND-C4D	-5.58	102.40	106.31
14	G	1101	CLA	C2C-C1C-NC	5.58	115.84	109.98
14	a	1124	CLA	C2C-C1C-NC	5.58	115.84	109.98
14	b	1022	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
14	H	1213	CLA	C2C-C1C-NC	5.58	115.84	109.98
14	A	1137	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	L	1501	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	a	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	1208	CLA	C2C-C1C-NC	5.58	115.84	109.98
14	T	1401	CLA	O2D-CGD-CBD	5.58	120.98	111.23
14	a	1128	CLA	C1C-C2C-C3C	-5.58	101.11	106.98
14	k	1401	CLA	O2D-CGD-CBD	5.57	120.98	111.23
14	H	1210	CLA	C2C-C1C-NC	5.57	115.84	109.98
14	A	1115	CLA	C4A-NA-C1A	5.57	109.22	106.68
14	H	1229	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
14	A	1118	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
14	B	1210	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
14	G	1104	CLA	C2C-C1C-NC	5.57	115.83	109.98
14	A	1122	CLA	C2C-C1C-NC	5.57	115.83	109.98
14	H	1212	CLA	O2D-CGD-CBD	5.57	120.96	111.23
14	H	1224	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
14	l	1501	CLA	C1C-C2C-C3C	-5.57	101.12	106.98
14	b	1217	CLA	C4A-NA-C1A	5.57	109.22	106.68
14	G	1104	CLA	C3D-C2D-C1D	-5.57	98.23	105.83
14	B	1201	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
14	A	1112	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
14	H	1210	CLA	C3B-C2B-C1B	-5.56	100.61	107.17
14	A	1128	CLA	C1C-C2C-C3C	-5.56	101.13	106.98
14	b	1229	CLA	C3B-C2B-C1B	-5.56	100.61	107.17
14	K	1401	CLA	O2D-CGD-CBD	5.56	120.95	111.23
14	a	1122	CLA	C2C-C1C-NC	5.56	115.82	109.98
15	b	1207	F6C	O2A-CGA-O1A	-5.56	109.72	123.63
18	H	4009	BCR	C24-C23-C22	-5.56	118.01	126.23
14	a	1102	CLA	C2C-C1C-NC	5.56	115.82	109.98
14	G	1124	CLA	C2C-C1C-NC	5.56	115.82	109.98
14	a	1131	CLA	C1C-C2C-C3C	-5.56	101.13	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1022	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
14	a	1118	CLA	C1C-C2C-C3C	-5.56	101.14	106.98
14	a	1116	CLA	C3B-C2B-C1B	-5.56	100.62	107.17
14	H	1022	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
14	A	1013	CLA	C3B-C2B-C1B	-5.55	100.62	107.17
14	G	1128	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
14	b	1213	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	b	1236	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
14	A	1101	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	G	1118	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
14	A	1105	CLA	C3B-C2B-C1B	-5.55	100.63	107.17
14	G	1116	CLA	C3B-C2B-C1B	-5.55	100.63	107.17
14	G	1130	CLA	C3B-C2B-C1B	-5.55	100.63	107.17
14	A	1106	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	B	1213	CLA	C2C-C1C-NC	5.55	115.81	109.98
14	H	1236	CLA	C1C-C2C-C3C	-5.55	101.15	106.98
14	B	1223	CLA	C3B-C2B-C1B	-5.55	100.63	107.17
14	A	1130	CLA	C3B-C2B-C1B	-5.54	100.63	107.17
14	A	1139	CLA	C2C-C1C-NC	5.54	115.81	109.98
14	U	1501	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	G	1112	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
15	B	1207	F6C	O2A-CGA-O1A	-5.54	109.76	123.63
14	A	1138	CLA	C2C-C1C-NC	5.54	115.80	109.98
14	b	1203	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	B	1218	CLA	O2D-CGD-CBD	5.54	120.92	111.23
14	U	1501	CLA	O2D-CGD-CBD	5.54	120.92	111.23
14	a	1137	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
14	A	1116	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
15	H	1207	F6C	O2A-CGA-O1A	-5.54	109.77	123.63
14	l	1501	CLA	O2D-CGD-CBD	5.54	120.91	111.23
14	b	1223	CLA	C3B-C2B-C1B	-5.54	100.64	107.17
14	G	1106	CLA	C2C-C1C-NC	5.54	115.80	109.98
14	B	1236	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
14	b	1212	CLA	O2D-CGD-CBD	5.53	120.90	111.23
14	b	1218	CLA	O2D-CGD-CBD	5.53	120.90	111.23
14	H	1201	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
14	H	1218	CLA	O2D-CGD-CBD	5.53	120.90	111.23
14	L	1501	CLA	O2D-CGD-CBD	5.53	120.90	111.23
14	G	1110	CLA	C2C-C1C-NC	5.53	115.79	109.98
14	a	1106	CLA	C2C-C1C-NC	5.53	115.79	109.98
18	b	4009	BCR	C24-C23-C22	-5.53	118.06	126.23
14	a	1140	CLA	C2C-C1C-NC	5.53	115.79	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1130	CLA	C3B-C2B-C1B	-5.53	100.65	107.17
14	H	1219	CLA	C3B-C2B-C1B	-5.53	100.66	107.17
14	a	1013	CLA	C3B-C2B-C1B	-5.53	100.66	107.17
14	A	1140	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	G	1138	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	a	1101	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	a	1110	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	b	1201	CLA	C3B-C2B-C1B	-5.52	100.66	107.17
14	H	1219	CLA	C2C-C1C-NC	5.52	115.78	109.98
15	A	1121	F6C	O2D-CGD-CBD	5.52	120.88	111.23
14	G	1139	CLA	C2C-C1C-NC	5.52	115.78	109.98
14	b	1233	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
14	a	1130	CLA	C1C-C2C-C3C	-5.52	101.17	106.98
14	B	1212	CLA	O2D-CGD-CBD	5.52	120.88	111.23
14	G	1105	CLA	C3B-C2B-C1B	-5.52	100.67	107.17
15	G	1121	F6C	O2D-CGD-CBD	5.52	120.87	111.23
14	G	1115	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	a	1105	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
14	b	1205	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	a	1122	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
14	H	1205	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	G	1013	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
14	b	1210	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	A	1124	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	H	1203	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	B	1233	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	B	1203	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
14	B	1205	CLA	C2C-C1C-NC	5.51	115.77	109.98
14	a	1120	CLA	O2D-CGD-CBD	5.51	120.86	111.23
14	B	1210	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	H	1223	CLA	C3B-C2B-C1B	-5.50	100.68	107.17
18	B	4009	BCR	C24-C23-C22	-5.50	118.09	126.23
14	G	1140	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	A	1122	CLA	O2D-CGD-CBD	5.50	120.85	111.23
14	b	1210	CLA	C3B-C2B-C1B	-5.50	100.69	107.17
14	H	1202	CLA	C3D-C2D-C1D	-5.50	98.32	105.83
14	A	1130	CLA	C1C-C2C-C3C	-5.50	101.19	106.98
14	b	1219	CLA	C2C-C1C-NC	5.50	115.76	109.98
14	A	1122	CLA	C3B-C2B-C1B	-5.50	100.69	107.17
14	G	1123	CLA	O2D-CGD-CBD	5.50	120.84	111.23
14	B	1202	CLA	C3D-C2D-C1D	-5.50	98.33	105.83
14	a	1112	CLA	C4A-NA-C1A	5.50	109.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1233	CLA	C1C-C2C-C3C	-5.50	101.20	106.98
14	G	1106	CLA	C2D-C1D-ND	5.50	115.57	110.13
14	A	1120	CLA	O2D-CGD-CBD	5.49	120.83	111.23
15	a	1121	F6C	O2D-CGD-CBD	5.49	120.83	111.23
14	H	1212	CLA	C2C-C1C-NC	5.49	115.75	109.98
14	A	1106	CLA	C2D-C1D-ND	5.49	115.56	110.13
14	B	1219	CLA	C3B-C2B-C1B	-5.49	100.69	107.17
14	G	1122	CLA	C3B-C2B-C1B	-5.49	100.69	107.17
14	b	1202	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
14	B	1212	CLA	C2C-C1C-NC	5.49	115.75	109.98
14	A	1116	CLA	C2C-C1C-NC	5.49	115.75	109.98
14	A	1107	CLA	O2D-CGD-CBD	5.49	120.83	111.23
14	b	1212	CLA	C2C-C1C-NC	5.49	115.75	109.98
14	b	1225	CLA	C2C-C1C-NC	5.48	115.74	109.98
14	B	1209	CLA	C2C-C1C-NC	5.48	115.74	109.98
14	H	1229	CLA	O2D-CGD-CBD	5.48	120.82	111.23
14	a	1122	CLA	O2D-CGD-CBD	5.48	120.82	111.23
14	B	1219	CLA	C2C-C1C-NC	5.48	115.74	109.98
15	B	1237	F6C	C2C-C1C-NC	5.48	116.01	110.33
14	G	1120	CLA	O2D-CGD-CBD	5.48	120.82	111.23
14	b	1212	CLA	C3D-C2D-C1D	-5.48	98.35	105.83
14	H	1228	CLA	O2D-CGD-CBD	5.48	120.81	111.23
14	a	1106	CLA	C2D-C1D-ND	5.48	115.55	110.13
14	a	1107	CLA	O2D-CGD-CBD	5.48	120.81	111.23
14	a	1132	CLA	C1C-C2C-C3C	-5.48	101.22	106.98
14	H	1201	CLA	O2A-CGA-O1A	-5.48	109.93	123.63
14	G	1116	CLA	C2C-C1C-NC	5.48	115.73	109.98
14	a	1116	CLA	C2C-C1C-NC	5.48	115.73	109.98
14	a	1115	CLA	C4A-NA-C1A	5.48	109.18	106.68
14	b	1218	CLA	C4A-NA-C1A	5.47	109.18	106.68
14	H	1212	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
14	a	1106	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
14	A	1106	CLA	C3D-C2D-C1D	-5.47	98.36	105.83
14	a	1108	CLA	C4A-NA-C1A	5.47	109.17	106.68
14	a	1126	CLA	O2A-CGA-O1A	-5.47	109.95	123.63
14	B	1222	CLA	C2C-C1C-NC	5.47	115.73	109.98
14	a	1123	CLA	O2D-CGD-CBD	5.47	120.79	111.23
14	A	1110	CLA	C2C-C1C-NC	5.47	115.72	109.98
14	G	1122	CLA	O2D-CGD-CBD	5.47	120.79	111.23
14	b	1229	CLA	O2D-CGD-CBD	5.47	120.78	111.23
14	B	1205	CLA	C3B-C2B-C1B	-5.47	100.73	107.17
14	A	1126	CLA	O2A-CGA-O1A	-5.46	109.96	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1130	CLA	C3D-C2D-C1D	-5.46	98.37	105.83
14	B	1201	CLA	O2A-CGA-O1A	-5.46	109.96	123.63
14	A	1110	CLA	O2D-CGD-CBD	5.46	120.78	111.23
14	G	1130	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
14	A	1132	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
14	H	1205	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
14	B	1229	CLA	O2D-CGD-CBD	5.46	120.78	111.23
14	b	1205	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
14	B	1212	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
14	G	1132	CLA	C1C-C2C-C3C	-5.46	101.24	106.98
14	G	1107	CLA	O2D-CGD-CBD	5.46	120.77	111.23
14	G	1106	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
14	a	1138	CLA	C2C-C1C-NC	5.46	115.72	109.98
14	A	1108	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	A	1111	CLA	C3B-C2B-C1B	-5.46	100.74	107.17
14	A	1123	CLA	O2D-CGD-CBD	5.46	120.77	111.23
14	G	1115	CLA	C3B-C2B-C1B	-5.46	100.74	107.17
14	H	1209	CLA	CAA-C2A-C3A	-5.46	98.26	113.00
14	U	1502	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
14	G	1126	CLA	O2A-CGA-O1A	-5.45	109.99	123.63
14	A	1115	CLA	C3B-C2B-C1B	-5.45	100.74	107.17
14	G	1112	CLA	C4A-NA-C1A	5.45	109.17	106.68
14	b	1219	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
14	a	1120	CLA	C1C-C2C-C3C	-5.45	101.25	106.98
14	G	1110	CLA	O2D-CGD-CBD	5.45	120.76	111.23
14	H	1023	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
14	b	1228	CLA	O2D-CGD-CBD	5.45	120.76	111.23
14	B	1228	CLA	O2D-CGD-CBD	5.45	120.76	111.23
14	b	1209	CLA	C2C-C1C-NC	5.45	115.70	109.98
14	H	1213	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
14	B	1213	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
14	B	1209	CLA	CAA-C2A-C3A	-5.45	98.28	113.00
14	b	1202	CLA	C2D-C1D-ND	5.45	115.52	110.13
14	B	1221	CLA	C2C-C1C-NC	5.45	115.70	109.98
14	b	1209	CLA	CAA-C2A-C3A	-5.44	98.29	113.00
14	H	1211	CLA	C2C-C1C-NC	5.44	115.70	109.98
14	b	1201	CLA	O2A-CGA-O1A	-5.44	110.01	123.63
14	b	1211	CLA	C2C-C1C-NC	5.44	115.70	109.98
14	A	1112	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	a	1110	CLA	O2D-CGD-CBD	5.44	120.74	111.23
14	a	1111	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
14	a	1115	CLA	C3B-C2B-C1B	-5.44	100.76	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	1401	CLA	C1C-C2C-C3C	-5.44	101.26	106.98
14	X	1701	CLA	C2C-C1C-NC	5.44	115.69	109.98
14	G	1111	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
14	H	1228	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	l	1502	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	B	1225	CLA	O2D-CGD-CBD	5.44	120.74	111.23
14	H	1225	CLA	C2C-C1C-NC	5.44	115.69	109.98
14	a	1107	CLA	C3B-C2B-C1B	-5.44	100.76	107.17
14	H	1218	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	H	1222	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	A	1135	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	L	1502	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
14	a	1130	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
15	b	1237	F6C	C2C-C1C-NC	5.43	115.96	110.33
18	L	4019	BCR	C3-C4-C5	-5.43	104.37	114.06
14	H	1209	CLA	C2C-C1C-NC	5.43	115.69	109.98
14	G	1130	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
14	H	1221	CLA	C2C-C1C-NC	5.43	115.69	109.98
14	H	1225	CLA	O2D-CGD-CBD	5.43	120.72	111.23
14	B	1218	CLA	C4A-NA-C1A	5.43	109.16	106.68
15	H	1237	F6C	C2C-C1C-NC	5.43	115.96	110.33
14	G	1115	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
14	B	1225	CLA	C2C-C1C-NC	5.43	115.68	109.98
18	B	4010	BCR	C15-C14-C13	-5.43	119.67	127.28
14	b	1213	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
14	b	1222	CLA	C2C-C1C-NC	5.43	115.68	109.98
14	A	1115	CLA	C3D-C2D-C1D	-5.43	98.43	105.83
14	b	1225	CLA	O2D-CGD-CBD	5.42	120.71	111.23
14	B	1202	CLA	C2D-C1D-ND	5.42	115.49	110.13
18	H	4010	BCR	C15-C14-C13	-5.42	119.67	127.28
14	A	1120	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
18	U	4019	BCR	C3-C4-C5	-5.42	104.39	114.06
14	G	1107	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
14	A	1107	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
18	b	4010	BCR	C15-C14-C13	-5.42	119.68	127.28
14	H	1222	CLA	C2C-C1C-NC	5.42	115.67	109.98
14	H	1202	CLA	C2D-C1D-ND	5.42	115.49	110.13
14	a	1102	CLA	O2A-CGA-O1A	-5.42	110.08	123.63
14	x	1701	CLA	C2C-C1C-NC	5.41	115.67	109.98
14	G	1113	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
14	U	1502	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	B	1203	CLA	C3B-C2B-C1B	-5.41	100.79	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1228	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
14	B	1021	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	B	1211	CLA	C2C-C1C-NC	5.41	115.66	109.98
14	b	1220	CLA	O2D-CGD-CBD	5.41	120.68	111.23
14	H	1021	CLA	C2D-C1D-ND	5.41	115.48	110.13
14	b	1231	CLA	C4A-NA-C1A	5.41	109.14	106.68
14	B	1235	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
14	b	1023	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	W	1701	CLA	C2C-C1C-NC	5.40	115.66	109.98
14	a	1113	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
18	b	4016	BCR	C15-C14-C13	-5.40	119.70	127.28
14	A	1111	CLA	C2C-C1C-NC	5.40	115.66	109.98
14	B	1023	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
14	a	1134	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	b	1021	CLA	C2D-C1D-ND	5.40	115.47	110.13
14	G	1102	CLA	O2A-CGA-O1A	-5.40	110.12	123.63
14	T	1401	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	A	1127	CLA	C1C-C2C-C3C	-5.40	101.30	106.98
14	B	1220	CLA	O2D-CGD-CBD	5.40	120.67	111.23
14	A	1113	CLA	C3D-C2D-C1D	-5.40	98.47	105.83
14	B	1228	CLA	C4A-NA-C1A	5.40	109.14	106.68
15	B	1237	F6C	O2D-CGD-CBD	5.40	120.66	111.23
14	L	1502	CLA	C2D-C1D-ND	5.40	115.47	110.13
18	l	4019	BCR	C3-C4-C5	-5.39	104.44	114.06
14	a	1127	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
14	H	1212	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
14	H	1220	CLA	O2D-CGD-CBD	5.39	120.65	111.23
14	a	1136	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	A	1116	CLA	C1C-C2C-C3C	-5.39	101.31	106.98
14	a	1013	CLA	O2D-CGD-CBD	5.39	120.65	111.23
14	a	1135	CLA	C4A-NA-C1A	5.39	109.14	106.68
14	a	1127	CLA	C2D-C1D-ND	5.39	115.46	110.13
14	A	1127	CLA	C2D-C1D-ND	5.39	115.46	110.13
14	H	1234	CLA	C1D-ND-C4D	-5.39	102.53	106.31
14	a	1109	CLA	C3B-C2B-C1B	-5.39	100.82	107.17
14	A	1102	CLA	O2A-CGA-O1A	-5.39	110.16	123.63
18	B	4016	BCR	C15-C14-C13	-5.39	119.72	127.28
14	b	1203	CLA	C3B-C2B-C1B	-5.38	100.82	107.17
14	a	1116	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	b	1228	CLA	C4A-NA-C1A	5.38	109.14	106.68
14	G	1134	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
15	H	1237	F6C	O2D-CGD-CBD	5.38	120.64	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1109	CLA	C1C-C2C-C3C	-5.38	101.32	106.98
14	a	1131	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
15	b	1238	F6C	C1A-C2A-C3A	-5.38	101.30	106.97
14	b	1221	CLA	C2C-C1C-NC	5.38	115.63	109.98
14	G	1108	CLA	C4A-NA-C1A	5.38	109.13	106.68
14	b	1239	CLA	C4A-NA-C1A	5.38	109.13	106.68
14	A	1013	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
14	G	1127	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	B	1228	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
15	A	1121	F6C	C1A-C2A-C3A	-5.38	101.31	106.97
14	G	1111	CLA	C2C-C1C-NC	5.38	115.63	109.98
14	l	1502	CLA	C2D-C1D-ND	5.38	115.45	110.13
14	H	1229	CLA	C1C-C2C-C3C	-5.38	101.33	106.98
14	k	1401	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	G	1120	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	b	1212	CLA	C3B-C2B-C1B	-5.37	100.83	107.17
14	A	1013	CLA	O2D-CGD-CBD	5.37	120.62	111.23
14	G	1126	CLA	C4A-NA-C1A	5.37	109.13	106.68
15	H	1207	F6C	O2D-CGD-O1D	-5.37	113.39	123.85
14	b	1229	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	a	1115	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
15	b	1207	F6C	O2D-CGD-O1D	-5.37	113.39	123.85
14	A	1104	CLA	O2D-CGD-CBD	5.37	120.62	111.23
18	R	4020	BCR	C24-C23-C22	-5.37	118.29	126.23
18	I	4020	BCR	C24-C23-C22	-5.37	118.29	126.23
14	G	1116	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	b	1211	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
14	H	1223	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	a	1104	CLA	O2D-CGD-CBD	5.37	120.61	111.23
14	H	1223	CLA	C2D-C1D-ND	5.37	115.44	110.13
14	H	1227	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	a	1109	CLA	C1C-C2C-C3C	-5.37	101.33	106.98
14	A	1134	CLA	C1C-C2C-C3C	-5.37	101.34	106.98
14	H	1235	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
14	A	1109	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
14	H	1203	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
14	H	1211	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
14	a	1111	CLA	C2C-C1C-NC	5.37	115.62	109.98
14	A	1012	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
14	G	1104	CLA	O2D-CGD-CBD	5.36	120.61	111.23
15	H	1237	F6C	CAA-C2A-C1A	-5.36	113.03	128.01
14	G	1127	CLA	O2A-CGA-O1A	-5.36	110.21	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1216	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	G	1013	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
18	H	4016	BCR	C15-C14-C13	-5.36	119.76	127.28
14	G	1111	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
14	B	1223	CLA	C1C-C2C-C3C	-5.36	101.34	106.98
14	b	1235	CLA	C3B-C2B-C1B	-5.36	100.85	107.17
14	b	1228	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
15	b	1237	F6C	O2D-CGD-CBD	5.36	120.60	111.23
15	b	1237	F6C	CAA-C2A-C1A	-5.36	113.05	128.01
14	B	1216	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
14	G	1105	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
14	G	1127	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
15	B	1238	F6C	C1A-C2A-C3A	-5.35	101.33	106.97
14	B	1208	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
14	b	1204	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
14	G	1013	CLA	O2D-CGD-CBD	5.35	120.58	111.23
14	a	1012	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
18	i	4020	BCR	C24-C23-C22	-5.35	118.32	126.23
14	A	1124	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
14	B	1229	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
15	a	1121	F6C	C1A-C2A-C3A	-5.35	101.34	106.97
14	b	1211	CLA	C1C-C2C-C3C	-5.35	101.35	106.98
14	a	1104	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
14	a	1108	CLA	C2C-C1C-NC	5.35	115.60	109.98
14	A	1124	CLA	O2D-CGD-CBD	5.35	120.58	111.23
15	B	1207	F6C	O2D-CGD-O1D	-5.35	113.44	123.85
15	B	1237	F6C	CAA-C2A-C1A	-5.35	113.07	128.01
14	H	1208	CLA	C3B-C2B-C1B	-5.35	100.87	107.17
14	a	1124	CLA	O2D-CGD-CBD	5.34	120.57	111.23
14	A	1127	CLA	O2A-CGA-O1A	-5.34	110.27	123.63
18	H	4014	BCR	C7-C8-C9	-5.34	118.34	126.23
14	a	1104	CLA	O2A-CGA-O1A	-5.34	110.27	123.63
14	b	1208	CLA	C3B-C2B-C1B	-5.34	100.88	107.17
14	B	1227	CLA	C1C-C2C-C3C	-5.34	101.37	106.98
15	H	1238	F6C	C1A-C2A-C3A	-5.34	101.35	106.97
14	a	1111	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	A	1111	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
14	A	1104	CLA	O2A-CGA-O1A	-5.34	110.28	123.63
14	B	1234	CLA	C1D-ND-C4D	-5.34	102.57	106.31
13	a	1011	CL0	O2A-CGA-O1A	-5.34	110.28	123.63
14	G	1135	CLA	C1C-C2C-C3C	-5.34	101.37	106.98
14	a	1013	CLA	C3D-C2D-C1D	-5.34	98.55	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1223	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
15	G	1121	F6C	C1A-C2A-C3A	-5.33	101.35	106.97
14	G	1109	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
14	a	1127	CLA	O2A-CGA-O1A	-5.33	110.29	123.63
14	G	1135	CLA	C4A-NA-C1A	5.33	109.11	106.68
14	B	1239	CLA	C4A-NA-C1A	5.33	109.11	106.68
14	G	1108	CLA	C2C-C1C-NC	5.33	115.58	109.98
14	A	1109	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
14	G	1131	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
14	B	1211	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
14	b	1222	CLA	C4A-NA-C1A	5.33	109.11	106.68
14	A	1136	CLA	C4A-NA-C1A	5.33	109.11	106.68
14	x	1701	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
14	A	1105	CLA	C1C-C2C-C3C	-5.33	101.37	106.98
18	i	4018	BCR	C24-C23-C22	-5.33	118.35	126.23
18	I	4018	BCR	C24-C23-C22	-5.33	118.35	126.23
14	G	1012	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
18	B	4014	BCR	C7-C8-C9	-5.33	118.35	126.23
14	B	1218	CLA	C1C-C2C-C3C	-5.33	101.38	106.98
14	B	1213	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	b	1213	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	H	1022	CLA	C3D-C2D-C1D	-5.33	98.56	105.83
14	G	1104	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
14	G	1103	CLA	C3B-C2B-C1B	-5.32	100.89	107.17
14	G	1123	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
14	A	1131	CLA	C3B-C2B-C1B	-5.32	100.89	107.17
14	B	1215	CLA	O2D-CGD-CBD	5.32	120.53	111.23
14	B	1217	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	A	1108	CLA	C2C-C1C-NC	5.32	115.57	109.98
14	H	1213	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	b	1234	CLA	C1D-ND-C4D	-5.32	102.58	106.31
14	b	1227	CLA	C1C-C2C-C3C	-5.32	101.38	106.98
14	B	1233	CLA	O2D-CGD-CBD	5.32	120.53	111.23
14	A	1012	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
14	G	1104	CLA	O2A-CGA-O1A	-5.32	110.32	123.63
14	G	1012	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
14	B	1223	CLA	C2D-C1D-ND	5.32	115.39	110.13
13	A	1011	CL0	O2A-CGA-O1A	-5.32	110.32	123.63
14	B	1212	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
14	B	1218	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
14	a	1105	CLA	C1C-C2C-C3C	-5.32	101.39	106.98
14	b	1216	CLA	C1C-C2C-C3C	-5.32	101.39	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1233	CLA	O2D-CGD-CBD	5.32	120.52	111.23
14	a	1103	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
14	H	1233	CLA	O2D-CGD-CBD	5.31	120.52	111.23
14	a	1135	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	G	1124	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	L	1501	CLA	C2D-C1D-ND	5.31	115.39	110.13
14	b	1218	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	H	1239	CLA	C4A-NA-C1A	5.31	109.10	106.68
14	A	1126	CLA	C4A-NA-C1A	5.31	109.10	106.68
14	B	1231	CLA	C4A-NA-C1A	5.31	109.10	106.68
18	R	4018	BCR	C24-C23-C22	-5.31	118.38	126.23
14	a	1124	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	a	1126	CLA	C2C-C1C-NC	5.31	115.56	109.98
14	B	1022	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	b	1022	CLA	C3D-C2D-C1D	-5.31	98.58	105.83
14	B	1209	CLA	C1C-C2C-C3C	-5.31	101.39	106.98
14	H	1211	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
14	G	1124	CLA	O2D-CGD-CBD	5.31	120.51	111.23
14	A	1107	CLA	C4A-NA-C1A	5.31	109.10	106.68
14	X	1701	CLA	C3B-C2B-C1B	-5.31	100.91	107.17
14	b	1215	CLA	O2D-CGD-CBD	5.31	120.51	111.23
14	H	1022	CLA	C2D-C1D-ND	5.31	115.38	110.13
14	A	1123	CLA	C1C-C2C-C3C	-5.31	101.40	106.98
14	x	1701	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	H	1236	CLA	C2D-C1D-ND	5.31	115.38	110.13
14	B	1236	CLA	C2D-C1D-ND	5.31	115.38	110.13
14	b	1220	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
14	G	1126	CLA	C2C-C1C-NC	5.31	115.55	109.98
14	A	1127	CLA	O2D-CGD-CBD	5.30	120.50	111.23
14	A	1136	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
14	a	1125	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
18	l	4022	BCR	C24-C23-C22	-5.30	118.39	126.23
14	a	1136	CLA	C1C-C2C-C3C	-5.30	101.40	106.98
18	b	4014	BCR	C7-C8-C9	-5.30	118.39	126.23
14	A	1104	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
14	b	1209	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
14	B	1204	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
14	H	1217	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
15	H	1238	F6C	O2D-CGD-CBD	5.30	120.49	111.23
14	a	1012	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
14	b	1217	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	H	1215	CLA	O2D-CGD-CBD	5.30	120.49	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1201	CLA	C1C-C2C-C3C	-5.30	101.41	106.98
13	G	1011	CL0	O2A-CGA-O1A	-5.30	110.38	123.63
14	H	1211	CLA	O2A-C1-C2	5.30	128.49	108.11
14	b	1211	CLA	O2A-C1-C2	5.30	128.49	108.11
14	B	1211	CLA	O2A-C1-C2	5.30	128.49	108.11
14	L	1501	CLA	C3D-C2D-C1D	-5.30	98.60	105.83
14	l	1501	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
18	G	4008	BCR	C24-C23-C22	-5.29	118.41	126.23
14	A	1112	CLA	O2A-CGA-O1A	-5.29	110.39	123.63
14	H	1218	CLA	C3B-C2B-C1B	-5.29	100.93	107.17
14	A	1103	CLA	C3B-C2B-C1B	-5.29	100.93	107.17
14	H	1204	CLA	C1C-C2C-C3C	-5.29	101.41	106.98
14	A	1126	CLA	C2C-C1C-NC	5.29	115.54	109.98
14	a	1125	CLA	C2C-C1C-NC	5.29	115.54	109.98
14	A	1135	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
18	a	4008	BCR	C24-C23-C22	-5.29	118.41	126.23
15	b	1230	F6C	C2D-C1D-ND	5.29	115.54	109.98
14	b	1215	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
18	L	4022	BCR	C24-C23-C22	-5.29	118.41	126.23
14	a	1123	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	b	1218	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	B	1021	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	B	1235	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
18	U	4022	BCR	C24-C23-C22	-5.29	118.41	126.23
14	G	1136	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	B	1211	CLA	C1C-C2C-C3C	-5.29	101.42	106.98
14	a	1133	CLA	O2A-CGA-O1A	-5.29	110.41	123.63
14	X	1701	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
14	H	1218	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
14	a	1125	CLA	O2A-CGA-O1A	-5.28	110.41	123.63
14	A	1125	CLA	C2C-C1C-NC	5.28	115.53	109.98
14	G	1102	CLA	C1C-C2C-C3C	-5.28	101.42	106.98
14	b	1223	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	U	1501	CLA	C3B-C2B-C1B	-5.28	100.94	107.17
14	A	1133	CLA	O2A-CGA-O1A	-5.28	110.42	123.63
14	a	1101	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
14	A	1102	CLA	C1C-C2C-C3C	-5.28	101.43	106.98
14	b	1021	CLA	O2D-CGD-CBD	5.28	120.46	111.23
14	H	1231	CLA	C4A-NA-C1A	5.28	109.09	106.68
14	A	1101	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
14	B	1215	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
14	b	1231	CLA	C1C-C2C-C3C	-5.28	101.43	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	l	1501	CLA	C2D-C1D-ND	5.28	115.35	110.13
14	G	1112	CLA	O2A-CGA-O1A	-5.28	110.43	123.63
14	G	1125	CLA	O2A-CGA-O1A	-5.28	110.43	123.63
14	A	1125	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
15	B	1207	F6C	C1-C2-C3	-5.27	117.56	126.20
14	H	1220	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	G	1124	CLA	C2D-C1D-ND	5.27	115.34	110.13
14	G	1138	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	W	1701	CLA	C3B-C2B-C1B	-5.27	100.95	107.17
14	a	1112	CLA	O2A-CGA-O1A	-5.27	110.44	123.63
14	B	1022	CLA	C2D-C1D-ND	5.27	115.34	110.13
14	G	1108	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	a	1127	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	B	1234	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	B	1220	CLA	C3D-C2D-C1D	-5.27	98.64	105.83
14	a	1102	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
14	b	1234	CLA	O2D-CGD-CBD	5.27	120.44	111.23
14	B	1231	CLA	C1C-C2C-C3C	-5.27	101.44	106.98
15	B	1230	F6C	C2D-C1D-ND	5.27	115.51	109.98
14	U	1501	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	A	1124	CLA	C2D-C1D-ND	5.26	115.33	110.13
14	H	1215	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	B	1229	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
14	a	1126	CLA	C4A-NA-C1A	5.26	109.08	106.68
14	W	1701	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
15	H	1230	F6C	C2D-C1D-ND	5.26	115.51	109.98
14	H	1021	CLA	O2D-CGD-CBD	5.26	120.43	111.23
14	l	1502	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
14	L	1503	CLA	C2D-C1D-ND	5.26	115.33	110.13
15	B	1207	F6C	C1C-C2C-C3C	-5.26	100.80	106.82
14	b	1201	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
14	H	1229	CLA	C3D-C2D-C1D	-5.26	98.66	105.83
14	G	1125	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
14	B	1217	CLA	O2A-CGA-O1A	-5.26	110.48	123.63
14	G	1125	CLA	C2C-C1C-NC	5.26	115.50	109.98
14	U	1501	CLA	C2D-C1D-ND	5.26	115.33	110.13
14	b	1217	CLA	O2A-CGA-O1A	-5.26	110.48	123.63
15	b	1207	F6C	C1-C2-C3	-5.26	117.58	126.20
14	G	1107	CLA	C4A-NA-C1A	5.26	109.08	106.68
14	H	1235	CLA	C1C-C2C-C3C	-5.26	101.45	106.98
14	G	1127	CLA	O2D-CGD-CBD	5.26	120.42	111.23
14	B	1021	CLA	O2D-CGD-CBD	5.26	120.42	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1101	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
14	H	1231	CLA	C1C-C2C-C3C	-5.25	101.45	106.98
14	G	1136	CLA	C4A-NA-C1A	5.25	109.08	106.68
14	H	1229	CLA	C2C-C1C-NC	5.25	115.50	109.98
15	B	1238	F6C	O2D-CGD-CBD	5.25	120.41	111.23
14	B	1232	CLA	C1C-C2C-C3C	-5.25	101.45	106.98
14	b	1222	CLA	C2D-C1D-ND	5.25	115.33	110.13
14	B	1021	CLA	C2C-C1C-NC	5.25	115.50	109.98
14	H	1209	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	H	1234	CLA	O2D-CGD-CBD	5.25	120.41	111.23
14	b	1229	CLA	C2C-C1C-NC	5.25	115.50	109.98
15	b	1207	F6C	C1C-C2C-C3C	-5.25	100.80	106.82
18	A	4008	BCR	C24-C23-C22	-5.25	118.47	126.23
14	X	1701	CLA	C2D-C1D-ND	5.25	115.32	110.13
14	A	1108	CLA	O2D-CGD-CBD	5.25	120.41	111.23
14	H	1217	CLA	O2A-CGA-O1A	-5.25	110.50	123.63
15	b	1238	F6C	O2D-CGD-CBD	5.25	120.41	111.23
14	G	1124	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	U	1503	CLA	C2D-C1D-ND	5.25	115.32	110.13
14	b	1235	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	A	1125	CLA	O2A-CGA-O1A	-5.25	110.50	123.63
14	U	1502	CLA	C3B-C2B-C1B	-5.25	100.98	107.17
14	A	1138	CLA	C1C-C2C-C3C	-5.25	101.46	106.98
14	b	1021	CLA	C2C-C1C-NC	5.24	115.49	109.98
14	G	1133	CLA	O2A-CGA-O1A	-5.24	110.52	123.63
14	b	1206	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	B	1201	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	A	1107	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	G	1106	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	H	1229	CLA	O2A-CGA-O1A	-5.24	110.52	123.63
14	G	1130	CLA	O2D-CGD-CBD	5.24	120.39	111.23
14	L	1501	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
14	U	1502	CLA	C1C-C2C-C3C	-5.24	101.47	106.98
14	b	1236	CLA	C2D-C1D-ND	5.24	115.31	110.13
14	H	1021	CLA	C2C-C1C-NC	5.24	115.48	109.98
18	G	4001	BCR	C7-C8-C9	-5.24	118.49	126.23
14	l	1501	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
14	L	1502	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
15	H	1207	F6C	C1-C2-C3	-5.23	117.62	126.20
14	k	1401	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
14	b	1229	CLA	O2A-CGA-O1A	-5.23	110.54	123.63
14	L	1502	CLA	C1C-C2C-C3C	-5.23	101.48	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1205	CLA	C2D-C1D-ND	5.23	115.30	110.13
14	a	1124	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	A	1115	CLA	C2D-C1D-ND	5.23	115.30	110.13
14	H	1021	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	G	1115	CLA	C2D-C1D-ND	5.23	115.30	110.13
14	b	1220	CLA	C2D-C1D-ND	5.23	115.30	110.13
15	H	1207	F6C	C1C-C2C-C3C	-5.23	100.83	106.82
14	b	1021	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	A	1106	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
14	G	1110	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
18	a	4001	BCR	C7-C8-C9	-5.23	118.50	126.23
14	l	1502	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
14	A	1113	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
14	b	1229	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
14	H	1220	CLA	C2D-C1D-ND	5.23	115.30	110.13
14	B	1205	CLA	C2D-C1D-ND	5.23	115.30	110.13
14	G	1129	CLA	C1C-C2C-C3C	-5.22	101.48	106.98
14	a	1108	CLA	O2D-CGD-CBD	5.22	120.36	111.23
14	H	1206	CLA	C1C-C2C-C3C	-5.22	101.49	106.98
14	B	1229	CLA	O2A-CGA-O1A	-5.22	110.57	123.63
18	B	4006	BCR	C7-C8-C9	-5.22	118.51	126.23
14	B	1220	CLA	C2D-C1D-ND	5.22	115.29	110.13
14	A	1140	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	a	1101	CLA	C2D-C1D-ND	5.22	115.29	110.13
14	b	1022	CLA	C2D-C1D-ND	5.22	115.29	110.13
14	A	1110	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
15	b	1207	F6C	C3A-C4A-NA	5.22	115.29	110.13
14	a	1108	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
14	a	1130	CLA	O2D-CGD-CBD	5.22	120.35	111.23
14	A	1139	CLA	O2D-CGD-CBD	5.22	120.35	111.23
14	a	1106	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	A	1138	CLA	C4A-NA-C1A	5.21	109.06	106.68
14	G	1113	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
14	W	1701	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	A	1112	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	A	1129	CLA	C1C-C2C-C3C	-5.21	101.50	106.98
14	T	1401	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
14	H	1203	CLA	O2D-CGD-CBD	5.21	120.33	111.23
14	a	1113	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
14	K	1401	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
14	G	1101	CLA	C2D-C1D-ND	5.21	115.28	110.13
14	a	1107	CLA	C4A-NA-C1A	5.21	109.05	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1112	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	B	1206	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	H	1210	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	A	1130	CLA	O2D-CGD-CBD	5.20	120.33	111.23
14	a	1138	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	H	1211	CLA	C4A-NA-C1A	5.20	109.05	106.68
14	K	1401	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
18	H	4006	BCR	C7-C8-C9	-5.20	118.54	126.23
18	A	4001	BCR	C7-C8-C9	-5.20	118.54	126.23
14	a	1140	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	B	1203	CLA	O2D-CGD-CBD	5.20	120.32	111.23
14	H	1208	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	a	1110	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
14	x	1701	CLA	C2D-C1D-ND	5.20	115.27	110.13
14	B	1217	CLA	C2D-C1D-ND	5.20	115.27	110.13
14	H	1022	CLA	O2A-CGA-O1A	-5.20	110.62	123.63
14	G	1107	CLA	C1C-C2C-C3C	-5.20	101.51	106.98
14	b	1210	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	A	1108	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	G	1140	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
14	a	1116	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
14	a	1129	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	B	1209	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
14	A	1124	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	G	1112	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	a	1139	CLA	O2D-CGD-CBD	5.19	120.31	111.23
14	a	1115	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	a	1124	CLA	C2D-C1D-ND	5.19	115.26	110.13
18	b	4006	BCR	C7-C8-C9	-5.19	118.56	126.23
15	B	1207	F6C	C3A-C4A-NA	5.19	115.26	110.13
14	a	1107	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	G	1139	CLA	O2D-CGD-CBD	5.19	120.30	111.23
14	b	1232	CLA	C1C-C2C-C3C	-5.19	101.52	106.98
14	b	1203	CLA	O2D-CGD-CBD	5.19	120.30	111.23
14	b	1208	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	B	1236	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
14	B	1229	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	b	1022	CLA	O2A-CGA-O1A	-5.19	110.66	123.63
14	b	1205	CLA	C2D-C1D-ND	5.19	115.26	110.13
14	B	1208	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	A	1116	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	B	1222	CLA	C2D-C1D-ND	5.18	115.25	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1208	CLA	O2A-CGA-O1A	-5.18	110.67	123.63
14	L	1503	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	A	1113	CLA	C2C-C1C-NC	5.18	115.42	109.98
14	B	1210	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
14	U	1503	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
15	B	1237	F6C	C4A-NA-C1A	5.18	109.95	106.31
14	H	1222	CLA	C2D-C1D-ND	5.18	115.25	110.13
14	b	1022	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	A	1101	CLA	C2D-C1D-ND	5.18	115.25	110.13
14	G	1108	CLA	C3D-C2D-C1D	-5.18	98.77	105.83
14	B	1211	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	A	1105	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	H	1232	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
14	B	1236	CLA	C1D-ND-C4D	-5.17	102.68	106.31
14	k	1401	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	a	1105	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
14	G	1138	CLA	C4A-NA-C1A	5.17	109.04	106.68
14	H	1236	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
15	H	1207	F6C	C3A-C4A-NA	5.17	115.24	110.13
14	B	1205	CLA	C1C-C2C-C3C	-5.17	101.54	106.98
14	B	1208	CLA	O2A-CGA-O1A	-5.17	110.70	123.63
14	b	1205	CLA	C1C-C2C-C3C	-5.17	101.55	106.98
14	G	1105	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	H	1022	CLA	C2C-C1C-NC	5.17	115.41	109.98
14	H	1236	CLA	C1D-ND-C4D	-5.17	102.69	106.31
14	B	1224	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
14	a	1113	CLA	C2C-C1C-NC	5.17	115.41	109.98
14	B	1231	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
14	b	1236	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
14	G	1116	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
14	G	1110	CLA	C2D-C1D-ND	5.16	115.24	110.13
14	B	1229	CLA	C2C-C1C-NC	5.16	115.41	109.98
14	H	1231	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
14	H	1208	CLA	O2A-CGA-O1A	-5.16	110.72	123.63
14	G	1112	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	G	1113	CLA	C2C-C1C-NC	5.16	115.40	109.98
14	a	1103	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
14	A	1101	CLA	C4A-NA-C1A	5.16	109.03	106.68
18	B	4004	BCR	C7-C8-C9	-5.16	118.61	126.23
14	H	1205	CLA	C1C-C2C-C3C	-5.16	101.56	106.98
14	a	1113	CLA	C2D-C1D-ND	5.16	115.23	110.13
14	l	1503	CLA	C2D-C1D-ND	5.16	115.23	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1211	CLA	C4A-NA-C1A	5.16	109.03	106.68
14	T	1401	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
14	A	1110	CLA	C2D-C1D-ND	5.15	115.23	110.13
14	B	1022	CLA	O2A-CGA-O1A	-5.15	110.74	123.63
14	B	1224	CLA	C2D-C1D-ND	5.15	115.23	110.13
14	H	1229	CLA	C2D-C1D-ND	5.15	115.22	110.13
15	H	1237	F6C	C2D-C1D-ND	5.15	115.39	109.98
14	b	1229	CLA	C2D-C1D-ND	5.15	115.22	110.13
14	H	1234	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
14	b	1231	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
14	H	1220	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	b	1234	CLA	O2A-CGA-O1A	-5.15	110.75	123.63
14	b	1208	CLA	C1C-C2C-C3C	-5.15	101.56	106.98
14	b	1023	CLA	O2D-CGD-CBD	5.15	120.23	111.23
14	b	1226	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	H	1208	CLA	C1C-C2C-C3C	-5.15	101.57	106.98
18	b	4004	BCR	C7-C8-C9	-5.15	118.62	126.23
14	B	1234	CLA	O2A-CGA-O1A	-5.15	110.76	123.63
14	a	1110	CLA	C2D-C1D-ND	5.14	115.22	110.13
14	l	1503	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	H	1224	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	a	1122	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
14	b	1209	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
14	G	1128	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	a	1137	CLA	C4A-NA-C1A	5.14	109.02	106.68
14	a	1138	CLA	C4A-NA-C1A	5.14	109.02	106.68
14	b	1202	CLA	C2C-C1C-NC	5.14	115.38	109.98
14	b	1220	CLA	C1C-C2C-C3C	-5.14	101.58	106.98
14	H	1213	CLA	C4A-NA-C1A	5.14	109.02	106.68
14	B	1023	CLA	O2D-CGD-CBD	5.14	120.21	111.23
14	a	1109	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	A	1112	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
14	A	1113	CLA	C2D-C1D-ND	5.13	115.21	110.13
14	B	1022	CLA	C2C-C1C-NC	5.13	115.37	109.98
14	B	1208	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
14	H	1217	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	B	1229	CLA	C1D-ND-C4D	-5.13	102.71	106.31
14	L	1502	CLA	C2C-C1C-NC	5.13	115.37	109.98
14	B	1220	CLA	C1C-C2C-C3C	-5.13	101.58	106.98
14	b	1234	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
14	b	1224	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	B	1022	CLA	C4A-NA-C1A	5.13	109.02	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1113	CLA	C2D-C1D-ND	5.13	115.20	110.13
18	H	4004	BCR	C7-C8-C9	-5.13	118.65	126.23
14	b	1217	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	H	1023	CLA	O2D-CGD-CBD	5.13	120.19	111.23
14	b	1224	CLA	C2D-C1D-ND	5.13	115.20	110.13
14	b	1229	CLA	C1D-ND-C4D	-5.13	102.72	106.31
14	G	1109	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
14	B	1232	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
14	a	1112	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
14	B	1202	CLA	C2C-C1C-NC	5.13	115.36	109.98
14	H	1209	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
14	a	1128	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	A	1109	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	H	1232	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	A	1122	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
14	a	1101	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
14	A	1115	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
14	H	1234	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
14	A	1128	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	H	1211	CLA	O2D-CGD-CBD	5.12	120.18	111.23
14	G	1117	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
14	G	1103	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	G	1132	CLA	C4A-NA-C1A	5.12	109.01	106.68
14	G	1122	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	b	1219	CLA	C3D-C2D-C1D	-5.12	98.85	105.83
14	A	1103	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
14	A	1117	CLA	C1C-C2C-C3C	-5.11	101.60	106.98
14	G	1111	CLA	C2D-C1D-ND	5.11	115.19	110.13
14	B	1227	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
14	a	1133	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	B	1221	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
14	a	1137	CLA	O2A-CGA-O1A	-5.11	110.85	123.63
14	A	1117	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
14	H	1202	CLA	C2C-C1C-NC	5.11	115.35	109.98
14	H	1219	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	H	1202	CLA	O2A-CGA-CBA	5.11	127.41	111.83
14	G	1133	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
14	G	1110	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	b	1212	CLA	C1C-C2C-C3C	-5.11	101.61	106.98
14	B	1235	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
15	H	1207	F6C	C3D-C2D-C1D	-5.11	98.44	105.83
15	b	1230	F6C	C2C-C1C-NC	5.10	115.62	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1137	CLA	C4A-NA-C1A	5.10	109.01	106.68
14	b	1202	CLA	O2A-CGA-CBA	5.10	127.40	111.83
14	a	1117	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
14	G	1137	CLA	O2A-CGA-O1A	-5.10	110.86	123.63
14	b	1023	CLA	O2A-CGA-O1A	-5.10	110.86	123.63
14	H	1227	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
14	b	1227	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
14	G	1132	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	B	1234	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
14	a	1137	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	G	1115	CLA	C1C-C2C-C3C	-5.10	101.62	106.98
14	B	1219	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
14	H	1216	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
15	b	1237	F6C	C2D-C1D-ND	5.09	115.33	109.98
14	G	1117	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
15	B	1237	F6C	C2D-C1D-ND	5.09	115.33	109.98
14	H	1221	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
14	U	1502	CLA	C2C-C1C-NC	5.09	115.33	109.98
15	H	1230	F6C	C1A-C2A-C3A	-5.09	101.61	106.97
14	a	1117	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
14	b	1216	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
14	A	1137	CLA	O2A-CGA-O1A	-5.09	110.89	123.63
14	A	1136	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	b	1232	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	a	1120	CLA	C1D-ND-C4D	-5.09	102.74	106.31
14	B	1202	CLA	O2A-CGA-CBA	5.09	127.35	111.83
15	b	1207	F6C	C3D-C2D-C1D	-5.09	98.46	105.83
14	A	1110	CLA	C1C-C2C-C3C	-5.09	101.63	106.98
14	A	1133	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	b	1235	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
14	H	1212	CLA	C1C-C2C-C3C	-5.08	101.63	106.98
14	b	1022	CLA	C2C-C1C-NC	5.08	115.32	109.98
14	B	1203	CLA	C4A-NA-C1A	5.08	109.00	106.68
14	l	1502	CLA	C2C-C1C-NC	5.08	115.32	109.98
14	a	1103	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	b	1211	CLA	O2D-CGD-CBD	5.08	120.11	111.23
14	A	1132	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	G	1101	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
14	G	1117	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
14	A	1134	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
15	H	1230	F6C	C2C-C1C-NC	5.08	115.59	110.33
14	G	1101	CLA	C4A-NA-C1A	5.08	109.00	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1204	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
14	a	1110	CLA	C1C-C2C-C3C	-5.08	101.64	106.98
14	B	1211	CLA	O2D-CGD-CBD	5.08	120.10	111.23
14	B	1023	CLA	O2A-CGA-O1A	-5.08	110.93	123.63
14	H	1235	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	a	1115	CLA	C1C-C2C-C3C	-5.07	101.64	106.98
14	a	1111	CLA	C2D-C1D-ND	5.07	115.15	110.13
15	B	1230	F6C	C2C-C1C-NC	5.07	115.59	110.33
14	G	1120	CLA	C1D-ND-C4D	-5.07	102.75	106.31
14	b	1206	CLA	O2D-CGD-CBD	5.07	120.10	111.23
14	H	1209	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
15	B	1207	F6C	C3D-C2D-C1D	-5.07	98.48	105.83
14	a	1134	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	H	1224	CLA	C2D-C1D-ND	5.07	115.15	110.13
14	H	1023	CLA	O2A-CGA-O1A	-5.07	110.94	123.63
14	a	1132	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	H	1206	CLA	O2D-CGD-CBD	5.07	120.10	111.23
14	H	1231	CLA	C2D-C1D-ND	5.07	115.14	110.13
14	A	1103	CLA	C1C-C2C-C3C	-5.07	101.65	106.98
14	B	1206	CLA	O2D-CGD-CBD	5.07	120.09	111.23
14	G	1134	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
14	A	1132	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
14	G	1137	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
15	B	1230	F6C	C3D-C2D-C1D	-5.07	98.49	105.83
15	B	1230	F6C	C1A-C2A-C3A	-5.07	101.63	106.97
14	H	1203	CLA	C4A-NA-C1A	5.07	108.99	106.68
14	G	1129	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
14	b	1204	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
14	a	1132	CLA	O2A-CGA-O1A	-5.07	110.95	123.63
15	b	1230	F6C	C3D-C2D-C1D	-5.07	98.49	105.83
14	b	1231	CLA	C2D-C1D-ND	5.06	115.14	110.13
14	A	1117	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
14	G	1132	CLA	O2A-CGA-O1A	-5.06	110.96	123.63
14	b	1209	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
14	X	1701	CLA	O2D-CGD-CBD	5.06	120.08	111.23
14	H	1204	CLA	O2A-CGA-O1A	-5.06	110.97	123.63
14	a	1101	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	H	1229	CLA	C1D-ND-C4D	-5.06	102.76	106.31
14	A	1012	CLA	O2A-CGA-O1A	-5.06	110.98	123.63
14	B	1233	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
14	b	1221	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
14	G	1101	CLA	C1C-C2C-C3C	-5.05	101.66	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1231	CLA	C2D-C1D-ND	5.05	115.13	110.13
14	A	1137	CLA	C3D-C2D-C1D	-5.05	98.93	105.83
15	H	1230	F6C	C3D-C2D-C1D	-5.05	98.51	105.83
14	A	1101	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
14	A	1111	CLA	C2D-C1D-ND	5.05	115.13	110.13
14	b	1236	CLA	C1D-ND-C4D	-5.05	102.77	106.31
14	H	1022	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	B	1214	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	a	1139	CLA	C1C-C2C-C3C	-5.05	101.67	106.98
14	X	1701	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	H	1228	CLA	C2D-C1D-ND	5.05	115.12	110.13
14	x	1701	CLA	O2D-CGD-CBD	5.05	120.05	111.23
14	a	1012	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	b	1228	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
14	G	1012	CLA	O2A-CGA-O1A	-5.05	111.00	123.63
14	a	1138	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
14	a	1132	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	b	1203	CLA	C4A-NA-C1A	5.05	108.98	106.68
14	a	1133	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
14	b	1206	CLA	C3D-C2D-C1D	-5.05	98.95	105.83
14	W	1701	CLA	O2D-CGD-CBD	5.05	120.05	111.23
14	a	1129	CLA	O2A-CGA-O1A	-5.04	111.01	123.63
14	b	1213	CLA	C1C-C2C-C3C	-5.04	101.67	106.98
14	b	1234	CLA	C2C-C1C-NC	5.04	115.28	109.98
14	A	1102	CLA	C4A-NA-C1A	5.04	108.98	106.68
15	H	1237	F6C	C4A-NA-C1A	5.04	109.85	106.31
14	H	1206	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
14	a	1120	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
14	a	1136	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
15	b	1237	F6C	C4A-NA-C1A	5.04	109.85	106.31
14	G	1103	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
14	A	1140	CLA	C2D-C1D-ND	5.04	115.11	110.13
14	b	1225	CLA	C1C-C2C-C3C	-5.04	101.68	106.98
14	a	1117	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	A	1138	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	b	1222	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	A	1129	CLA	O2A-CGA-O1A	-5.04	111.03	123.63
14	B	1231	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	B	1209	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
14	H	1233	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
14	A	1120	CLA	C1D-ND-C4D	-5.03	102.78	106.31
14	G	1138	CLA	C3D-C2D-C1D	-5.03	98.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1218	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
14	B	1236	CLA	C4A-NA-C1A	5.03	108.97	106.68
14	A	1101	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	B	1212	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
18	I	4018	BCR	C15-C14-C13	-5.03	120.22	127.28
14	B	1228	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
14	B	1226	CLA	C4A-NA-C1A	5.03	108.97	106.68
15	b	1230	F6C	C1A-C2A-C3A	-5.03	101.67	106.97
14	H	1213	CLA	C1C-C2C-C3C	-5.03	101.69	106.98
14	b	1231	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	B	1216	CLA	C3B-C2B-C1B	-5.03	101.25	107.17
14	B	1206	CLA	C3D-C2D-C1D	-5.03	98.97	105.83
14	H	1226	CLA	O2A-CGA-O1A	-5.03	111.06	123.63
14	A	1013	CLA	C2B-C1B-NB	5.02	115.54	110.33
14	b	1214	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
14	b	1226	CLA	O2A-CGA-O1A	-5.02	111.06	123.63
14	A	1139	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	H	1216	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	a	1101	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	a	1140	CLA	C2D-C1D-ND	5.02	115.09	110.13
14	G	1133	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
14	H	1228	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
14	b	1233	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
14	H	1225	CLA	C1C-C2C-C3C	-5.02	101.70	106.98
14	B	1234	CLA	C2C-C1C-NC	5.02	115.25	109.98
15	B	1238	F6C	C2C-C1C-NC	5.02	115.53	110.33
14	G	1012	CLA	O2D-CGD-CBD	5.02	120.00	111.23
15	H	1237	F6C	C3D-C2D-C1D	-5.02	98.57	105.83
14	H	1226	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	a	1102	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	b	1216	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	a	1119	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	B	1225	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
14	G	1136	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	B	1226	CLA	O2A-CGA-O1A	-5.01	111.09	123.63
15	G	1121	F6C	C1C-C2C-C3C	-5.01	101.08	106.82
14	H	1214	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
14	G	1139	CLA	C1C-C2C-C3C	-5.01	101.71	106.98
14	B	1228	CLA	C2D-C1D-ND	5.01	115.08	110.13
14	A	1115	CLA	O2A-CGA-O1A	-5.01	111.10	123.63
14	G	1120	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
14	H	1232	CLA	C3B-C2B-C1B	-5.01	101.27	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1232	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
14	A	1131	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
14	G	1118	CLA	O2A-CGA-O1A	-5.00	111.11	123.63
14	H	1231	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	A	1133	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
14	G	1139	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	B	1222	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
14	A	1134	CLA	C3B-C2B-C1B	-5.00	101.27	107.17
14	G	1102	CLA	C4A-NA-C1A	5.00	108.96	106.68
14	B	1213	CLA	C4A-NA-C1A	5.00	108.96	106.68
15	A	1121	F6C	C1C-C2C-C3C	-5.00	101.09	106.82
14	G	1140	CLA	C2D-C1D-ND	5.00	115.07	110.13
14	a	1013	CLA	C2B-C1B-NB	5.00	115.51	110.33
14	H	1218	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	b	1213	CLA	C4A-NA-C1A	5.00	108.96	106.68
14	a	1115	CLA	O2A-CGA-O1A	-5.00	111.13	123.63
14	a	1127	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
14	U	1503	CLA	C1C-C2C-C3C	-5.00	101.73	106.98
14	A	1132	CLA	C4A-NA-C1A	5.00	108.96	106.68
14	G	1127	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
15	a	1121	F6C	C1C-C2C-C3C	-5.00	101.10	106.82
14	A	1012	CLA	O2D-CGD-CBD	4.99	119.96	111.23
14	a	1012	CLA	O2D-CGD-CBD	4.99	119.96	111.23
14	H	1211	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	G	1131	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	A	1120	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
14	A	1119	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
14	H	1234	CLA	C2C-C1C-NC	4.99	115.22	109.98
14	A	1137	CLA	C4A-NA-C1A	4.99	108.96	106.68
15	b	1237	F6C	C3D-C2D-C1D	-4.99	98.61	105.83
14	G	1115	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
14	b	1236	CLA	C4A-NA-C1A	4.99	108.95	106.68
14	A	1118	CLA	O2A-CGA-O1A	-4.99	111.15	123.63
14	a	1129	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
14	b	1239	CLA	C3D-C2D-C1D	-4.99	99.03	105.83
14	a	1140	CLA	C1C-C2C-C3C	-4.98	101.74	106.98
14	B	1211	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	B	1215	CLA	C4A-NA-C1A	4.98	108.95	106.68
14	A	1123	CLA	O2A-CGA-O1A	-4.98	111.16	123.63
14	B	1226	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	a	1122	CLA	O2A-CGA-O1A	-4.98	111.16	123.63
14	G	1013	CLA	C2B-C1B-NB	4.98	115.49	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1134	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
14	b	1228	CLA	C2D-C1D-ND	4.98	115.06	110.13
14	A	1128	CLA	O2A-CGA-O1A	-4.98	111.17	123.63
14	a	1134	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
14	A	1139	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	a	1128	CLA	O2A-CGA-O1A	-4.98	111.17	123.63
14	a	1131	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
14	H	1222	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	B	1213	CLA	C1C-C2C-C3C	-4.98	101.74	106.98
14	a	1139	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	H	1239	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	H	1226	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
14	T	1401	CLA	C2D-C1D-ND	4.98	115.05	110.13
14	G	1128	CLA	O2A-CGA-O1A	-4.98	111.18	123.63
15	B	1237	F6C	C3D-C2D-C1D	-4.98	98.63	105.83
14	b	1226	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
18	R	4018	BCR	C15-C14-C13	-4.98	120.30	127.28
18	i	4018	BCR	C15-C14-C13	-4.97	120.30	127.28
14	B	1213	CLA	C2D-C1D-ND	4.97	115.05	110.13
14	b	1232	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
14	A	1129	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
14	A	1127	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
14	b	1218	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	G	1122	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
14	B	1239	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	b	1217	CLA	O2D-CGD-CBD	4.97	119.92	111.23
14	a	1118	CLA	O2A-CGA-O1A	-4.97	111.19	123.63
14	A	1110	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
14	B	1233	CLA	O2A-CGA-O1A	-4.97	110.55	123.33
14	B	1233	CLA	C4A-NA-C1A	4.97	108.95	106.68
14	H	1213	CLA	C2D-C1D-ND	4.97	115.04	110.13
14	l	1503	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
14	B	1205	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	b	1211	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
14	k	1401	CLA	C2D-C1D-ND	4.97	115.04	110.13
14	H	1205	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	H	1233	CLA	O2A-CGA-O1A	-4.96	110.56	123.33
14	a	1123	CLA	O2A-CGA-O1A	-4.96	111.21	123.63
14	b	1205	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	A	1119	CLA	O2A-C1-C2	4.96	127.21	108.11
14	B	1221	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	A	1114	CLA	C3D-C2D-C1D	-4.96	99.06	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1119	CLA	O2A-C1-C2	4.96	127.21	108.11
14	K	1401	CLA	C2D-C1D-ND	4.96	115.04	110.13
14	W	1701	CLA	C4A-NA-C1A	4.96	108.94	106.68
14	B	1225	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
14	G	1140	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
14	G	1123	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
14	B	1224	CLA	O2A-CGA-O1A	-4.96	111.22	123.63
14	a	1109	CLA	O2D-CGD-CBD	4.96	119.90	111.23
14	A	1109	CLA	O2D-CGD-CBD	4.96	119.90	111.23
14	B	1217	CLA	O2D-CGD-CBD	4.96	119.90	111.23
14	A	1140	CLA	C1C-C2C-C3C	-4.96	101.77	106.98
14	A	1122	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
14	b	1208	CLA	C2D-C1D-ND	4.96	115.03	110.13
14	X	1701	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
14	H	1221	CLA	O2A-CGA-O1A	-4.96	111.23	123.63
14	G	1119	CLA	O2A-C1-C2	4.96	127.18	108.11
14	G	1114	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
14	B	1216	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
14	a	1127	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
14	a	1101	CLA	C1D-ND-C4D	-4.95	102.84	106.31
14	G	1123	CLA	O2A-CGA-O1A	-4.95	111.24	123.63
14	G	1119	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
14	b	1233	CLA	O2A-CGA-O1A	-4.95	110.60	123.33
14	H	1236	CLA	C4A-NA-C1A	4.95	108.94	106.68
14	b	1224	CLA	O2A-CGA-O1A	-4.95	111.25	123.63
14	b	1201	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	H	1217	CLA	O2D-CGD-CBD	4.95	119.88	111.23
14	G	1109	CLA	O2D-CGD-CBD	4.95	119.88	111.23
14	H	1224	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
14	B	1221	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
14	a	1114	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
14	B	1222	CLA	O2A-CGA-O1A	-4.95	111.26	123.63
14	B	1208	CLA	C4A-NA-C1A	4.94	108.94	106.68
14	H	1225	CLA	O2A-CGA-O1A	-4.94	111.26	123.63
14	L	1503	CLA	C1D-ND-C4D	-4.94	102.84	106.31
14	b	1213	CLA	C2D-C1D-ND	4.94	115.02	110.13
14	b	1225	CLA	O2A-CGA-O1A	-4.94	111.26	123.63
14	b	1221	CLA	O2A-CGA-O1A	-4.94	111.26	123.63
14	a	1123	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	H	1224	CLA	C1C-C2C-C3C	-4.94	101.78	106.98
14	H	1222	CLA	O2A-CGA-O1A	-4.94	111.27	123.63
14	a	1110	CLA	C3B-C2B-C1B	-4.94	101.34	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1206	CLA	C4A-NA-C1A	4.94	108.93	106.68
14	A	1123	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	B	1201	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
14	x	1701	CLA	O2A-CGA-O1A	-4.94	111.28	123.63
14	G	1124	CLA	C1D-ND-C4D	-4.94	102.85	106.31
15	b	1238	F6C	C2C-C1C-NC	4.94	115.44	110.33
14	G	1129	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
14	B	1224	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
14	H	1217	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	G	1127	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	A	1119	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
14	L	1503	CLA	C1C-C2C-C3C	-4.93	101.79	106.98
14	W	1701	CLA	O2A-CGA-O1A	-4.93	111.29	123.63
14	B	1217	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	b	1222	CLA	O2A-CGA-O1A	-4.93	111.30	123.63
14	B	1206	CLA	O2A-CGA-O1A	-4.93	110.65	123.33
14	H	1221	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
14	B	1214	CLA	O2A-CGA-O1A	-4.93	111.30	123.63
14	a	1119	CLA	C1C-C2C-C3C	-4.93	101.80	106.98
14	G	1110	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	H	1214	CLA	O2A-CGA-O1A	-4.93	111.30	123.63
14	U	1503	CLA	C1D-ND-C4D	-4.93	102.86	106.31
14	b	1217	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
14	a	1123	CLA	C4A-NA-C1A	4.93	108.93	106.68
14	A	1127	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
14	H	1201	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
14	H	1219	CLA	C2D-C1D-ND	4.92	115.00	110.13
14	A	1124	CLA	C1D-ND-C4D	-4.92	102.86	106.31
14	a	1136	CLA	O2A-CGA-CBA	4.92	126.85	111.83
14	G	1101	CLA	C1D-ND-C4D	-4.92	102.86	106.31
14	b	1228	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
14	b	1215	CLA	C4A-NA-C1A	4.92	108.92	106.68
14	b	1221	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
14	b	1214	CLA	O2A-CGA-O1A	-4.92	111.32	123.63
14	a	1101	CLA	O2A-CGA-O1A	-4.92	110.68	123.33
14	H	1208	CLA	C2D-C1D-ND	4.92	115.00	110.13
14	B	1219	CLA	C2D-C1D-ND	4.92	115.00	110.13
14	b	1206	CLA	O2A-CGA-O1A	-4.92	110.68	123.33
14	G	1135	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
15	H	1238	F6C	C2C-C1C-NC	4.92	115.43	110.33
14	G	1140	CLA	O2A-CGA-O1A	-4.92	111.33	123.63
14	a	1118	CLA	C3D-C2D-C1D	-4.91	99.12	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1140	CLA	O2A-CGA-O1A	-4.91	111.34	123.63
14	H	1206	CLA	O2A-CGA-O1A	-4.91	110.70	123.33
14	G	1101	CLA	O2A-CGA-O1A	-4.91	110.70	123.33
14	B	1208	CLA	C2D-C1D-ND	4.91	114.98	110.13
14	B	1228	CLA	O2A-CGA-O1A	-4.91	111.35	123.63
14	A	1111	CLA	O2A-CGA-O1A	-4.91	111.36	123.63
15	b	1207	F6C	CAA-C2A-C1A	-4.91	114.30	128.01
14	b	1233	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	b	1219	CLA	C2D-C1D-ND	4.90	114.98	110.13
14	A	1125	CLA	OBD-CAD-C3D	-4.90	116.95	128.42
14	x	1701	CLA	C4A-NA-C1A	4.90	108.92	106.68
14	G	1123	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
18	b	4013	BCR	C24-C23-C22	-4.90	118.98	126.23
14	A	1140	CLA	O2A-CGA-O1A	-4.90	111.37	123.63
15	B	1207	F6C	CAA-C2A-C1A	-4.90	114.32	128.01
14	a	1125	CLA	OBD-CAD-C3D	-4.90	116.96	128.42
14	A	1109	CLA	C2D-C1D-ND	4.90	114.97	110.13
14	A	1136	CLA	O2A-CGA-CBA	4.90	126.77	111.83
14	A	1118	CLA	C4A-NA-C1A	4.90	108.91	106.68
14	A	1101	CLA	O2A-CGA-O1A	-4.90	110.73	123.33
14	H	1233	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
18	H	4013	BCR	C24-C23-C22	-4.90	118.99	126.23
14	a	1124	CLA	C1D-ND-C4D	-4.90	102.88	106.31
14	H	1228	CLA	O2A-CGA-O1A	-4.90	111.38	123.63
14	G	1136	CLA	O2A-CGA-CBA	4.90	126.77	111.83
14	a	1111	CLA	O2A-CGA-O1A	-4.89	111.38	123.63
14	G	1118	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	b	1212	CLA	C1D-ND-C4D	-4.89	102.88	106.31
14	G	1118	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
15	H	1207	F6C	CAA-C2A-C1A	-4.89	114.34	128.01
14	A	1118	CLA	C3D-C2D-C1D	-4.89	99.15	105.83
14	H	1234	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	b	1224	CLA	C1C-C2C-C3C	-4.89	101.83	106.98
14	A	1106	CLA	C1D-ND-C4D	-4.89	102.88	106.31
14	a	1109	CLA	C2D-C1D-ND	4.89	114.97	110.13
14	A	1105	CLA	C2D-C1D-ND	4.89	114.96	110.13
14	G	1106	CLA	C1D-ND-C4D	-4.89	102.88	106.31
14	G	1111	CLA	O2A-CGA-O1A	-4.89	111.41	123.63
14	a	1135	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
14	a	1123	CLA	C3B-C2B-C1B	-4.88	101.41	107.17
14	a	1135	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	G	1125	CLA	OBD-CAD-C3D	-4.88	117.01	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1135	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
14	A	1101	CLA	C1D-ND-C4D	-4.88	102.89	106.31
18	V	4021	BCR	C33-C5-C6	-4.88	119.16	124.48
14	G	1105	CLA	C2D-C1D-ND	4.88	114.95	110.13
14	H	1209	CLA	O2A-CGA-O1A	-4.88	110.79	123.33
14	B	1209	CLA	O2A-CGA-O1A	-4.88	110.79	123.33
14	b	1233	CLA	C3B-C2B-C1B	-4.87	101.42	107.17
14	H	1215	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	H	1233	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	G	1109	CLA	C2D-C1D-ND	4.87	114.95	110.13
14	A	1116	CLA	C2D-C1D-ND	4.87	114.94	110.13
14	B	1233	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
14	a	1105	CLA	C2D-C1D-ND	4.87	114.94	110.13
14	B	1221	CLA	C2D-C1D-ND	4.87	114.94	110.13
14	A	1135	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
14	b	1234	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	G	1119	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
14	b	1209	CLA	O2A-CGA-O1A	-4.86	110.82	123.33
14	A	1135	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
14	H	1206	CLA	C4A-NA-C1A	4.86	108.90	106.68
14	H	1208	CLA	C4A-NA-C1A	4.86	108.90	106.68
18	M	4021	BCR	C33-C5-C6	-4.86	119.18	124.48
14	A	1126	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
14	A	1108	CLA	C1C-C2C-C3C	-4.86	101.87	106.98
14	H	1204	CLA	C2D-C1D-ND	4.86	114.94	110.13
14	G	1105	CLA	C4A-NA-C1A	4.86	108.90	106.68
14	G	1123	CLA	C4A-NA-C1A	4.86	108.90	106.68
18	B	4013	BCR	C24-C23-C22	-4.86	119.05	126.23
14	G	1140	CLA	C4A-NA-C1A	4.86	108.89	106.68
14	b	1021	CLA	C3B-C2B-C1B	-4.86	101.45	107.17
14	B	1235	CLA	C4A-NA-C1A	4.86	108.89	106.68
14	A	1123	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
14	b	1215	CLA	C2D-C1D-ND	4.85	114.93	110.13
14	a	1108	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
14	G	1131	CLA	O2A-CGA-O1A	-4.85	111.49	123.63
14	a	1113	CLA	O2A-CGA-O1A	-4.85	110.85	123.33
14	b	1204	CLA	C2D-C1D-ND	4.85	114.93	110.13
14	A	1107	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
14	A	1131	CLA	O2A-CGA-O1A	-4.85	111.49	123.63
14	a	1107	CLA	O2A-CGA-O1A	-4.85	110.86	123.33
14	B	1228	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
14	l	1503	CLA	C1D-ND-C4D	-4.85	102.91	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1213	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	a	1131	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	a	1116	CLA	C2D-C1D-ND	4.85	114.92	110.13
14	G	1124	CLA	O2A-CGA-O1A	-4.85	111.50	123.63
14	B	1206	CLA	C4A-NA-C1A	4.85	108.89	106.68
14	G	1139	CLA	C2D-C1D-ND	4.85	114.92	110.13
14	H	1228	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
14	l	1501	CLA	O2A-CGA-O1A	-4.84	111.51	123.63
14	G	1126	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
14	b	1210	CLA	C2D-C1D-ND	4.84	114.92	110.13
14	B	1021	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
14	A	1139	CLA	C2D-C1D-ND	4.84	114.92	110.13
14	a	1106	CLA	C1D-ND-C4D	-4.84	102.92	106.31
14	G	1113	CLA	O2A-CGA-O1A	-4.84	110.88	123.33
18	A	4002	BCR	C24-C23-C22	-4.84	119.08	126.23
14	G	1134	CLA	C4A-NA-C1A	4.84	108.89	106.68
14	A	1116	CLA	O2A-CGA-O1A	-4.84	111.52	123.63
14	H	1210	CLA	C2D-C1D-ND	4.84	114.91	110.13
14	A	1124	CLA	O2A-CGA-O1A	-4.83	111.54	123.63
14	G	1108	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
14	G	1107	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	A	1108	CLA	O2A-CGA-O1A	-4.83	110.91	123.33
14	H	1213	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
14	B	1213	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
14	B	1223	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
18	G	4002	BCR	C24-C23-C22	-4.83	119.09	126.23
14	b	1208	CLA	C4A-NA-C1A	4.83	108.88	106.68
14	B	1215	CLA	C2D-C1D-ND	4.83	114.91	110.13
14	G	1108	CLA	O2A-CGA-O1A	-4.83	110.92	123.33
14	b	1223	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
14	a	1116	CLA	O2A-CGA-O1A	-4.83	111.55	123.63
14	A	1113	CLA	O2A-CGA-O1A	-4.83	110.92	123.33
14	G	1110	CLA	C1D-ND-C4D	-4.83	102.93	106.31
14	H	1223	CLA	O2A-CGA-O1A	-4.83	111.56	123.63
18	a	4002	BCR	C24-C23-C22	-4.83	119.10	126.23
18	b	4010	BCR	C7-C8-C9	-4.82	119.10	126.23
14	H	1215	CLA	C2D-C1D-ND	4.82	114.90	110.13
14	T	1401	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	K	1401	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	a	1124	CLA	O2A-CGA-O1A	-4.82	111.56	123.63
14	G	1013	CLA	O2A-CGA-O1A	-4.82	111.56	123.63
14	H	1235	CLA	C4A-NA-C1A	4.82	108.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1139	CLA	C2D-C1D-ND	4.82	114.90	110.13
18	m	4021	BCR	C33-C5-C6	-4.82	119.22	124.48
14	a	1139	CLA	O2A-CGA-O1A	-4.82	110.94	123.33
14	G	1132	CLA	C2D-C1D-ND	4.82	114.90	110.13
14	B	1219	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
14	a	1126	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
14	U	1501	CLA	O2A-CGA-O1A	-4.82	111.57	123.63
14	A	1110	CLA	C1D-ND-C4D	-4.82	102.93	106.31
14	b	1228	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
15	B	1238	F6C	O2A-CGA-O1A	-4.82	111.58	123.63
14	A	1013	CLA	O2A-CGA-O1A	-4.82	111.58	123.63
18	H	4010	BCR	C7-C8-C9	-4.81	119.11	126.23
14	B	1210	CLA	C2D-C1D-ND	4.81	114.89	110.13
14	B	1212	CLA	C1D-ND-C4D	-4.81	102.94	106.31
14	a	1118	CLA	C4A-NA-C1A	4.81	108.87	106.68
14	A	1123	CLA	C4A-NA-C1A	4.81	108.87	106.68
14	a	1013	CLA	O2A-CGA-O1A	-4.81	111.59	123.63
14	l	1502	CLA	C1D-ND-C4D	-4.81	102.94	106.31
14	H	1021	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
18	A	4007	BCR	C24-C23-C22	-4.81	119.12	126.23
14	G	1116	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
14	L	1501	CLA	O2A-CGA-O1A	-4.81	111.60	123.63
14	G	1139	CLA	O2A-CGA-O1A	-4.81	110.97	123.33
14	b	1225	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
14	a	1108	CLA	O2A-CGA-O1A	-4.81	110.97	123.33
14	B	1234	CLA	C4A-NA-C1A	4.80	108.87	106.68
14	H	1212	CLA	C1D-ND-C4D	-4.80	102.94	106.31
18	G	4007	BCR	C24-C23-C22	-4.80	119.13	126.23
14	a	1105	CLA	C4A-NA-C1A	4.80	108.87	106.68
18	a	4007	BCR	C24-C23-C22	-4.80	119.13	126.23
14	A	1132	CLA	C2D-C1D-ND	4.80	114.88	110.13
14	l	1503	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
14	a	1110	CLA	C1D-ND-C4D	-4.80	102.94	106.31
15	H	1238	F6C	O2A-CGA-O1A	-4.80	111.62	123.63
14	A	1105	CLA	C4A-NA-C1A	4.80	108.87	106.68
15	b	1238	F6C	O2A-CGA-O1A	-4.80	111.63	123.63
14	A	1139	CLA	O2A-CGA-O1A	-4.80	111.00	123.33
14	H	1219	CLA	C1C-C2C-C3C	-4.80	101.94	106.98
14	a	1132	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	b	1219	CLA	C1C-C2C-C3C	-4.79	101.94	106.98
14	G	1111	CLA	C1-C2-C3	-4.79	118.34	126.20
14	G	1134	CLA	O2A-CGA-O1A	-4.79	111.01	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1232	CLA	C4A-NA-C1A	4.79	108.86	106.68
14	A	1134	CLA	C4A-NA-C1A	4.79	108.86	106.68
14	a	1111	CLA	C1-C2-C3	-4.79	118.35	126.20
14	b	1221	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	A	1111	CLA	C1-C2-C3	-4.79	118.35	126.20
14	b	1210	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
14	B	1224	CLA	C4A-NA-C1A	4.79	108.86	106.68
14	B	1204	CLA	C2D-C1D-ND	4.79	114.87	110.13
14	U	1502	CLA	C1D-ND-C4D	-4.79	102.95	106.31
14	b	1021	CLA	O2A-CGA-O1A	-4.79	111.65	123.63
14	H	1225	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
14	B	1210	CLA	O2A-CGA-O1A	-4.79	111.66	123.63
14	H	1021	CLA	C1D-ND-C4D	-4.78	102.95	106.31
14	H	1202	CLA	C1D-ND-C4D	-4.78	102.96	106.31
14	a	1134	CLA	O2A-CGA-O1A	-4.78	111.03	123.33
14	B	1225	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
14	A	1102	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
14	L	1502	CLA	C1D-ND-C4D	-4.78	102.96	106.31
14	b	1235	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	A	1134	CLA	O2A-CGA-O1A	-4.78	111.04	123.33
14	H	1210	CLA	O2A-CGA-O1A	-4.78	111.68	123.63
14	G	1107	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
14	G	1123	CLA	C2D-C1D-ND	4.78	114.85	110.13
14	B	1222	CLA	O2A-CGA-CBA	4.78	126.40	111.83
14	b	1202	CLA	C1D-ND-C4D	-4.77	102.96	106.31
14	a	1102	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
14	b	1222	CLA	O2A-CGA-CBA	4.77	126.38	111.83
14	H	1021	CLA	O2A-CGA-O1A	-4.77	111.70	123.63
14	H	1224	CLA	C4A-NA-C1A	4.77	108.85	106.68
14	B	1021	CLA	O2A-CGA-O1A	-4.77	111.70	123.63
18	B	4010	BCR	C7-C8-C9	-4.77	119.18	126.23
14	G	1116	CLA	C2D-C1D-ND	4.77	114.84	110.13
14	H	1222	CLA	O2A-CGA-CBA	4.76	126.36	111.83
14	H	1236	CLA	O2A-CGA-O1A	-4.76	111.08	123.33
14	H	1222	CLA	C1C-C2C-C3C	-4.76	101.97	106.98
14	a	1128	CLA	C2D-C1D-ND	4.76	114.84	110.13
14	U	1503	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
14	L	1503	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
14	B	1021	CLA	C1D-ND-C4D	-4.76	102.97	106.31
18	b	4009	BCR	C15-C14-C13	-4.76	120.60	127.28
14	H	1221	CLA	C2D-C1D-ND	4.76	114.84	110.13
14	a	1134	CLA	C4A-NA-C1A	4.76	108.85	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1102	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
14	b	1236	CLA	O2A-CGA-O1A	-4.76	111.10	123.33
14	b	1231	CLA	O2A-CGA-O1A	-4.76	111.73	123.63
14	B	1222	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
14	B	1236	CLA	O2A-CGA-O1A	-4.75	111.11	123.33
14	a	1012	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	B	1231	CLA	O2A-CGA-O1A	-4.75	111.74	123.63
14	G	1128	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	a	1119	CLA	C1-C2-C3	-4.75	118.42	126.20
14	b	1021	CLA	C1D-ND-C4D	-4.75	102.98	106.31
14	A	1012	CLA	C2D-C1D-ND	4.75	114.83	110.13
14	a	1140	CLA	C4A-NA-C1A	4.75	108.84	106.68
14	a	1107	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
18	H	4009	BCR	C15-C14-C13	-4.75	120.62	127.28
14	H	1233	CLA	C2D-C1D-ND	4.75	114.82	110.13
14	a	1133	CLA	C2D-C1D-ND	4.75	114.82	110.13
14	A	1140	CLA	C4A-NA-C1A	4.75	108.84	106.68
14	A	1123	CLA	C2D-C1D-ND	4.74	114.82	110.13
14	b	1232	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	B	1232	CLA	C4A-NA-C1A	4.74	108.84	106.68
14	b	1021	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	A	1107	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	H	1209	CLA	C2D-C1D-ND	4.74	114.82	110.13
14	H	1204	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
18	B	4017	BCR	C24-C23-C22	-4.74	119.22	126.23
14	G	1119	CLA	C1-C2-C3	-4.74	118.43	126.20
14	b	1204	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	H	1021	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
14	H	1231	CLA	O2A-CGA-O1A	-4.74	111.77	123.63
15	H	1230	F6C	O2A-CGA-O1A	-4.74	111.14	123.33
14	b	1233	CLA	C2D-C1D-ND	4.74	114.82	110.13
14	A	1133	CLA	C2D-C1D-ND	4.74	114.81	110.13
14	B	1225	CLA	C2D-C1D-ND	4.74	114.81	110.13
14	G	1139	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
15	B	1230	F6C	O2A-CGA-O1A	-4.73	111.17	123.33
14	b	1222	CLA	C1C-C2C-C3C	-4.73	102.00	106.98
14	H	1231	CLA	C1D-ND-C4D	-4.73	102.99	106.31
14	H	1202	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
14	B	1202	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
14	B	1225	CLA	C4A-NA-C1A	4.73	108.83	106.68
14	a	1108	CLA	C2D-C1D-ND	4.73	114.80	110.13
14	A	1108	CLA	C2D-C1D-ND	4.73	114.80	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1204	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
14	A	1114	CLA	O2A-CGA-O1A	-4.72	111.18	123.33
14	G	1108	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	a	1114	CLA	O2A-CGA-O1A	-4.72	111.18	123.33
14	b	1239	CLA	C2D-C1D-ND	4.72	114.80	110.13
18	b	4017	BCR	C24-C23-C22	-4.72	119.25	126.23
14	B	1021	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
14	A	1128	CLA	C2D-C1D-ND	4.72	114.80	110.13
14	A	1119	CLA	C1-C2-C3	-4.72	118.46	126.20
14	B	1218	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
14	B	1202	CLA	C1D-ND-C4D	-4.72	103.00	106.31
14	b	1224	CLA	C4A-NA-C1A	4.72	108.83	106.68
14	a	1122	CLA	C2D-C1D-ND	4.72	114.79	110.13
15	b	1230	F6C	O2A-CGA-O1A	-4.72	111.20	123.33
14	G	1114	CLA	O2A-CGA-O1A	-4.72	111.20	123.33
18	B	4009	BCR	C15-C14-C13	-4.72	120.67	127.28
14	k	1401	CLA	C4A-NA-C1A	4.71	108.83	106.68
14	B	1217	CLA	C1D-ND-C4D	-4.71	103.00	106.31
14	a	1139	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
14	b	1225	CLA	C2D-C1D-ND	4.71	114.79	110.13
14	G	1133	CLA	C2D-C1D-ND	4.71	114.79	110.13
18	A	4003	BCR	C24-C23-C22	-4.71	119.26	126.23
15	b	1207	F6C	O2A-CGA-CBA	4.71	126.20	111.83
14	k	1401	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
14	b	1022	CLA	O2A-C1-C2	4.71	126.23	108.11
14	A	1136	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
14	B	1022	CLA	O2A-C1-C2	4.71	126.23	108.11
14	H	1022	CLA	O2A-C1-C2	4.71	126.23	108.11
14	A	1122	CLA	C2D-C1D-ND	4.71	114.79	110.13
14	B	1233	CLA	C2D-C1D-ND	4.71	114.79	110.13
14	a	1105	CLA	O2A-CGA-O1A	-4.71	111.22	123.33
15	H	1207	F6C	O2A-CGA-CBA	4.71	126.19	111.83
14	a	1136	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
18	H	4017	BCR	C24-C23-C22	-4.71	119.27	126.23
14	H	1225	CLA	C4A-NA-C1A	4.71	108.83	106.68
14	A	1136	CLA	C2D-C1D-ND	4.70	114.78	110.13
14	a	1124	CLA	C4A-NA-C1A	4.70	108.83	106.68
14	A	1119	CLA	O2D-CGD-CBD	4.70	119.45	111.23
14	b	1203	CLA	O2A-CGA-O1A	-4.70	111.86	123.63
14	H	1212	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
14	H	1218	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
14	H	1225	CLA	C2D-C1D-ND	4.70	114.78	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1212	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
15	B	1207	F6C	O2A-CGA-CBA	4.70	126.17	111.83
14	A	1105	CLA	O2A-CGA-O1A	-4.70	111.24	123.33
14	K	1401	CLA	O2A-CGA-O1A	-4.70	111.25	123.33
14	G	1012	CLA	C2D-C1D-ND	4.70	114.78	110.13
14	H	1239	CLA	C2D-C1D-ND	4.70	114.78	110.13
14	G	1126	CLA	C1C-C2C-C3C	-4.70	102.04	106.98
14	b	1202	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
14	a	1110	CLA	O2A-CGA-O1A	-4.70	111.26	123.33
14	a	1123	CLA	C2D-C1D-ND	4.70	114.77	110.13
14	G	1105	CLA	O2A-CGA-O1A	-4.70	111.26	123.33
14	b	1231	CLA	C1D-ND-C4D	-4.69	103.02	106.31
14	G	1135	CLA	O2D-CGD-CBD	4.69	119.44	111.23
14	b	1218	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	B	1235	CLA	C2D-C1D-ND	4.69	114.77	110.13
14	T	1401	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	H	1203	CLA	C1D-ND-C4D	-4.69	103.02	106.31
14	H	1232	CLA	O2A-CGA-O1A	-4.69	111.27	123.33
14	A	1118	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
14	H	1203	CLA	O2A-CGA-O1A	-4.69	111.90	123.63
14	B	1203	CLA	O2A-CGA-O1A	-4.69	111.90	123.63
14	H	1211	CLA	C2D-C1D-ND	4.69	114.77	110.13
14	G	1136	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
14	A	1139	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
14	a	1126	CLA	C1C-C2C-C3C	-4.69	102.05	106.98
14	B	1239	CLA	C2D-C1D-ND	4.69	114.76	110.13
14	a	1119	CLA	O2D-CGD-CBD	4.69	119.42	111.23
14	b	1203	CLA	C1D-ND-C4D	-4.68	103.03	106.31
14	A	1135	CLA	O2D-CGD-CBD	4.68	119.42	111.23
14	B	1209	CLA	C2D-C1D-ND	4.68	114.76	110.13
15	G	1121	F6C	C3D-C2D-C1D	-4.68	99.05	105.83
14	b	1212	CLA	O2A-CGA-O1A	-4.68	111.29	123.33
14	G	1119	CLA	O2D-CGD-CBD	4.68	119.41	111.23
14	H	1215	CLA	O2A-CGA-CBA	4.68	126.10	111.83
14	a	1135	CLA	O2D-CGD-CBD	4.68	119.41	111.23
14	B	1220	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
14	H	1022	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
14	A	1124	CLA	C4A-NA-C1A	4.68	108.81	106.68
14	B	1022	CLA	C1C-C2C-C3C	-4.68	102.06	106.98
14	b	1211	CLA	C1-C2-C3	-4.68	118.53	126.20
14	H	1235	CLA	C2D-C1D-ND	4.68	114.75	110.13
14	G	1122	CLA	C2D-C1D-ND	4.68	114.75	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1219	CLA	O2A-CGA-O1A	-4.67	111.31	123.33
14	b	1215	CLA	O2A-CGA-CBA	4.67	126.09	111.83
14	B	1232	CLA	O2A-CGA-O1A	-4.67	111.31	123.33
14	B	1215	CLA	O2A-CGA-CBA	4.67	126.09	111.83
14	b	1209	CLA	C2D-C1D-ND	4.67	114.75	110.13
14	A	1134	CLA	C2D-C1D-ND	4.67	114.75	110.13
14	b	1219	CLA	O2A-CGA-O1A	-4.67	111.31	123.33
15	B	1207	F6C	O2A-C1-C2	4.67	126.08	108.11
14	b	1235	CLA	C2D-C1D-ND	4.67	114.75	110.13
15	H	1207	F6C	O2A-C1-C2	4.67	126.08	108.11
15	b	1207	F6C	O2A-C1-C2	4.67	126.08	108.11
14	b	1220	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
14	A	1126	CLA	C1C-C2C-C3C	-4.67	102.07	106.98
14	b	1211	CLA	C2D-C1D-ND	4.67	114.75	110.13
14	G	1136	CLA	C2D-C1D-ND	4.66	114.74	110.13
14	B	1211	CLA	C2D-C1D-ND	4.66	114.74	110.13
14	H	1220	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
14	B	1239	CLA	O2A-CGA-O1A	-4.66	111.97	123.63
14	b	1220	CLA	O2A-CGA-O1A	-4.66	111.97	123.63
14	a	1118	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
14	H	1239	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
14	G	1124	CLA	C4A-NA-C1A	4.66	108.80	106.68
18	B	4005	BCR	C33-C5-C6	-4.66	119.40	124.48
14	B	1220	CLA	O2A-CGA-O1A	-4.66	111.98	123.63
14	H	1211	CLA	C1-C2-C3	-4.66	118.57	126.20
14	B	1231	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	G	1110	CLA	O2A-CGA-O1A	-4.65	111.36	123.33
14	b	1232	CLA	O2A-CGA-O1A	-4.65	111.36	123.33
14	A	1110	CLA	O2A-CGA-O1A	-4.65	111.36	123.33
14	H	1219	CLA	O2A-CGA-O1A	-4.65	111.37	123.33
14	B	1220	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	H	1218	CLA	CMD-C2D-C1D	4.65	132.92	124.73
14	a	1139	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	a	1102	CLA	O2A-CGA-CBA	4.65	126.01	111.83
14	A	1139	CLA	C1D-ND-C4D	-4.65	103.05	106.31
14	H	1220	CLA	O2A-CGA-O1A	-4.65	112.00	123.63
14	B	1218	CLA	CMD-C2D-C1D	4.65	132.91	124.73
14	G	1118	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
14	H	1236	CLA	C3B-C2B-C1B	-4.64	101.69	107.17
18	a	4003	BCR	C24-C23-C22	-4.64	119.36	126.23
14	G	1112	CLA	C2D-C1D-ND	4.64	114.72	110.13
14	a	1112	CLA	C2D-C1D-ND	4.64	114.72	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1220	CLA	C1D-ND-C4D	-4.64	103.05	106.31
14	G	1102	CLA	O2A-CGA-CBA	4.64	125.99	111.83
18	G	4003	BCR	C24-C23-C22	-4.64	119.37	126.23
14	a	1136	CLA	C2D-C1D-ND	4.64	114.72	110.13
14	a	1134	CLA	C2D-C1D-ND	4.64	114.72	110.13
15	H	1238	F6C	C1C-C2C-C3C	-4.64	101.50	106.82
14	G	1106	CLA	O2A-CGA-O1A	-4.64	112.02	123.63
15	B	1238	F6C	C1C-C2C-C3C	-4.64	101.50	106.82
14	G	1122	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
14	b	1239	CLA	O2A-CGA-O1A	-4.64	112.03	123.63
14	A	1113	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
15	A	1121	F6C	C3D-C2D-C1D	-4.64	99.12	105.83
14	A	1112	CLA	O2A-CGA-CBA	4.63	125.97	111.83
14	b	1216	CLA	C2D-C1D-ND	4.63	114.71	110.13
15	a	1121	F6C	C3D-C2D-C1D	-4.63	99.12	105.83
14	G	1112	CLA	O2A-CGA-CBA	4.63	125.96	111.83
14	a	1112	CLA	O2A-CGA-CBA	4.63	125.96	111.83
14	b	1218	CLA	CMD-C2D-C1D	4.63	132.89	124.73
14	b	1227	CLA	O2A-CGA-O1A	-4.63	111.42	123.33
14	b	1236	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
14	H	1227	CLA	O2A-CGA-O1A	-4.63	111.42	123.33
14	A	1111	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
14	A	1102	CLA	O2A-CGA-CBA	4.63	125.95	111.83
14	B	1203	CLA	C1D-ND-C4D	-4.63	103.06	106.31
15	G	1121	F6C	O2A-CGA-O1A	-4.63	111.43	123.33
15	A	1121	F6C	O2A-CGA-O1A	-4.63	111.43	123.33
14	G	1111	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
14	B	1211	CLA	C1-C2-C3	-4.62	118.62	126.20
14	G	1134	CLA	C2D-C1D-ND	4.62	114.70	110.13
15	B	1237	F6C	C1C-C2C-C3C	-4.62	101.52	106.82
14	B	1216	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	a	1113	CLA	C1C-C2C-C3C	-4.62	102.12	106.98
14	T	1401	CLA	C1D-ND-C4D	-4.62	103.07	106.31
14	H	1215	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
14	H	1216	CLA	C2D-C1D-ND	4.62	114.70	110.13
14	B	1236	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
14	b	1215	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
14	a	1106	CLA	O2A-CGA-O1A	-4.62	112.08	123.63
14	a	1129	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
14	b	1217	CLA	C1D-ND-C4D	-4.62	103.07	106.31
15	a	1121	F6C	O2A-CGA-O1A	-4.62	111.46	123.33
14	H	1232	CLA	C2D-C1D-ND	4.62	114.69	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1106	CLA	O2A-CGA-O1A	-4.62	112.08	123.63
14	G	1129	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
14	G	1139	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	G	1126	CLA	C2D-C1D-ND	4.61	114.69	110.13
14	A	1126	CLA	C2D-C1D-ND	4.61	114.69	110.13
15	H	1207	F6C	C2D-C1D-ND	4.61	114.83	109.98
14	H	1211	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	B	1232	CLA	C2D-C1D-ND	4.61	114.69	110.13
15	b	1238	F6C	C1C-C2C-C3C	-4.61	101.54	106.82
14	H	1216	CLA	C4A-NA-C1A	4.61	108.78	106.68
14	B	1227	CLA	O2A-CGA-O1A	-4.61	111.48	123.33
14	b	1022	CLA	C1C-C2C-C3C	-4.61	102.13	106.98
14	G	1114	CLA	C3B-C2B-C1B	-4.61	101.74	107.17
18	b	4005	BCR	C33-C5-C6	-4.61	119.46	124.48
20	i	5006	LMG	O7-C10-C11	4.61	121.45	111.48
14	G	1125	CLA	C1-C2-C3	-4.61	118.65	126.20
18	H	4005	BCR	C33-C5-C6	-4.61	119.46	124.48
14	A	1127	CLA	C1-C2-C3	-4.61	118.65	126.20
14	a	1137	CLA	C2D-C1D-ND	4.61	114.69	110.13
14	H	1217	CLA	C1D-ND-C4D	-4.61	103.08	106.31
14	a	1127	CLA	C1-C2-C3	-4.61	118.65	126.20
14	X	1701	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
14	A	1112	CLA	C2D-C1D-ND	4.60	114.68	110.13
14	G	1130	CLA	C2D-C1D-ND	4.60	114.68	110.13
14	a	1114	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
14	b	1222	CLA	C1D-ND-C4D	-4.60	103.08	106.31
14	U	1502	CLA	O2A-CGA-O1A	-4.60	112.12	123.63
20	R	5006	LMG	O7-C10-C11	4.60	121.43	111.48
15	B	1207	F6C	C2D-C1D-ND	4.60	114.81	109.98
14	b	1232	CLA	C2D-C1D-ND	4.60	114.68	110.13
14	G	1113	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
18	U	4022	BCR	C33-C5-C6	-4.60	119.47	124.48
14	B	1215	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
14	b	1225	CLA	C4A-NA-C1A	4.60	108.78	106.68
14	G	1127	CLA	C1-C2-C3	-4.60	118.67	126.20
14	L	1502	CLA	O2A-CGA-O1A	-4.60	112.13	123.63
14	a	1130	CLA	C2D-C1D-ND	4.60	114.67	110.13
14	G	1109	CLA	O2A-CGA-O1A	-4.60	112.13	123.63
20	I	5006	LMG	O7-C10-C11	4.59	121.42	111.48
14	a	1111	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
14	a	1125	CLA	C1-C2-C3	-4.59	118.67	126.20
14	A	1138	CLA	C2D-C1D-ND	4.59	114.67	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	1502	CLA	C4A-NA-C1A	4.59	108.77	106.68
14	G	1138	CLA	C2B-C1B-NB	4.59	115.09	110.33
14	A	1109	CLA	O2A-CGA-O1A	-4.59	112.15	123.63
14	A	1114	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
14	k	1401	CLA	C1D-ND-C4D	-4.59	103.09	106.31
14	A	1125	CLA	C1-C2-C3	-4.59	118.68	126.20
14	U	1502	CLA	C4A-NA-C1A	4.59	108.77	106.68
14	l	1502	CLA	O2A-CGA-O1A	-4.59	112.16	123.63
14	B	1225	CLA	C3D-C2D-C1D	-4.58	99.57	105.83
14	a	1138	CLA	C2B-C1B-NB	4.58	115.08	110.33
14	a	1109	CLA	O2A-CGA-O1A	-4.58	112.16	123.63
15	H	1237	F6C	C1C-C2C-C3C	-4.58	101.57	106.82
14	H	1206	CLA	C2D-C1D-ND	4.58	114.66	110.13
14	H	1220	CLA	C1D-ND-C4D	-4.58	103.10	106.31
14	a	1135	CLA	O2A-CGA-O1A	-4.58	112.17	123.63
14	a	1122	CLA	C1C-C2C-C3C	-4.58	102.17	106.98
14	B	1218	CLA	C1D-ND-C4D	-4.58	103.10	106.31
18	I	4018	BCR	C4-C5-C6	-4.58	116.52	122.70
14	a	1118	CLA	C2D-C1D-ND	4.58	114.66	110.13
15	B	1207	F6C	C4A-C3A-C2A	-4.58	100.18	106.97
15	b	1207	F6C	C2D-C1D-ND	4.58	114.79	109.98
14	l	1502	CLA	C4A-NA-C1A	4.57	108.77	106.68
14	B	1219	CLA	C4A-NA-C1A	4.57	108.77	106.68
14	b	1206	CLA	C2D-C1D-ND	4.57	114.65	110.13
14	A	1119	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
15	b	1237	F6C	C1C-C2C-C3C	-4.57	101.58	106.82
14	A	1130	CLA	O2A-CGA-O1A	-4.57	112.19	123.63
14	a	1102	CLA	C2B-C1B-NB	4.57	115.07	110.33
14	A	1130	CLA	C2D-C1D-ND	4.57	114.65	110.13
14	H	1218	CLA	C1D-ND-C4D	-4.57	103.11	106.31
14	b	1211	CLA	C1D-ND-C4D	-4.57	103.11	106.31
14	G	1126	CLA	C2B-C1B-NB	4.57	115.06	110.33
14	b	1219	CLA	C4A-NA-C1A	4.57	108.76	106.68
14	G	1138	CLA	C2D-C1D-ND	4.57	114.65	110.13
14	K	1401	CLA	C1D-ND-C4D	-4.57	103.11	106.31
14	A	1135	CLA	O2A-CGA-O1A	-4.57	112.21	123.63
14	a	1126	CLA	C2D-C1D-ND	4.56	114.64	110.13
18	i	4018	BCR	C4-C5-C6	-4.56	116.54	122.70
14	b	1216	CLA	C4A-NA-C1A	4.56	108.76	106.68
14	G	1135	CLA	O2A-CGA-O1A	-4.56	112.21	123.63
18	l	4022	BCR	C33-C5-C6	-4.56	119.50	124.48
14	A	1129	CLA	C3D-C2D-C1D	-4.56	99.60	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1219	CLA	C4A-NA-C1A	4.56	108.76	106.68
18	R	4018	BCR	C4-C5-C6	-4.56	116.54	122.70
15	b	1207	F6C	C4A-C3A-C2A	-4.56	100.21	106.97
14	G	1113	CLA	C4A-NA-C1A	4.56	108.76	106.68
14	B	1206	CLA	C2D-C1D-ND	4.56	114.64	110.13
14	G	1103	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
14	a	1130	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
14	G	1130	CLA	O2A-CGA-O1A	-4.56	112.23	123.63
14	a	1107	CLA	C2D-C1D-ND	4.55	114.63	110.13
14	a	1113	CLA	C4A-NA-C1A	4.55	108.76	106.68
14	B	1223	CLA	C4A-NA-C1A	4.55	108.76	106.68
15	H	1207	F6C	C4A-C3A-C2A	-4.55	100.21	106.97
15	G	1121	F6C	C2D-C1D-ND	4.55	114.77	109.98
14	x	1701	CLA	C1C-C2C-C3C	-4.55	102.19	106.98
14	a	1119	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
14	b	1225	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
14	A	1138	CLA	C2B-C1B-NB	4.55	115.04	110.33
18	L	4022	BCR	C33-C5-C6	-4.55	119.52	124.48
14	a	1109	CLA	C1D-ND-C4D	-4.55	103.12	106.31
14	H	1220	CLA	C1-C2-C3	-4.55	118.75	126.20
14	G	1140	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
14	b	1023	CLA	C1D-ND-C4D	-4.55	103.12	106.31
14	A	1140	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
14	A	1120	CLA	O2A-CGA-O1A	-4.54	111.64	123.33
14	H	1225	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
14	b	1202	CLA	C1C-C2C-C3C	-4.54	102.20	106.98
14	A	1126	CLA	C2B-C1B-NB	4.54	115.04	110.33
14	A	1122	CLA	C1C-C2C-C3C	-4.54	102.20	106.98
14	B	1220	CLA	C1-C2-C3	-4.54	118.76	126.20
14	G	1119	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
14	U	1502	CLA	CHD-C1D-ND	-4.54	118.41	124.80
14	A	1137	CLA	C2D-C1D-ND	4.54	114.62	110.13
14	L	1502	CLA	CHD-C1D-ND	-4.54	118.41	124.80
14	G	1120	CLA	O2A-CGA-O1A	-4.54	111.66	123.33
14	A	1103	CLA	O2A-CGA-O1A	-4.54	112.28	123.63
14	H	1223	CLA	C4A-NA-C1A	4.54	108.75	106.68
14	a	1120	CLA	O2A-CGA-O1A	-4.54	111.66	123.33
14	B	1202	CLA	C1C-C2C-C3C	-4.54	102.21	106.98
14	A	1102	CLA	C2B-C1B-NB	4.54	115.03	110.33
14	A	1118	CLA	C2D-C1D-ND	4.53	114.61	110.13
14	A	1133	CLA	O2A-CGA-CBA	4.53	125.66	111.83
14	b	1220	CLA	C1-C2-C3	-4.53	118.77	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1103	CLA	O2A-CGA-O1A	-4.53	112.29	123.63
14	a	1133	CLA	O2A-CGA-CBA	4.53	125.66	111.83
14	G	1107	CLA	C2D-C1D-ND	4.53	114.61	110.13
14	G	1111	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	a	1132	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	A	1132	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	G	1118	CLA	C2D-C1D-ND	4.53	114.61	110.13
14	b	1218	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	B	1211	CLA	C1D-ND-C4D	-4.53	103.13	106.31
14	W	1701	CLA	C1C-C2C-C3C	-4.53	102.22	106.98
14	H	1214	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
14	a	1115	CLA	C1D-ND-C4D	-4.53	103.14	106.31
14	B	1228	CLA	C1D-ND-C4D	-4.53	103.14	106.31
14	a	1138	CLA	C2D-C1D-ND	4.53	114.61	110.13
14	H	1202	CLA	C1C-C2C-C3C	-4.52	102.22	106.98
14	G	1133	CLA	O2A-CGA-CBA	4.52	125.63	111.83
13	a	1011	CL0	CHA-C1A-C2A	-4.52	122.69	133.31
14	H	1204	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	B	1206	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
14	G	1137	CLA	C2D-C1D-ND	4.52	114.60	110.13
14	a	1103	CLA	C2D-C1D-ND	4.52	114.60	110.13
13	A	1011	CL0	CHA-C1A-C2A	-4.52	122.70	133.31
14	b	1214	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
14	H	1222	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	H	1228	CLA	C1D-ND-C4D	-4.52	103.14	106.31
14	A	1107	CLA	C2D-C1D-ND	4.51	114.59	110.13
14	b	1210	CLA	CAC-C3C-C4C	4.51	130.66	124.79
14	H	1206	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
14	a	1140	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
14	B	1214	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
14	B	1221	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
15	A	1121	F6C	C2D-C1D-ND	4.51	114.72	109.98
14	G	1102	CLA	C2B-C1B-NB	4.51	115.00	110.33
14	b	1206	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
14	l	1502	CLA	CHD-C1D-ND	-4.50	118.47	124.80
13	G	1011	CL0	CHA-C1A-C2A	-4.50	122.74	133.31
14	a	1126	CLA	C2B-C1B-NB	4.50	114.99	110.33
14	A	1109	CLA	C1D-ND-C4D	-4.50	103.16	106.31
14	A	1103	CLA	C2D-C1D-ND	4.50	114.58	110.13
14	H	1221	CLA	C1C-C2C-C3C	-4.50	102.25	106.98
14	a	1113	CLA	C1D-ND-C4D	-4.50	103.16	106.31
14	G	1135	CLA	C2D-C1D-ND	4.50	114.58	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1113	CLA	C1D-ND-C4D	-4.49	103.16	106.31
14	B	1210	CLA	CAC-C3C-C4C	4.49	130.64	124.79
14	B	1229	CLA	O2A-CGA-CBA	4.49	125.53	111.83
14	H	1229	CLA	O2A-CGA-CBA	4.49	125.53	111.83
14	G	1103	CLA	C2D-C1D-ND	4.49	114.57	110.13
14	B	1216	CLA	C4A-NA-C1A	4.49	108.73	106.68
14	G	1115	CLA	C1D-ND-C4D	-4.49	103.16	106.31
14	b	1204	CLA	C1D-ND-C4D	-4.49	103.16	106.31
14	G	1114	CLA	C4A-NA-C1A	4.49	108.73	106.68
14	G	1132	CLA	C1D-ND-C4D	-4.49	103.16	106.31
15	a	1121	F6C	C2D-C1D-ND	4.49	114.69	109.98
14	H	1210	CLA	CAC-C3C-C4C	4.49	130.63	124.79
14	G	1109	CLA	C1D-ND-C4D	-4.48	103.17	106.31
14	a	1135	CLA	C2D-C1D-ND	4.48	114.56	110.13
14	B	1210	CLA	O2A-C1-C2	4.48	125.35	108.11
14	a	1127	CLA	C1D-ND-C4D	-4.48	103.17	106.31
14	H	1210	CLA	O2A-C1-C2	4.48	125.34	108.11
14	A	1127	CLA	C1D-ND-C4D	-4.48	103.17	106.31
14	b	1210	CLA	O2A-C1-C2	4.47	125.33	108.11
14	a	1105	CLA	C1D-ND-C4D	-4.47	103.17	106.31
14	H	1209	CLA	C1D-ND-C4D	-4.47	103.17	106.31
14	a	1111	CLA	C1D-ND-C4D	-4.47	103.17	106.31
14	A	1115	CLA	C1D-ND-C4D	-4.47	103.17	106.31
14	A	1111	CLA	C4A-NA-C1A	4.47	108.72	106.68
14	b	1229	CLA	O2A-CGA-CBA	4.47	125.46	111.83
14	G	1117	CLA	C2D-C1D-ND	4.47	114.55	110.13
14	B	1023	CLA	C1D-ND-C4D	-4.47	103.18	106.31
14	B	1222	CLA	C1D-ND-C4D	-4.47	103.18	106.31
14	b	1232	CLA	O2D-CGD-CBD	4.47	119.04	111.23
14	H	1023	CLA	C1D-ND-C4D	-4.46	103.18	106.31
14	A	1111	CLA	C1D-ND-C4D	-4.46	103.18	106.31
15	b	1237	F6C	O2A-CGA-O1A	-4.46	112.46	123.63
14	B	1210	CLA	C1D-ND-C4D	-4.46	103.18	106.31
14	b	1221	CLA	C1C-C2C-C3C	-4.46	102.29	106.98
14	G	1127	CLA	C1D-ND-C4D	-4.46	103.18	106.31
14	b	1228	CLA	C1D-ND-C4D	-4.46	103.18	106.31
18	a	4008	BCR	C7-C8-C9	-4.46	119.64	126.23
15	H	1237	F6C	O2A-CGA-O1A	-4.46	112.47	123.63
15	B	1237	F6C	O2A-CGA-O1A	-4.46	112.47	123.63
14	B	1232	CLA	O2D-CGD-CBD	4.46	119.03	111.23
14	A	1135	CLA	C2D-C1D-ND	4.46	114.54	110.13
18	G	4008	BCR	C7-C8-C9	-4.46	119.64	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1105	CLA	C1D-ND-C4D	-4.46	103.19	106.31
18	A	4011	BCR	C24-C23-C22	-4.46	119.64	126.23
14	H	1210	CLA	C1C-C2C-C3C	-4.45	102.30	106.98
14	G	1111	CLA	C4A-NA-C1A	4.45	108.71	106.68
14	G	1113	CLA	C1D-ND-C4D	-4.45	103.19	106.31
14	B	1201	CLA	C2D-C1D-ND	4.44	114.52	110.13
14	b	1223	CLA	C4A-NA-C1A	4.44	108.70	106.68
14	b	1201	CLA	C2D-C1D-ND	4.44	114.52	110.13
14	A	1116	CLA	C4A-NA-C1A	4.44	108.70	106.68
14	A	1108	CLA	C2B-C1B-NB	4.44	114.93	110.33
14	l	1503	CLA	O2A-CGA-O1A	-4.44	112.53	123.63
14	b	1226	CLA	O2A-CGA-CBA	4.44	125.36	111.83
14	H	1232	CLA	O2D-CGD-CBD	4.43	118.98	111.23
14	G	1105	CLA	C1D-ND-C4D	-4.43	103.20	106.31
14	H	1233	CLA	C1D-ND-C4D	-4.43	103.20	106.31
14	a	1108	CLA	C2B-C1B-NB	4.43	114.92	110.33
14	B	1204	CLA	C1D-ND-C4D	-4.43	103.20	106.31
14	B	1209	CLA	C1D-ND-C4D	-4.43	103.20	106.31
18	G	4003	BCR	C7-C8-C9	-4.43	119.68	126.23
14	b	1234	CLA	O2A-CGA-CBA	4.43	125.35	111.83
14	a	1124	CLA	C2B-C1B-NB	4.43	114.92	110.33
18	G	4011	BCR	C24-C23-C22	-4.43	119.68	126.23
14	G	1124	CLA	C2B-C1B-NB	4.43	114.92	110.33
14	L	1503	CLA	O2A-CGA-O1A	-4.43	112.55	123.63
14	H	1234	CLA	O2A-CGA-CBA	4.42	125.33	111.83
14	H	1226	CLA	O2A-CGA-CBA	4.42	125.32	111.83
14	U	1503	CLA	O2A-CGA-O1A	-4.42	112.56	123.63
14	H	1201	CLA	C2D-C1D-ND	4.42	114.50	110.13
14	b	1210	CLA	C1D-ND-C4D	-4.42	103.21	106.31
14	B	1226	CLA	O2A-CGA-CBA	4.42	125.32	111.83
14	a	1111	CLA	C4A-NA-C1A	4.42	108.69	106.68
14	A	1117	CLA	C2D-C1D-ND	4.42	114.50	110.13
14	H	1219	CLA	C1D-ND-C4D	-4.42	103.21	106.31
14	b	1219	CLA	C1D-ND-C4D	-4.42	103.21	106.31
18	H	4004	BCR	C3-C4-C5	-4.42	106.18	114.06
14	A	1113	CLA	C4A-NA-C1A	4.42	108.69	106.68
14	a	1013	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
18	a	4003	BCR	C7-C8-C9	-4.42	119.70	126.23
14	X	1701	CLA	C1D-ND-C4D	-4.42	103.21	106.31
18	A	4008	BCR	C7-C8-C9	-4.42	119.70	126.23
14	b	1210	CLA	C1-C2-C3	-4.41	118.96	126.20
14	a	1117	CLA	C2D-C1D-ND	4.41	114.49	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1210	CLA	C1-C2-C3	-4.41	118.97	126.20
14	G	1108	CLA	C2B-C1B-NB	4.41	114.90	110.33
14	B	1219	CLA	C1D-ND-C4D	-4.41	103.22	106.31
14	H	1210	CLA	C1D-ND-C4D	-4.41	103.22	106.31
18	a	4011	BCR	C24-C23-C22	-4.41	119.71	126.23
14	B	1210	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
14	b	1209	CLA	C1D-ND-C4D	-4.41	103.22	106.31
18	b	4004	BCR	C3-C4-C5	-4.40	106.20	114.06
14	B	1205	CLA	O2A-CGA-CBA	4.40	125.26	111.83
14	B	1210	CLA	C1-C2-C3	-4.40	118.98	126.20
14	A	1124	CLA	C2B-C1B-NB	4.40	114.89	110.33
14	A	1114	CLA	C4A-NA-C1A	4.40	108.69	106.68
14	B	1234	CLA	O2A-CGA-CBA	4.40	125.25	111.83
14	b	1233	CLA	C1D-ND-C4D	-4.40	103.22	106.31
14	B	1226	CLA	C2D-C1D-ND	4.40	114.48	110.13
14	H	1205	CLA	O2A-CGA-CBA	4.40	125.24	111.83
14	a	1114	CLA	C4A-NA-C1A	4.40	108.69	106.68
14	A	1131	CLA	C2D-C1D-ND	4.40	114.48	110.13
14	G	1013	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
14	b	1210	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
18	B	4004	BCR	C3-C4-C5	-4.39	106.22	114.06
15	B	1230	F6C	C4A-NA-C1A	4.39	109.39	106.31
14	G	1129	CLA	C2D-C1D-ND	4.39	114.47	110.13
14	H	1226	CLA	C2D-C1D-ND	4.39	114.47	110.13
14	W	1701	CLA	C1D-ND-C4D	-4.39	103.23	106.31
18	A	4003	BCR	C7-C8-C9	-4.39	119.74	126.23
14	b	1205	CLA	O2A-CGA-CBA	4.39	125.22	111.83
14	B	1235	CLA	O2A-CGA-CBA	4.39	125.21	111.83
14	a	1112	CLA	C2B-C1B-NB	4.39	114.87	110.33
14	a	1129	CLA	C2D-C1D-ND	4.39	114.47	110.13
14	G	1012	CLA	O2A-CGA-CBA	4.38	125.20	111.83
14	G	1125	CLA	O2A-CGA-CBA	4.38	125.20	111.83
14	A	1013	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
14	B	1229	CLA	CAA-C2A-C3A	-4.38	101.16	113.00
14	B	1234	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
14	A	1012	CLA	O2A-CGA-CBA	4.38	125.19	111.83
14	G	1125	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	H	1235	CLA	O2A-CGA-CBA	4.38	125.18	111.83
14	a	1135	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	a	1140	CLA	C1D-ND-C4D	-4.38	103.24	106.31
14	B	1213	CLA	O2A-C1-C2	4.38	124.95	108.11
18	m	4021	BCR	C15-C14-C13	-4.37	121.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1213	CLA	O2A-C1-C2	4.37	124.94	108.11
15	H	1230	F6C	C4A-NA-C1A	4.37	109.38	106.31
14	b	1226	CLA	C2D-C1D-ND	4.37	114.45	110.13
14	b	1234	CLA	C1C-C2C-C3C	-4.37	102.38	106.98
15	H	1237	F6C	C1-C2-C3	-4.37	119.03	126.20
14	G	1135	CLA	C1D-ND-C4D	-4.37	103.25	106.31
15	b	1230	F6C	C4A-NA-C1A	4.37	109.38	106.31
14	H	1229	CLA	CAA-C2A-C3A	-4.37	101.19	113.00
14	b	1229	CLA	CAA-C2A-C3A	-4.37	101.19	113.00
14	A	1134	CLA	C1D-ND-C4D	-4.37	103.25	106.31
15	B	1237	F6C	C1-C2-C3	-4.37	119.04	126.20
14	G	1131	CLA	C2D-C1D-ND	4.37	114.45	110.13
14	G	1112	CLA	C2B-C1B-NB	4.37	114.85	110.33
14	a	1012	CLA	O2A-CGA-CBA	4.37	125.15	111.83
14	A	1135	CLA	C1D-ND-C4D	-4.37	103.25	106.31
14	b	1213	CLA	O2A-C1-C2	4.37	124.91	108.11
14	B	1201	CLA	C2B-C1B-NB	4.36	114.85	110.33
14	a	1116	CLA	C4A-NA-C1A	4.36	108.67	106.68
14	A	1129	CLA	C2D-C1D-ND	4.36	114.44	110.13
15	A	1121	F6C	C3A-C4A-NA	4.36	114.44	110.13
14	a	1125	CLA	O2A-CGA-CBA	4.36	125.14	111.83
14	G	1129	CLA	C4A-NA-C1A	4.36	108.67	106.68
18	V	4021	BCR	C15-C14-C13	-4.36	121.16	127.28
14	B	1211	CLA	C1-O2A-CGA	4.36	127.20	116.65
14	b	1208	CLA	O2A-CGA-CBA	4.36	125.13	111.83
14	b	1235	CLA	O2A-CGA-CBA	4.36	125.12	111.83
14	A	1125	CLA	O2A-CGA-CBA	4.36	125.12	111.83
14	G	1116	CLA	C4A-NA-C1A	4.36	108.67	106.68
14	B	1233	CLA	C1D-ND-C4D	-4.36	103.25	106.31
14	a	1131	CLA	C2D-C1D-ND	4.36	114.44	110.13
14	H	1211	CLA	C1-O2A-CGA	4.36	127.19	116.65
14	H	1234	CLA	C1C-C2C-C3C	-4.35	102.40	106.98
15	a	1121	F6C	CMA-C3A-C4A	-4.35	117.06	124.73
14	b	1229	CLA	C4A-NA-C1A	4.35	108.67	106.68
14	A	1131	CLA	C4A-NA-C1A	4.35	108.67	106.68
14	a	1125	CLA	C1D-ND-C4D	-4.35	103.26	106.31
15	b	1237	F6C	C1-C2-C3	-4.35	119.07	126.20
14	B	1208	CLA	O2A-CGA-CBA	4.35	125.10	111.83
14	A	1112	CLA	C2B-C1B-NB	4.35	114.84	110.33
14	x	1701	CLA	C1D-ND-C4D	-4.35	103.26	106.31
14	b	1211	CLA	C1-O2A-CGA	4.35	127.17	116.65
14	H	1208	CLA	O2A-CGA-CBA	4.34	125.07	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	M	4021	BCR	C15-C14-C13	-4.34	121.19	127.28
18	H	4017	BCR	C38-C26-C25	-4.34	119.75	124.48
14	G	1136	CLA	C1D-ND-C4D	-4.33	103.27	106.31
14	b	1216	CLA	O2A-CGA-O1A	-4.33	112.79	123.63
14	a	1119	CLA	O2A-CGA-O1A	-4.33	112.79	123.63
14	a	1102	CLA	C2D-C1D-ND	4.33	114.41	110.13
14	B	1216	CLA	O2A-CGA-O1A	-4.33	112.80	123.63
15	b	1238	F6C	C2D-C1D-ND	4.33	114.53	109.98
14	a	1129	CLA	C4A-NA-C1A	4.33	108.65	106.68
15	G	1121	F6C	C3A-C4A-NA	4.33	114.41	110.13
15	a	1121	F6C	C3A-C4A-NA	4.33	114.41	110.13
14	G	1110	CLA	C4A-NA-C1A	4.32	108.65	106.68
14	A	1119	CLA	O2A-CGA-O1A	-4.32	112.81	123.63
14	G	1140	CLA	C1D-ND-C4D	-4.32	103.28	106.31
14	a	1128	CLA	O2A-CGA-CBA	4.32	125.02	111.83
15	H	1207	F6C	C1A-C2A-C3A	-4.32	102.42	106.97
14	H	1239	CLA	C1-C2-C3	-4.32	119.12	126.20
15	B	1238	F6C	C2D-C1D-ND	4.32	114.52	109.98
14	H	1216	CLA	O2A-CGA-O1A	-4.32	112.82	123.63
15	G	1121	F6C	CMA-C3A-C4A	-4.32	117.12	124.73
14	G	1119	CLA	O2A-CGA-O1A	-4.32	112.83	123.63
15	A	1121	F6C	CMA-C3A-C4A	-4.32	117.13	124.73
14	B	1203	CLA	CAA-C2A-C3A	-4.32	101.33	113.00
14	A	1128	CLA	O2A-CGA-CBA	4.32	124.99	111.83
15	b	1207	F6C	C4-C3-C5	4.31	122.72	115.23
14	b	1023	CLA	O2A-CGA-CBA	4.31	124.99	111.83
14	G	1131	CLA	C4A-NA-C1A	4.31	108.65	106.68
14	A	1140	CLA	C1D-ND-C4D	-4.31	103.29	106.31
14	A	1102	CLA	C2D-C1D-ND	4.31	114.39	110.13
14	G	1134	CLA	C1D-ND-C4D	-4.31	103.29	106.31
18	A	4001	BCR	C28-C27-C26	-4.30	106.38	114.06
18	b	4017	BCR	C38-C26-C25	-4.30	119.79	124.48
14	B	1239	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
14	b	1201	CLA	C2B-C1B-NB	4.30	114.79	110.33
20	B	5002	LMG	O7-C10-C11	4.30	120.78	111.48
14	H	1201	CLA	C2B-C1B-NB	4.30	114.78	110.33
18	G	4001	BCR	C28-C27-C26	-4.30	106.39	114.06
14	B	1023	CLA	O2A-CGA-CBA	4.30	124.94	111.83
15	B	1207	F6C	C4-C3-C5	4.30	122.69	115.23
14	H	1203	CLA	CAA-C2A-C3A	-4.30	101.39	113.00
18	a	4001	BCR	C28-C27-C26	-4.30	106.39	114.06
14	H	1022	CLA	C1D-ND-C4D	-4.30	103.30	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1207	F6C	C1A-C2A-C3A	-4.30	102.44	106.97
14	G	1102	CLA	C2D-C1D-ND	4.30	114.38	110.13
14	a	1119	CLA	C2D-C1D-ND	4.30	114.38	110.13
15	B	1207	F6C	C1A-C2A-C3A	-4.30	102.45	106.97
14	A	1125	CLA	C1D-ND-C4D	-4.30	103.30	106.31
20	b	5002	LMG	O7-C10-C11	4.30	120.77	111.48
15	H	1207	F6C	C4-C3-C5	4.29	122.68	115.23
14	b	1217	CLA	O2A-CGA-CBA	4.29	124.92	111.83
14	b	1239	CLA	C1-C2-C3	-4.29	119.16	126.20
14	B	1239	CLA	C1-C2-C3	-4.29	119.16	126.20
14	H	1023	CLA	O2A-CGA-CBA	4.29	124.92	111.83
15	H	1238	F6C	C2D-C1D-ND	4.29	114.49	109.98
14	b	1203	CLA	CAA-C2A-C3A	-4.29	101.41	113.00
14	a	1131	CLA	C4A-NA-C1A	4.29	108.64	106.68
14	H	1217	CLA	O2A-CGA-CBA	4.29	124.91	111.83
14	b	1225	CLA	C1D-ND-C4D	-4.29	103.30	106.31
14	G	1128	CLA	O2A-CGA-CBA	4.29	124.91	111.83
14	H	1225	CLA	O2A-CGA-CBA	4.29	124.91	111.83
18	B	4017	BCR	C38-C26-C25	-4.29	119.81	124.48
14	B	1225	CLA	O2A-CGA-CBA	4.28	124.90	111.83
14	a	1110	CLA	C4A-NA-C1A	4.28	108.63	106.68
14	B	1217	CLA	O2A-CGA-CBA	4.28	124.89	111.83
14	B	1022	CLA	C1D-ND-C4D	-4.28	103.31	106.31
14	B	1229	CLA	C4A-NA-C1A	4.28	108.63	106.68
20	H	5002	LMG	O7-C10-C11	4.28	120.74	111.48
14	b	1225	CLA	O2A-CGA-CBA	4.27	124.87	111.83
14	b	1239	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
15	B	1207	F6C	CMA-C3A-C4A	-4.27	117.20	124.73
14	G	1122	CLA	O2A-CGA-CBA	4.27	124.86	111.83
15	H	1207	F6C	CMA-C3A-C4A	-4.27	117.20	124.73
14	a	1138	CLA	O2A-CGA-O1A	-4.27	112.95	123.63
15	B	1238	F6C	O2A-C1-C2	4.27	124.53	108.11
14	b	1203	CLA	O2A-CGA-CBA	4.27	124.84	111.83
14	A	1136	CLA	C1D-ND-C4D	-4.26	103.32	106.31
15	b	1238	F6C	O2A-C1-C2	4.26	124.51	108.11
14	a	1129	CLA	C1D-ND-C4D	-4.26	103.32	106.31
15	b	1207	F6C	CMA-C3A-C4A	-4.26	117.22	124.73
14	G	1119	CLA	C2D-C1D-ND	4.26	114.34	110.13
14	A	1125	CLA	O2A-C1-C2	4.26	124.49	108.11
14	G	1125	CLA	O2A-C1-C2	4.26	124.49	108.11
14	a	1125	CLA	O2A-C1-C2	4.26	124.49	108.11
14	a	1134	CLA	C1D-ND-C4D	-4.26	103.33	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1136	CLA	C1D-ND-C4D	-4.26	103.33	106.31
14	A	1122	CLA	O2A-CGA-CBA	4.25	124.81	111.83
15	H	1238	F6C	O2A-C1-C2	4.25	124.48	108.11
14	a	1122	CLA	O2A-CGA-CBA	4.25	124.81	111.83
14	H	1223	CLA	C1D-ND-C4D	-4.25	103.33	106.31
14	A	1131	CLA	O2A-CGA-CBA	4.25	124.80	111.83
14	A	1133	CLA	O2A-C1-C2	4.25	124.47	108.11
14	B	1203	CLA	O2A-CGA-CBA	4.25	124.80	111.83
14	A	1138	CLA	O2A-CGA-O1A	-4.25	113.00	123.63
14	G	1130	CLA	C2B-C1B-NB	4.25	114.73	110.33
14	b	1023	CLA	C2B-C1B-NB	4.25	114.73	110.33
14	b	1208	CLA	C1D-ND-C4D	-4.25	103.33	106.31
14	A	1013	CLA	O2A-CGA-CBA	4.25	124.79	111.83
14	H	1225	CLA	C1D-ND-C4D	-4.25	103.33	106.31
14	A	1110	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	a	1133	CLA	C1-C2-C3	-4.24	119.24	126.20
14	B	1023	CLA	C2B-C1B-NB	4.24	114.73	110.33
14	G	1129	CLA	C1D-ND-C4D	-4.24	103.33	106.31
14	H	1203	CLA	O2A-CGA-CBA	4.24	124.78	111.83
14	G	1131	CLA	O2A-CGA-CBA	4.24	124.78	111.83
14	a	1133	CLA	O2A-C1-C2	4.24	124.44	108.11
14	a	1114	CLA	C2D-C1D-ND	4.24	114.33	110.13
14	a	1137	CLA	O2A-CGA-CBA	4.24	124.76	111.83
14	A	1119	CLA	C2D-C1D-ND	4.24	114.32	110.13
14	G	1133	CLA	O2A-C1-C2	4.24	124.42	108.11
14	a	1013	CLA	O2A-CGA-CBA	4.24	124.76	111.83
14	G	1124	CLA	O2A-C1-C2	4.24	124.41	108.11
14	A	1124	CLA	O2A-C1-C2	4.24	124.41	108.11
14	a	1130	CLA	C2B-C1B-NB	4.24	114.72	110.33
14	a	1131	CLA	O2A-CGA-CBA	4.24	124.75	111.83
14	a	1132	CLA	O2A-CGA-CBA	4.23	124.75	111.83
14	B	1213	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	G	1133	CLA	C1-C2-C3	-4.23	119.26	126.20
14	G	1013	CLA	O2A-CGA-CBA	4.23	124.74	111.83
14	U	1502	CLA	O2A-C1-C2	4.23	124.39	108.11
14	B	1214	CLA	C2D-C1D-ND	4.23	114.31	110.13
14	B	1210	CLA	C2B-C1B-NB	4.23	114.71	110.33
14	A	1129	CLA	C4A-NA-C1A	4.23	108.61	106.68
18	L	4019	BCR	C38-C26-C25	-4.23	119.87	124.48
14	L	1502	CLA	O2A-C1-C2	4.23	124.39	108.11
14	A	1132	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
14	a	1124	CLA	O2A-C1-C2	4.23	124.38	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1216	CLA	C1D-ND-C4D	-4.23	103.34	106.31
14	H	1239	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
14	A	1133	CLA	C1-C2-C3	-4.23	119.27	126.20
14	H	1201	CLA	O2A-CGA-CBA	4.23	124.72	111.83
14	l	1502	CLA	O2A-C1-C2	4.23	124.37	108.11
14	H	1213	CLA	C1D-ND-C4D	-4.23	103.35	106.31
14	H	1219	CLA	C2B-C1B-NB	4.23	114.71	110.33
18	G	4011	BCR	C38-C26-C25	-4.22	119.87	124.48
14	H	1023	CLA	C2B-C1B-NB	4.22	114.71	110.33
14	G	1132	CLA	O2D-CGD-O1D	-4.22	115.62	123.85
14	G	1137	CLA	O2A-CGA-CBA	4.22	124.71	111.83
14	G	1132	CLA	O2A-CGA-CBA	4.22	124.71	111.83
18	H	4017	BCR	C3-C4-C5	-4.22	106.53	114.06
14	H	1229	CLA	C4A-NA-C1A	4.22	108.61	106.68
18	B	4005	BCR	C38-C26-C25	-4.22	119.88	124.48
14	G	1138	CLA	O2A-CGA-O1A	-4.22	113.07	123.63
14	a	1132	CLA	O2D-CGD-O1D	-4.22	115.63	123.85
14	H	1208	CLA	C1D-ND-C4D	-4.22	103.35	106.31
14	B	1223	CLA	C1D-ND-C4D	-4.22	103.35	106.31
18	H	4005	BCR	C38-C26-C25	-4.22	119.88	124.48
14	a	1104	CLA	O2A-CGA-CBA	4.22	124.69	111.83
14	b	1213	CLA	O2A-CGA-CBA	4.22	124.69	111.83
14	A	1103	CLA	C1-C2-C3	-4.22	119.29	126.20
14	B	1201	CLA	O2A-CGA-CBA	4.21	124.69	111.83
14	l	1502	CLA	C1-C2-C3	-4.21	119.29	126.20
14	L	1502	CLA	C1-C2-C3	-4.21	119.29	126.20
14	A	1114	CLA	C2D-C1D-ND	4.21	114.30	110.13
14	A	1104	CLA	O2A-CGA-CBA	4.21	124.68	111.83
14	B	1213	CLA	O2A-CGA-CBA	4.21	124.68	111.83
14	A	1130	CLA	C2B-C1B-NB	4.21	114.69	110.33
14	G	1103	CLA	C1-C2-C3	-4.21	119.30	126.20
18	A	4011	BCR	C38-C26-C25	-4.21	119.89	124.48
14	G	1104	CLA	O2A-CGA-CBA	4.21	124.67	111.83
14	A	1132	CLA	O2A-CGA-CBA	4.21	124.67	111.83
14	A	1137	CLA	O2A-CGA-CBA	4.21	124.67	111.83
14	A	1126	CLA	C1D-ND-C4D	-4.21	103.36	106.31
14	A	1117	CLA	O2A-CGA-O1A	-4.21	113.10	123.63
18	a	4011	BCR	C38-C26-C25	-4.21	119.89	124.48
18	B	4017	BCR	C3-C4-C5	-4.21	106.56	114.06
14	H	1210	CLA	C2B-C1B-NB	4.21	114.69	110.33
15	B	1207	F6C	C4A-NA-C1A	4.21	109.26	106.31
14	B	1225	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	l	4019	BCR	C38-C26-C25	-4.20	119.90	124.48
14	a	1129	CLA	O2A-CGA-CBA	4.20	124.65	111.83
14	B	1221	CLA	O2A-C1-C2	4.20	124.28	108.11
14	U	1502	CLA	C1-C2-C3	-4.20	119.31	126.20
14	G	1117	CLA	O2A-CGA-O1A	-4.20	113.12	123.63
14	G	1126	CLA	C1D-ND-C4D	-4.20	103.36	106.31
15	H	1207	F6C	C4A-NA-C1A	4.20	109.26	106.31
14	b	1201	CLA	O2A-CGA-CBA	4.20	124.64	111.83
18	b	4017	BCR	C3-C4-C5	-4.20	106.57	114.06
18	U	4019	BCR	C38-C26-C25	-4.20	119.90	124.48
14	B	1227	CLA	C3D-C2D-C1D	-4.20	100.11	105.83
14	a	1117	CLA	O2A-CGA-O1A	-4.19	113.14	123.63
14	H	1214	CLA	O2A-CGA-CBA	4.19	124.62	111.83
14	b	1221	CLA	O2A-C1-C2	4.19	124.24	108.11
18	I	4018	BCR	C38-C26-C25	-4.19	119.91	124.48
14	G	1129	CLA	O2A-CGA-CBA	4.19	124.62	111.83
14	B	1208	CLA	C1D-ND-C4D	-4.19	103.37	106.31
14	A	1139	CLA	C4A-NA-C1A	4.19	108.59	106.68
14	H	1213	CLA	O2A-CGA-CBA	4.19	124.61	111.83
14	b	1223	CLA	C1D-ND-C4D	-4.19	103.37	106.31
14	A	1129	CLA	O2A-CGA-CBA	4.19	124.60	111.83
14	H	1221	CLA	O2A-C1-C2	4.19	124.22	108.11
14	H	1235	CLA	C1D-ND-C4D	-4.19	103.38	106.31
14	b	1213	CLA	C1D-ND-C4D	-4.19	103.38	106.31
14	a	1131	CLA	O2A-C1-C2	4.19	124.22	108.11
14	B	1214	CLA	O2A-CGA-CBA	4.18	124.59	111.83
14	b	1225	CLA	O2A-C1-C2	4.18	124.20	108.11
14	A	1129	CLA	C1D-ND-C4D	-4.18	103.38	106.31
14	G	1131	CLA	O2A-C1-C2	4.18	124.20	108.11
14	H	1022	CLA	O2A-CGA-CBA	4.18	124.58	111.83
14	B	1225	CLA	O2A-C1-C2	4.18	124.19	108.11
14	b	1214	CLA	C2D-C1D-ND	4.18	114.26	110.13
14	b	1214	CLA	O2A-CGA-CBA	4.18	124.57	111.83
14	H	1214	CLA	C2D-C1D-ND	4.18	114.26	110.13
14	A	1131	CLA	O2A-C1-C2	4.18	124.18	108.11
14	H	1225	CLA	O2A-C1-C2	4.18	124.18	108.11
14	G	1114	CLA	C2D-C1D-ND	4.18	114.26	110.13
14	b	1022	CLA	C1D-ND-C4D	-4.17	103.38	106.31
14	a	1124	CLA	C1-C2-C3	-4.17	119.36	126.20
14	b	1227	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
14	b	1210	CLA	C4A-NA-C1A	4.17	108.58	106.68
18	B	4013	BCR	C7-C8-C9	-4.17	120.06	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1235	CLA	C1D-ND-C4D	-4.17	103.39	106.31
18	G	4002	BCR	C19-C18-C17	4.17	125.57	119.01
18	a	4002	BCR	C19-C18-C17	4.17	125.57	119.01
14	a	1103	CLA	C1-C2-C3	-4.17	119.37	126.20
14	b	1022	CLA	O2A-CGA-CBA	4.17	124.54	111.83
14	b	1216	CLA	C1D-ND-C4D	-4.17	103.39	106.31
14	L	1501	CLA	C1D-ND-C4D	-4.17	103.39	106.31
18	A	4002	BCR	C19-C18-C17	4.17	125.56	119.01
14	b	1210	CLA	C2B-C1B-NB	4.17	114.65	110.33
14	B	1022	CLA	O2A-CGA-CBA	4.17	124.54	111.83
14	a	1109	CLA	O2A-CGA-CBA	4.16	124.53	111.83
14	A	1124	CLA	C1-C2-C3	-4.16	119.37	126.20
14	G	1109	CLA	O2A-CGA-CBA	4.16	124.53	111.83
15	b	1238	F6C	C3D-C2D-C1D	-4.16	99.80	105.83
14	A	1109	CLA	O2A-CGA-CBA	4.16	124.53	111.83
15	B	1238	F6C	C3D-C2D-C1D	-4.16	99.80	105.83
14	H	1228	CLA	O2A-CGA-CBA	4.16	124.52	111.83
18	H	4013	BCR	C7-C8-C9	-4.16	120.08	126.23
15	b	1207	F6C	C4A-NA-C1A	4.16	109.23	106.31
14	b	1219	CLA	C2B-C1B-NB	4.16	114.64	110.33
14	G	1124	CLA	CHD-C1D-ND	-4.16	118.95	124.80
14	a	1126	CLA	C1D-ND-C4D	-4.16	103.39	106.31
14	B	1219	CLA	C2B-C1B-NB	4.16	114.64	110.33
14	A	1131	CLA	CHD-C1D-ND	-4.16	118.95	124.80
14	G	1131	CLA	CHD-C1D-ND	-4.16	118.95	124.80
14	B	1210	CLA	C4A-NA-C1A	4.16	108.58	106.68
15	H	1238	F6C	C3D-C2D-C1D	-4.15	99.81	105.83
14	H	1227	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
18	b	4013	BCR	C7-C8-C9	-4.15	120.09	126.23
14	a	1131	CLA	CHD-C1D-ND	-4.15	118.96	124.80
14	B	1228	CLA	O2A-CGA-CBA	4.15	124.49	111.83
18	b	4005	BCR	C38-C26-C25	-4.15	119.96	124.48
14	b	1228	CLA	O2A-CGA-CBA	4.15	124.48	111.83
14	G	1124	CLA	C1-C2-C3	-4.15	119.40	126.20
14	b	1235	CLA	C1D-ND-C4D	-4.14	103.41	106.31
14	H	1216	CLA	C1D-ND-C4D	-4.14	103.41	106.31
14	A	1108	CLA	C1D-ND-C4D	-4.14	103.41	106.31
18	B	4014	BCR	C33-C5-C6	-4.14	119.97	124.48
18	H	4009	BCR	C38-C26-C25	-4.13	119.97	124.48
18	b	4014	BCR	C33-C5-C6	-4.13	119.97	124.48
14	H	1210	CLA	C4A-NA-C1A	4.13	108.56	106.68
14	l	1501	CLA	C1D-ND-C4D	-4.13	103.42	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	4018	BCR	C38-C26-C25	-4.13	119.98	124.48
18	A	4011	BCR	C33-C5-C6	-4.13	119.98	124.48
16	b	2002	PQN	C14-C13-C15	4.13	122.39	115.23
14	A	1124	CLA	CHD-C1D-ND	-4.12	119.00	124.80
18	H	4014	BCR	C33-C5-C6	-4.12	119.98	124.48
14	b	1224	CLA	C1D-ND-C4D	-4.12	103.42	106.31
16	B	2002	PQN	C14-C13-C15	4.12	122.38	115.23
14	A	1111	CLA	O2A-CGA-CBA	4.12	124.39	111.83
14	a	1124	CLA	CHD-C1D-ND	-4.12	119.01	124.80
18	B	4009	BCR	C38-C26-C25	-4.12	119.99	124.48
13	G	1011	CL0	O2A-CGA-CBA	4.12	124.38	111.83
14	a	1139	CLA	C4A-NA-C1A	4.11	108.56	106.68
14	A	1103	CLA	CAA-C2A-C3A	-4.11	101.88	113.00
16	H	2002	PQN	C14-C13-C15	4.11	122.37	115.23
14	a	1103	CLA	CAA-C2A-C3A	-4.11	101.89	113.00
13	a	1011	CL0	O2A-CGA-CBA	4.11	124.37	111.83
18	b	4009	BCR	C38-C26-C25	-4.11	120.00	124.48
14	A	1128	CLA	C1-C2-C3	-4.11	119.47	126.20
18	G	4011	BCR	C3-C4-C5	-4.11	106.73	114.06
14	a	1013	CLA	C2C-C1C-NC	4.11	114.30	109.98
14	G	1111	CLA	O2A-CGA-CBA	4.11	124.36	111.83
14	G	1133	CLA	C1D-ND-C4D	-4.11	103.43	106.31
14	A	1116	CLA	C1D-ND-C4D	-4.11	103.43	106.31
14	B	1224	CLA	C1D-ND-C4D	-4.11	103.43	106.31
18	a	4011	BCR	C3-C4-C5	-4.10	106.74	114.06
14	A	1140	CLA	O2A-CGA-CBA	4.10	124.35	111.83
14	H	1205	CLA	C1D-ND-C4D	-4.10	103.43	106.31
18	A	4011	BCR	C3-C4-C5	-4.10	106.74	114.06
14	a	1140	CLA	O2A-CGA-CBA	4.10	124.34	111.83
14	G	1103	CLA	CAA-C2A-C3A	-4.10	101.92	113.00
18	a	4011	BCR	C33-C5-C6	-4.10	120.01	124.48
14	G	1140	CLA	O2A-CGA-CBA	4.10	124.33	111.83
14	G	1013	CLA	C2C-C1C-NC	4.10	114.29	109.98
14	U	1501	CLA	C1D-ND-C4D	-4.10	103.44	106.31
13	A	1011	CL0	O2A-CGA-CBA	4.10	124.33	111.83
18	i	4018	BCR	C38-C26-C25	-4.10	120.02	124.48
14	G	1109	CLA	O2A-C1-C2	4.09	123.86	108.11
14	a	1111	CLA	O2A-CGA-CBA	4.09	124.31	111.83
18	G	4011	BCR	C33-C5-C6	-4.09	120.02	124.48
14	A	1109	CLA	O2A-C1-C2	4.09	123.85	108.11
14	X	1701	CLA	O2A-CGA-CBA	4.09	124.31	111.83
14	B	1205	CLA	C1D-ND-C4D	-4.09	103.44	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1013	CLA	C2C-C1C-NC	4.09	114.27	109.98
14	x	1701	CLA	O2A-CGA-CBA	4.09	124.29	111.83
14	A	1133	CLA	C1D-ND-C4D	-4.09	103.44	106.31
14	a	1109	CLA	O2A-C1-C2	4.08	123.83	108.11
14	G	1128	CLA	C1-C2-C3	-4.08	119.51	126.20
14	G	1117	CLA	C2B-C1B-NB	4.08	114.56	110.33
14	H	1222	CLA	C2B-C1B-NB	4.08	114.56	110.33
14	W	1701	CLA	O2A-CGA-CBA	4.08	124.26	111.83
14	A	1127	CLA	O2A-CGA-CBA	4.08	124.26	111.83
14	G	1108	CLA	C1D-ND-C4D	-4.07	103.45	106.31
14	H	1224	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	G	1118	CLA	O2A-CGA-CBA	4.07	124.25	111.83
14	G	1122	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	A	1122	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	a	1116	CLA	C2B-C1B-NB	4.07	114.55	110.33
14	a	1108	CLA	C1D-ND-C4D	-4.07	103.46	106.31
14	G	1127	CLA	O2A-CGA-CBA	4.07	124.24	111.83
14	A	1113	CLA	C2B-C1B-NB	4.07	114.54	110.33
14	b	1224	CLA	C1-C2-C3	-4.07	119.53	126.20
14	G	1139	CLA	C4A-NA-C1A	4.06	108.53	106.68
14	b	1222	CLA	C2B-C1B-NB	4.06	114.54	110.33
14	A	1137	CLA	O2D-CGD-O1D	-4.06	115.94	123.85
14	A	1118	CLA	O2A-CGA-CBA	4.06	124.22	111.83
14	a	1122	CLA	C1D-ND-C4D	-4.06	103.46	106.31
14	G	1106	CLA	C2B-C1B-NB	4.06	114.53	110.33
14	a	1106	CLA	C2B-C1B-NB	4.06	114.53	110.33
14	B	1235	CLA	C2B-C1B-NB	4.06	114.53	110.33
14	A	1123	CLA	O2A-CGA-CBA	4.06	124.21	111.83
14	A	1117	CLA	C2B-C1B-NB	4.06	114.53	110.33
14	b	1205	CLA	C1D-ND-C4D	-4.06	103.47	106.31
14	G	1113	CLA	C2B-C1B-NB	4.05	114.53	110.33
14	a	1128	CLA	C1-C2-C3	-4.05	119.55	126.20
14	a	1127	CLA	O2A-CGA-CBA	4.05	124.20	111.83
14	G	1116	CLA	C1D-ND-C4D	-4.05	103.47	106.31
13	G	1011	CL0	C1C-CHC-C4B	4.05	130.56	116.07
13	a	1011	CL0	C1C-CHC-C4B	4.05	130.56	116.07
15	b	1237	F6C	CMA-C3A-C4A	-4.05	117.60	124.73
14	H	1224	CLA	O2A-CGA-CBA	4.05	124.18	111.83
14	a	1118	CLA	O2A-CGA-CBA	4.05	124.18	111.83
14	G	1103	CLA	C1D-ND-C4D	-4.05	103.47	106.31
14	b	1224	CLA	O2A-CGA-CBA	4.05	124.17	111.83
15	B	1237	F6C	CMA-C3A-C4A	-4.05	117.60	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1116	CLA	C2B-C1B-NB	4.04	114.52	110.33
14	B	1224	CLA	O2A-CGA-CBA	4.04	124.17	111.83
13	A	1011	CL0	C1C-CHC-C4B	4.04	130.54	116.07
14	a	1103	CLA	C1D-ND-C4D	-4.04	103.48	106.31
14	B	1221	CLA	C1D-ND-C4D	-4.04	103.48	106.31
13	A	1011	CL0	C1-C2-C3	-4.04	119.58	126.20
14	G	1123	CLA	O2A-CGA-CBA	4.04	124.16	111.83
13	a	1011	CL0	C1-C2-C3	-4.04	119.58	126.20
14	B	1224	CLA	C1-C2-C3	-4.04	119.58	126.20
14	A	1103	CLA	C1D-ND-C4D	-4.04	103.48	106.31
14	H	1224	CLA	C1-C2-C3	-4.04	119.58	126.20
14	a	1137	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
14	a	1133	CLA	C1D-ND-C4D	-4.04	103.48	106.31
14	G	1103	CLA	O2A-CGA-CBA	4.04	124.14	111.83
14	G	1137	CLA	O2D-CGD-O1D	-4.03	115.99	123.85
18	b	4010	BCR	C3-C4-C5	-4.03	106.86	114.06
14	a	1111	CLA	C2B-C1B-NB	4.03	114.51	110.33
14	a	1117	CLA	C2B-C1B-NB	4.03	114.51	110.33
15	H	1237	F6C	CMA-C3A-C4A	-4.03	117.63	124.73
14	a	1113	CLA	C2B-C1B-NB	4.03	114.50	110.33
14	a	1118	CLA	C1D-ND-C4D	-4.03	103.49	106.31
18	B	4010	BCR	C3-C4-C5	-4.03	106.87	114.06
14	a	1123	CLA	O2A-CGA-CBA	4.02	124.11	111.83
14	G	1111	CLA	C2B-C1B-NB	4.02	114.50	110.33
14	A	1111	CLA	C2B-C1B-NB	4.02	114.50	110.33
14	b	1232	CLA	C1D-ND-C4D	-4.02	103.49	106.31
14	a	1103	CLA	O2A-CGA-CBA	4.02	124.10	111.83
13	G	1011	CL0	C1-C2-C3	-4.02	119.61	126.20
14	A	1115	CLA	C1-C2-C3	-4.02	119.61	126.20
14	a	1115	CLA	C1-C2-C3	-4.02	119.61	126.20
14	a	1116	CLA	C1D-ND-C4D	-4.02	103.49	106.31
14	A	1103	CLA	O2A-CGA-CBA	4.02	124.08	111.83
14	a	1102	CLA	O2A-C1-C2	4.01	123.53	108.11
14	b	1211	CLA	C2B-C1B-NB	4.01	114.48	110.33
14	A	1102	CLA	O2A-C1-C2	4.01	123.53	108.11
14	H	1228	CLA	CHD-C1D-ND	-4.00	119.17	124.80
14	G	1115	CLA	C1-C2-C3	-4.00	119.64	126.20
14	G	1116	CLA	C2B-C1B-NB	4.00	114.48	110.33
14	B	1228	CLA	CHD-C1D-ND	-4.00	119.17	124.80
14	a	1107	CLA	C1D-ND-C4D	-4.00	103.50	106.31
14	H	1211	CLA	C2B-C1B-NB	4.00	114.48	110.33
14	B	1222	CLA	C2B-C1B-NB	4.00	114.47	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1232	CLA	C1D-ND-C4D	-4.00	103.50	106.31
14	G	1102	CLA	O2A-C1-C2	4.00	123.50	108.11
14	H	1203	CLA	O2A-C1-C2	4.00	123.50	108.11
14	B	1203	CLA	O2A-C1-C2	4.00	123.49	108.11
14	H	1235	CLA	C2B-C1B-NB	4.00	114.47	110.33
14	b	1235	CLA	C2B-C1B-NB	4.00	114.47	110.33
18	H	4010	BCR	C3-C4-C5	-3.99	106.93	114.06
14	A	1137	CLA	C1D-ND-C4D	-3.99	103.51	106.31
14	A	1106	CLA	C2B-C1B-NB	3.99	114.47	110.33
14	G	1104	CLA	CHD-C1D-ND	-3.99	119.18	124.80
14	b	1203	CLA	O2A-C1-C2	3.99	123.47	108.11
18	G	4007	BCR	C38-C26-C25	-3.99	120.13	124.48
14	G	1118	CLA	C1D-ND-C4D	-3.99	103.51	106.31
14	b	1228	CLA	CHD-C1D-ND	-3.99	119.19	124.80
14	A	1013	CLA	O2A-C1-C2	3.98	123.43	108.11
14	b	1221	CLA	C1D-ND-C4D	-3.98	103.52	106.31
14	B	1204	CLA	C2B-C1B-NB	3.98	114.45	110.33
14	B	1229	CLA	C2B-C1B-NB	3.98	114.45	110.33
14	b	1203	CLA	C1-C2-C3	-3.98	119.67	126.20
14	G	1013	CLA	O2A-C1-C2	3.98	123.42	108.11
14	a	1115	CLA	O2A-CGA-CBA	3.98	123.97	111.83
14	a	1013	CLA	O2A-C1-C2	3.98	123.42	108.11
14	A	1115	CLA	O2A-CGA-CBA	3.98	123.96	111.83
14	b	1204	CLA	C2B-C1B-NB	3.98	114.45	110.33
14	H	1232	CLA	C1D-ND-C4D	-3.98	103.52	106.31
14	G	1107	CLA	C1D-ND-C4D	-3.97	103.52	106.31
14	G	1115	CLA	O2A-CGA-CBA	3.97	123.94	111.83
14	H	1210	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
14	A	1104	CLA	CHD-C1D-ND	-3.97	119.22	124.80
14	a	1012	CLA	O2A-C1-C2	3.97	123.38	108.11
14	H	1204	CLA	C2B-C1B-NB	3.97	114.44	110.33
18	b	4013	BCR	C33-C5-C6	-3.96	120.16	124.48
14	b	1210	CLA	O2D-CGD-O1D	-3.96	116.13	123.85
18	a	4007	BCR	C38-C26-C25	-3.96	120.16	124.48
18	A	4007	BCR	C38-C26-C25	-3.96	120.16	124.48
14	A	1107	CLA	C1D-ND-C4D	-3.96	103.53	106.31
14	A	1012	CLA	O2A-C1-C2	3.96	123.36	108.11
14	G	1112	CLA	C1D-ND-C4D	-3.96	103.53	106.31
14	B	1211	CLA	C2B-C1B-NB	3.96	114.43	110.33
14	b	1204	CLA	CHD-C1D-ND	-3.96	119.23	124.80
14	A	1116	CLA	O2A-C1-C2	3.96	123.34	108.11
14	a	1104	CLA	CHD-C1D-ND	-3.96	119.23	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1012	CLA	O2A-C1-C2	3.96	123.33	108.11
14	G	1136	CLA	C2B-C1B-NB	3.96	114.43	110.33
14	a	1137	CLA	C1D-ND-C4D	-3.96	103.54	106.31
14	B	1211	CLA	O2A-CGA-O1A	-3.96	113.73	123.63
15	H	1238	F6C	C1-C2-C3	-3.95	119.72	126.20
14	A	1136	CLA	C2B-C1B-NB	3.95	114.42	110.33
15	B	1238	F6C	C1-C2-C3	-3.95	119.72	126.20
14	W	1701	CLA	C1-C2-C3	-3.95	119.73	126.20
14	x	1701	CLA	C1-C2-C3	-3.95	119.73	126.20
14	H	1221	CLA	C1D-ND-C4D	-3.95	103.54	106.31
14	H	1239	CLA	C1D-ND-C4D	-3.95	103.54	106.31
14	H	1211	CLA	O2A-CGA-O1A	-3.95	113.75	123.63
14	b	1223	CLA	C2B-C1B-NB	3.95	114.42	110.33
18	A	4003	BCR	C28-C27-C26	-3.95	107.02	114.06
14	b	1214	CLA	C4A-NA-C1A	3.95	108.48	106.68
14	G	1116	CLA	O2A-C1-C2	3.95	123.30	108.11
15	b	1238	F6C	C1-C2-C3	-3.95	119.73	126.20
18	B	4013	BCR	C33-C5-C6	-3.95	120.18	124.48
14	b	1211	CLA	O2A-CGA-O1A	-3.95	113.76	123.63
14	a	1116	CLA	O2A-C1-C2	3.94	123.29	108.11
15	H	1207	F6C	CHB-C4A-C3A	-3.94	117.28	125.49
14	G	1126	CLA	O2A-CGA-CBA	3.94	123.86	111.83
15	B	1207	F6C	CHB-C4A-C3A	-3.94	117.29	125.49
14	A	1126	CLA	O2A-CGA-CBA	3.94	123.85	111.83
14	H	1204	CLA	CHD-C1D-ND	-3.94	119.26	124.80
14	a	1136	CLA	C2B-C1B-NB	3.94	114.41	110.33
14	H	1221	CLA	O2A-CGA-CBA	3.94	123.85	111.83
14	a	1126	CLA	O2A-CGA-CBA	3.94	123.85	111.83
14	b	1221	CLA	O2A-CGA-CBA	3.94	123.84	111.83
18	H	4013	BCR	C33-C5-C6	-3.94	120.19	124.48
14	A	1132	CLA	C1-C2-C3	-3.94	119.75	126.20
14	B	1203	CLA	C1-C2-C3	-3.94	119.75	126.20
14	B	1221	CLA	O2A-CGA-CBA	3.93	123.83	111.83
14	X	1701	CLA	C1-C2-C3	-3.93	119.75	126.20
14	G	1123	CLA	C1D-ND-C4D	-3.93	103.55	106.31
14	B	1239	CLA	C1D-ND-C4D	-3.93	103.55	106.31
18	I	4020	BCR	C38-C26-C25	-3.93	120.19	124.48
14	G	1132	CLA	C1-C2-C3	-3.93	119.76	126.20
14	G	1105	CLA	C2B-C1B-NB	3.93	114.40	110.33
14	A	1123	CLA	C1D-ND-C4D	-3.93	103.56	106.31
14	B	1204	CLA	CHD-C1D-ND	-3.93	119.28	124.80
14	B	1210	CLA	O2D-CGD-O1D	-3.93	116.21	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1207	F6C	CHB-C4A-C3A	-3.92	117.32	125.49
14	A	1118	CLA	C1D-ND-C4D	-3.92	103.56	106.31
14	A	1105	CLA	C2B-C1B-NB	3.92	114.39	110.33
18	a	4003	BCR	C28-C27-C26	-3.92	107.07	114.06
14	H	1203	CLA	C1-C2-C3	-3.92	119.78	126.20
18	G	4003	BCR	C28-C27-C26	-3.92	107.07	114.06
14	H	1229	CLA	C2B-C1B-NB	3.92	114.39	110.33
14	b	1215	CLA	O2A-CGA-O1A	-3.91	113.84	123.63
14	B	1215	CLA	CHD-C1D-ND	-3.91	119.29	124.80
14	b	1239	CLA	C1D-ND-C4D	-3.91	103.57	106.31
14	H	1227	CLA	C4A-NA-C1A	3.91	108.46	106.68
18	G	4002	BCR	C34-C9-C10	-3.91	116.48	122.82
14	X	1701	CLA	O2A-C1-C2	3.91	123.15	108.11
14	b	1223	CLA	O2A-CGA-CBA	3.91	123.75	111.83
14	H	1215	CLA	O2A-CGA-O1A	-3.91	113.85	123.63
18	R	4020	BCR	C38-C26-C25	-3.91	120.22	124.48
14	B	1216	CLA	C2B-C1B-NB	3.91	114.38	110.33
18	a	4002	BCR	C34-C9-C10	-3.91	116.49	122.82
14	H	1216	CLA	C2B-C1B-NB	3.91	114.38	110.33
14	H	1223	CLA	C2B-C1B-NB	3.91	114.38	110.33
14	G	1129	CLA	O2D-CGD-O1D	-3.91	116.25	123.85
14	x	1701	CLA	O2A-C1-C2	3.91	123.14	108.11
14	H	1215	CLA	CHD-C1D-ND	-3.91	119.31	124.80
14	b	1216	CLA	C2B-C1B-NB	3.90	114.38	110.33
14	W	1701	CLA	O2A-C1-C2	3.90	123.12	108.11
14	B	1215	CLA	O2A-CGA-O1A	-3.90	113.87	123.63
14	H	1223	CLA	O2A-CGA-CBA	3.90	123.73	111.83
14	b	1215	CLA	CHD-C1D-ND	-3.90	119.31	124.80
14	b	1214	CLA	C1-C2-C3	-3.90	119.81	126.20
14	a	1129	CLA	O2D-CGD-O1D	-3.90	116.26	123.85
14	B	1223	CLA	C2B-C1B-NB	3.89	114.36	110.33
14	H	1214	CLA	C1-C2-C3	-3.89	119.82	126.20
14	B	1223	CLA	O2A-CGA-CBA	3.89	123.71	111.83
18	a	4001	BCR	C15-C14-C13	-3.89	121.82	127.28
14	G	1136	CLA	CHD-C1D-ND	-3.89	119.33	124.80
18	A	4002	BCR	C34-C9-C10	-3.89	116.51	122.82
14	a	1132	CLA	C1-C2-C3	-3.89	119.82	126.20
14	H	1209	CLA	C4A-NA-C1A	3.89	108.45	106.68
18	G	4008	BCR	C15-C14-C13	-3.89	121.82	127.28
14	H	1223	CLA	C1-C2-C3	-3.89	119.83	126.20
14	B	1214	CLA	C1-C2-C3	-3.89	119.83	126.20
14	H	1213	CLA	C2B-C1B-NB	3.89	114.36	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1136	CLA	CHD-C1D-ND	-3.89	119.33	124.80
18	i	4020	BCR	C38-C26-C25	-3.88	120.25	124.48
14	B	1213	CLA	C2B-C1B-NB	3.88	114.35	110.33
14	a	1136	CLA	CHD-C1D-ND	-3.88	119.34	124.80
18	B	4006	BCR	C24-C23-C22	-3.88	120.49	126.23
14	b	1223	CLA	C1-C2-C3	-3.88	119.84	126.20
14	a	1112	CLA	C1D-ND-C4D	-3.88	103.59	106.31
18	A	4008	BCR	C15-C14-C13	-3.88	121.83	127.28
14	A	1129	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
14	b	1229	CLA	C2B-C1B-NB	3.88	114.35	110.33
14	a	1123	CLA	C1D-ND-C4D	-3.87	103.59	106.31
14	B	1223	CLA	C1-C2-C3	-3.87	119.85	126.20
14	b	1227	CLA	C4A-NA-C1A	3.87	108.45	106.68
14	B	1227	CLA	C4A-NA-C1A	3.87	108.45	106.68
14	a	1105	CLA	C2B-C1B-NB	3.87	114.34	110.33
14	A	1115	CLA	C2B-C1B-NB	3.87	114.34	110.33
14	G	1137	CLA	C1D-ND-C4D	-3.87	103.59	106.31
14	A	1112	CLA	C1D-ND-C4D	-3.87	103.59	106.31
14	a	1115	CLA	C2B-C1B-NB	3.87	114.34	110.33
14	b	1213	CLA	C2B-C1B-NB	3.87	114.34	110.33
18	G	4001	BCR	C15-C14-C13	-3.87	121.85	127.28
14	G	1012	CLA	C4A-NA-C1A	3.87	108.44	106.68
14	l	1503	CLA	O2A-CGA-CBA	3.87	123.63	111.83
14	A	1116	CLA	O2A-CGA-CBA	3.87	123.63	111.83
14	G	1105	CLA	CHD-C1D-ND	-3.87	119.36	124.80
14	A	1105	CLA	CHD-C1D-ND	-3.86	119.36	124.80
14	H	1220	CLA	O2A-CGA-CBA	3.86	123.62	111.83
14	B	1220	CLA	O2A-CGA-CBA	3.86	123.62	111.83
14	G	1104	CLA	C1-C2-C3	-3.86	119.87	126.20
18	b	4006	BCR	C24-C23-C22	-3.86	120.52	126.23
14	H	1214	CLA	C4A-NA-C1A	3.86	108.44	106.68
14	L	1503	CLA	O2A-CGA-CBA	3.86	123.60	111.83
14	H	1239	CLA	O2A-CGA-CBA	3.86	123.60	111.83
18	a	4008	BCR	C15-C14-C13	-3.86	121.87	127.28
14	G	1116	CLA	O2A-CGA-CBA	3.86	123.60	111.83
18	H	4013	BCR	C38-C26-C25	-3.86	120.28	124.48
14	a	1012	CLA	C4A-NA-C1A	3.86	108.44	106.68
14	b	1226	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
14	a	1105	CLA	CHD-C1D-ND	-3.86	119.38	124.80
14	A	1104	CLA	C1-C2-C3	-3.85	119.88	126.20
14	H	1220	CLA	O2A-C1-C2	3.85	122.93	108.11
14	a	1104	CLA	C1-C2-C3	-3.85	119.89	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4006	BCR	C24-C23-C22	-3.85	120.54	126.23
14	b	1220	CLA	O2A-CGA-CBA	3.85	123.57	111.83
18	A	4001	BCR	C15-C14-C13	-3.85	121.88	127.28
14	G	1115	CLA	C2B-C1B-NB	3.85	114.32	110.33
14	a	1116	CLA	O2A-CGA-CBA	3.85	123.57	111.83
14	b	1239	CLA	O2A-CGA-CBA	3.85	123.56	111.83
15	b	1238	F6C	O2A-CGA-CBA	3.85	123.56	111.83
15	B	1238	F6C	O2A-CGA-CBA	3.85	123.56	111.83
14	B	1231	CLA	O2A-CGA-CBA	3.85	123.56	111.83
14	b	1220	CLA	O2A-C1-C2	3.85	122.91	108.11
14	b	1201	CLA	C1D-ND-C4D	-3.85	103.61	106.31
14	B	1201	CLA	C1D-ND-C4D	-3.85	103.61	106.31
14	b	1231	CLA	O2A-CGA-CBA	3.85	123.56	111.83
15	H	1238	F6C	O2A-CGA-CBA	3.84	123.56	111.83
15	b	1230	F6C	C4A-C3A-C2A	-3.84	101.27	106.97
14	H	1201	CLA	C1D-ND-C4D	-3.84	103.61	106.31
14	A	1131	CLA	C2B-C1B-NB	3.84	114.31	110.33
14	U	1503	CLA	O2A-CGA-CBA	3.84	123.55	111.83
14	B	1239	CLA	O2A-CGA-CBA	3.84	123.55	111.83
14	H	1208	CLA	C2B-C1B-NB	3.84	114.31	110.33
14	H	1231	CLA	O2A-CGA-CBA	3.84	123.53	111.83
14	a	1131	CLA	C2B-C1B-NB	3.84	114.31	110.33
14	B	1220	CLA	O2A-C1-C2	3.84	122.87	108.11
14	B	1209	CLA	C2B-C1B-NB	3.83	114.30	110.33
14	B	1214	CLA	C4A-NA-C1A	3.83	108.43	106.68
14	B	1208	CLA	C2B-C1B-NB	3.83	114.30	110.33
14	A	1134	CLA	C2B-C1B-NB	3.83	114.30	110.33
19	A	5001	LHG	O7-C7-C8	3.83	119.76	111.48
18	b	4013	BCR	C15-C14-C13	-3.82	121.92	127.28
18	B	4013	BCR	C38-C26-C25	-3.82	120.31	124.48
15	H	1230	F6C	C4A-C3A-C2A	-3.82	101.30	106.97
14	b	1222	CLA	O2A-C1-C2	3.82	122.81	108.11
19	a	5001	LHG	O7-C7-C8	3.82	119.74	111.48
14	G	1132	CLA	C2B-C1B-NB	3.82	114.29	110.33
14	B	1209	CLA	C4A-NA-C1A	3.82	108.42	106.68
14	a	1012	CLA	CHD-C1D-ND	-3.82	119.43	124.80
15	a	1121	F6C	C4A-C3A-C2A	-3.82	101.31	106.97
15	B	1230	F6C	C4A-C3A-C2A	-3.82	101.31	106.97
15	A	1121	F6C	C4A-C3A-C2A	-3.82	101.31	106.97
14	B	1220	CLA	CMA-C3A-C4A	3.81	122.03	111.77
14	H	1226	CLA	C3B-C2B-C1B	-3.81	102.67	107.17
14	G	1118	CLA	O2A-C1-C2	3.81	122.78	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1209	CLA	C2B-C1B-NB	3.81	114.28	110.33
14	B	1205	CLA	C2B-C1B-NB	3.81	114.28	110.33
14	b	1220	CLA	CMA-C3A-C4A	3.81	122.02	111.77
14	A	1138	CLA	C1D-ND-C4D	-3.81	103.64	106.31
14	H	1222	CLA	O2A-C1-C2	3.81	122.77	108.11
18	A	4002	BCR	C38-C26-C25	-3.81	120.33	124.48
18	H	4013	BCR	C15-C14-C13	-3.81	121.94	127.28
14	B	1222	CLA	O2A-C1-C2	3.81	122.76	108.11
14	G	1138	CLA	C1D-ND-C4D	-3.81	103.64	106.31
14	b	1229	CLA	CHD-C1D-ND	-3.81	119.44	124.80
15	G	1121	F6C	C4A-C3A-C2A	-3.81	101.32	106.97
14	G	1131	CLA	C2B-C1B-NB	3.81	114.27	110.33
14	H	1204	CLA	C4A-NA-C1A	3.81	108.42	106.68
14	A	1012	CLA	C4A-NA-C1A	3.81	108.42	106.68
14	B	1226	CLA	C3B-C2B-C1B	-3.81	102.68	107.17
14	b	1215	CLA	C1D-ND-C4D	-3.80	103.64	106.31
14	H	1220	CLA	CMA-C3A-C4A	3.80	121.99	111.77
19	G	5001	LHG	O7-C7-C8	3.80	119.70	111.48
14	B	1201	CLA	C1-C2-C3	-3.80	119.97	126.20
14	B	1204	CLA	C4A-NA-C1A	3.80	108.41	106.68
18	b	4013	BCR	C38-C26-C25	-3.80	120.34	124.48
14	A	1118	CLA	O2A-C1-C2	3.80	122.71	108.11
14	B	1229	CLA	CHD-C1D-ND	-3.80	119.46	124.80
14	a	1118	CLA	O2A-C1-C2	3.79	122.71	108.11
14	G	1012	CLA	CHD-C1D-ND	-3.79	119.46	124.80
14	A	1132	CLA	C2B-C1B-NB	3.79	114.26	110.33
18	b	4006	BCR	C33-C5-C6	-3.79	120.34	124.48
14	A	1130	CLA	C4A-NA-C1A	3.79	108.41	106.68
14	b	1208	CLA	C2B-C1B-NB	3.79	114.26	110.33
18	G	4002	BCR	C38-C26-C25	-3.79	120.35	124.48
14	b	1209	CLA	C4A-NA-C1A	3.79	108.41	106.68
14	a	1132	CLA	C2B-C1B-NB	3.79	114.25	110.33
14	H	1201	CLA	C1-C2-C3	-3.79	119.99	126.20
14	B	1231	CLA	C1-C2-C3	-3.79	119.99	126.20
19	H	5004	LHG	O7-C7-C8	3.78	119.67	111.48
14	G	1134	CLA	C2B-C1B-NB	3.78	114.25	110.33
14	H	1209	CLA	C2B-C1B-NB	3.78	114.25	110.33
14	H	1205	CLA	C2B-C1B-NB	3.78	114.25	110.33
14	b	1229	CLA	C4-C3-C5	3.78	121.79	115.23
18	H	4006	BCR	C33-C5-C6	-3.78	120.36	124.48
14	b	1224	CLA	C2B-C1B-NB	3.78	114.24	110.33
18	a	4002	BCR	C38-C26-C25	-3.78	120.36	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1236	CLA	CHD-C1D-ND	-3.78	119.49	124.80
14	A	1117	CLA	O2D-CGD-O1D	-3.78	116.50	123.85
14	b	1201	CLA	C1-C2-C3	-3.78	120.01	126.20
18	H	4004	BCR	C38-C26-C25	-3.77	120.37	124.48
18	B	4006	BCR	C33-C5-C6	-3.77	120.37	124.48
14	a	1117	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
14	b	1231	CLA	C1-C2-C3	-3.77	120.02	126.20
14	A	1115	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	b	1227	CLA	C1D-ND-C4D	-3.77	103.67	106.31
14	G	1012	CLA	CMB-C2B-C1B	3.77	131.16	125.42
14	H	1229	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	A	1012	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	H	1231	CLA	C1-C2-C3	-3.77	120.02	126.20
14	H	1229	CLA	C4-C3-C5	3.77	121.77	115.23
19	b	5004	LHG	O7-C7-C8	3.77	119.63	111.48
19	B	5004	LHG	O7-C7-C8	3.77	119.63	111.48
14	a	1114	CLA	C2B-C1B-NB	3.77	114.23	110.33
14	G	1132	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	a	1115	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	A	1116	CLA	CHD-C1D-ND	-3.77	119.50	124.80
14	a	1116	CLA	CHD-C1D-ND	-3.77	119.50	124.80
18	B	4016	BCR	C33-C5-C6	-3.76	120.38	124.48
14	b	1215	CLA	C2B-C1B-NB	3.76	114.23	110.33
14	a	1134	CLA	C2B-C1B-NB	3.76	114.23	110.33
18	B	4013	BCR	C15-C14-C13	-3.76	122.00	127.28
15	B	1238	F6C	C4A-C3A-C2A	-3.76	101.39	106.97
14	b	1204	CLA	C4A-NA-C1A	3.76	108.39	106.68
14	A	1137	CLA	C2B-C1B-NB	3.76	114.22	110.33
14	H	1215	CLA	C1D-ND-C4D	-3.76	103.67	106.31
14	B	1215	CLA	C1D-ND-C4D	-3.76	103.68	106.31
14	a	1122	CLA	C2B-C1B-NB	3.76	114.22	110.33
14	A	1122	CLA	C2B-C1B-NB	3.76	114.22	110.33
15	b	1238	F6C	C3A-C4A-NA	3.76	113.84	110.13
14	G	1116	CLA	CHD-C1D-ND	-3.76	119.52	124.80
18	b	4016	BCR	C33-C5-C6	-3.76	120.39	124.48
15	H	1238	F6C	C4A-C3A-C2A	-3.75	101.40	106.97
14	B	1217	CLA	C1-C2-C3	-3.75	120.05	126.20
14	H	1023	CLA	C1-C2-C3	-3.75	120.05	126.20
14	L	1503	CLA	O2A-C1-C2	3.75	122.55	108.11
14	b	1217	CLA	C1-C2-C3	-3.75	120.05	126.20
18	b	4017	BCR	C15-C14-C13	-3.75	122.02	127.28
14	G	1117	CLA	O2D-CGD-O1D	-3.75	116.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1021	CLA	CAA-C2A-C3A	-3.75	102.87	113.00
14	b	1021	CLA	CAA-C2A-C3A	-3.75	102.87	113.00
14	G	1114	CLA	C2B-C1B-NB	3.75	114.21	110.33
15	b	1238	F6C	C4A-C3A-C2A	-3.75	101.41	106.97
14	H	1227	CLA	C1D-ND-C4D	-3.75	103.68	106.31
14	B	1235	CLA	CHD-C1D-ND	-3.75	119.53	124.80
18	A	4007	BCR	C33-C5-C6	-3.75	120.40	124.48
14	B	1236	CLA	CHD-C1D-ND	-3.75	119.53	124.80
14	H	1215	CLA	C2B-C1B-NB	3.75	114.21	110.33
14	H	1224	CLA	C2B-C1B-NB	3.75	114.21	110.33
14	B	1229	CLA	C4-C3-C5	3.75	121.73	115.23
14	H	1021	CLA	CAA-C2A-C3A	-3.75	102.88	113.00
14	a	1137	CLA	C2B-C1B-NB	3.75	114.21	110.33
14	b	1239	CLA	CAC-C3C-C2C	3.74	134.44	127.56
15	H	1238	F6C	C3A-C4A-NA	3.74	113.83	110.13
20	G	5005	LMG	O7-C10-C11	3.74	119.58	111.48
14	U	1503	CLA	O2A-C1-C2	3.74	122.52	108.11
18	B	4017	BCR	C15-C14-C13	-3.74	122.03	127.28
18	H	4016	BCR	C33-C5-C6	-3.74	120.40	124.48
18	b	4004	BCR	C38-C26-C25	-3.74	120.40	124.48
14	a	1132	CLA	CHD-C1D-ND	-3.74	119.53	124.80
14	l	1503	CLA	O2A-C1-C2	3.74	122.51	108.11
14	b	1205	CLA	C2B-C1B-NB	3.74	114.21	110.33
14	B	1239	CLA	CAC-C3C-C2C	3.74	134.43	127.56
15	B	1238	F6C	C3A-C4A-NA	3.74	113.83	110.13
14	B	1227	CLA	C1D-ND-C4D	-3.74	103.69	106.31
18	H	4017	BCR	C15-C14-C13	-3.74	122.03	127.28
20	L	5007	LMG	O7-C10-C11	3.74	119.57	111.48
14	H	1239	CLA	CAC-C3C-C2C	3.74	134.43	127.56
14	G	1128	CLA	O2A-C1-C2	3.74	122.50	108.11
14	B	1224	CLA	C2B-C1B-NB	3.74	114.20	110.33
14	a	1128	CLA	O2A-C1-C2	3.74	122.50	108.11
14	a	1132	CLA	O2A-C1-C2	3.74	122.50	108.11
14	G	1122	CLA	C2B-C1B-NB	3.74	114.20	110.33
14	A	1132	CLA	O2A-C1-C2	3.74	122.49	108.11
20	A	5005	LMG	O7-C10-C11	3.74	119.56	111.48
14	b	1023	CLA	C1-C2-C3	-3.74	120.08	126.20
14	b	1214	CLA	O2A-C1-C2	3.74	122.48	108.11
14	A	1114	CLA	C2B-C1B-NB	3.74	114.20	110.33
18	a	4007	BCR	C33-C5-C6	-3.74	120.41	124.48
14	H	1224	CLA	O2A-C1-C2	3.74	122.48	108.11
14	a	1130	CLA	C4A-NA-C1A	3.73	108.38	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1217	CLA	C1-C2-C3	-3.73	120.08	126.20
14	B	1023	CLA	C1-C2-C3	-3.73	120.08	126.20
14	B	1206	CLA	C2B-C1B-NB	3.73	114.20	110.33
14	G	1130	CLA	CHD-C1D-ND	-3.73	119.55	124.80
14	A	1132	CLA	CHD-C1D-ND	-3.73	119.55	124.80
18	A	4002	BCR	C8-C9-C10	3.73	124.88	119.01
14	B	1224	CLA	O2A-C1-C2	3.73	122.47	108.11
14	A	1012	CLA	CMB-C2B-C1B	3.73	131.10	125.42
14	B	1226	CLA	CHD-C1D-ND	-3.73	119.55	124.80
14	G	1115	CLA	CHD-C1D-ND	-3.73	119.55	124.80
14	a	1012	CLA	CMB-C2B-C1B	3.73	131.10	125.42
14	G	1132	CLA	O2A-C1-C2	3.73	122.46	108.11
14	H	1209	CLA	CHD-C1D-ND	-3.73	119.56	124.80
18	G	4002	BCR	C8-C9-C10	3.73	124.87	119.01
14	B	1204	CLA	O2A-CGA-CBA	3.73	123.19	111.83
14	H	1204	CLA	O2A-CGA-CBA	3.72	123.19	111.83
14	H	1214	CLA	O2A-C1-C2	3.72	122.44	108.11
14	a	1109	CLA	C2B-C1B-NB	3.72	114.19	110.33
14	B	1209	CLA	CHD-C1D-ND	-3.72	119.56	124.80
14	H	1217	CLA	O2A-C1-C2	3.72	122.44	108.11
14	A	1128	CLA	O2A-C1-C2	3.72	122.44	108.11
14	B	1217	CLA	O2A-C1-C2	3.72	122.44	108.11
14	H	1235	CLA	CHD-C1D-ND	-3.72	119.56	124.80
14	H	1023	CLA	O2A-C1-C2	3.72	122.43	108.11
14	b	1224	CLA	O2A-C1-C2	3.72	122.43	108.11
14	B	1214	CLA	O2A-C1-C2	3.72	122.43	108.11
14	G	1137	CLA	C2B-C1B-NB	3.72	114.19	110.33
20	l	5007	LMG	O7-C10-C11	3.72	119.53	111.48
14	b	1204	CLA	O2A-CGA-CBA	3.72	123.18	111.83
20	a	5005	LMG	O7-C10-C11	3.72	119.53	111.48
14	b	1217	CLA	O2A-C1-C2	3.72	122.41	108.11
14	G	1109	CLA	C2B-C1B-NB	3.72	114.18	110.33
14	B	1215	CLA	C2B-C1B-NB	3.71	114.18	110.33
18	b	4016	BCR	C24-C23-C22	-3.71	120.74	126.23
18	B	4016	BCR	C24-C23-C22	-3.71	120.74	126.23
20	U	5007	LMG	O7-C10-C11	3.71	119.51	111.48
14	b	1236	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	a	1103	CLA	O2A-C1-C2	3.71	122.39	108.11
14	b	1209	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	b	1235	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	G	1111	CLA	O2A-C1-C2	3.71	122.38	108.11
14	a	1111	CLA	O2A-C1-C2	3.71	122.38	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1130	CLA	CHD-C1D-ND	-3.71	119.58	124.80
14	a	1114	CLA	C1D-ND-C4D	-3.71	103.71	106.31
14	a	1138	CLA	C1D-ND-C4D	-3.71	103.71	106.31
14	B	1023	CLA	O2A-C1-C2	3.71	122.37	108.11
18	B	4004	BCR	C38-C26-C25	-3.71	120.44	124.48
18	H	4016	BCR	C24-C23-C22	-3.71	120.75	126.23
14	A	1108	CLA	CHD-C1D-ND	-3.70	119.59	124.80
14	G	1103	CLA	C2B-C1B-NB	3.70	114.17	110.33
14	H	1212	CLA	C2B-C1B-NB	3.70	114.17	110.33
14	A	1103	CLA	O2A-C1-C2	3.70	122.35	108.11
14	H	1231	CLA	O2A-C1-C2	3.70	122.35	108.11
14	H	1226	CLA	CHD-C1D-ND	-3.70	119.59	124.80
14	a	1116	CLA	C1-C2-C3	-3.70	120.13	126.20
18	U	4019	BCR	C30-C25-C24	3.70	125.69	115.65
18	G	4007	BCR	C33-C5-C6	-3.70	120.45	124.48
14	b	1216	CLA	C1-C2-C3	-3.70	120.14	126.20
14	A	1111	CLA	O2A-C1-C2	3.70	122.34	108.11
14	b	1212	CLA	C2B-C1B-NB	3.70	114.16	110.33
18	l	4019	BCR	C30-C25-C24	3.70	125.68	115.65
14	a	1012	CLA	C1D-ND-C4D	-3.70	103.72	106.31
14	a	1102	CLA	C1D-ND-C4D	-3.70	103.72	106.31
14	H	1222	CLA	CAA-CBA-CGA	-3.70	102.71	113.21
14	b	1023	CLA	O2A-C1-C2	3.70	122.33	108.11
14	H	1206	CLA	C2B-C1B-NB	3.70	114.16	110.33
14	x	1701	CLA	C2B-C1B-NB	3.70	114.16	110.33
18	a	4002	BCR	C8-C9-C10	3.69	124.82	119.01
14	B	1222	CLA	CAA-CBA-CGA	-3.69	102.72	113.21
14	G	1106	CLA	O2A-CGA-CBA	3.69	123.09	111.83
14	G	1103	CLA	O2A-C1-C2	3.69	122.31	108.11
14	G	1108	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	b	1206	CLA	C2B-C1B-NB	3.69	114.15	110.33
14	b	1231	CLA	O2A-C1-C2	3.69	122.30	108.11
14	G	1124	CLA	O2A-CGA-CBA	3.69	123.08	111.83
14	b	1222	CLA	CAA-CBA-CGA	-3.69	102.74	113.21
14	B	1210	CLA	CHD-C1D-ND	-3.69	119.61	124.80
14	H	1210	CLA	CHD-C1D-ND	-3.68	119.62	124.80
14	b	1226	CLA	CHD-C1D-ND	-3.68	119.62	124.80
18	L	4019	BCR	C30-C25-C24	3.68	125.64	115.65
14	a	1124	CLA	O2A-CGA-CBA	3.68	123.06	111.83
14	B	1231	CLA	O2A-C1-C2	3.68	122.28	108.11
14	b	1228	CLA	C2B-C1B-NB	3.68	114.14	110.33
14	A	1102	CLA	C1D-ND-C4D	-3.68	103.73	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1208	CLA	CHD-C1D-ND	-3.68	119.62	124.80
14	A	1124	CLA	O2A-CGA-CBA	3.68	123.05	111.83
14	G	1130	CLA	C1D-ND-C4D	-3.68	103.73	106.31
14	X	1701	CLA	C2B-C1B-NB	3.68	114.14	110.33
14	B	1216	CLA	C1-C2-C3	-3.68	120.17	126.20
14	H	1211	CLA	CHD-C1D-ND	-3.68	119.63	124.80
14	a	1106	CLA	O2A-CGA-CBA	3.68	123.04	111.83
14	H	1216	CLA	C1-C2-C3	-3.67	120.18	126.20
14	G	1116	CLA	C1-C2-C3	-3.67	120.18	126.20
14	b	1210	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	G	1130	CLA	C4A-NA-C1A	3.67	108.35	106.68
14	A	1106	CLA	O2A-CGA-CBA	3.67	123.03	111.83
14	G	1012	CLA	C1-C2-C3	-3.67	120.18	126.20
14	A	1130	CLA	CHD-C1D-ND	-3.67	119.64	124.80
14	B	1234	CLA	O2A-C1-C2	3.67	122.23	108.11
14	a	1140	CLA	C4-C3-C5	3.67	121.59	115.23
14	a	1103	CLA	C2B-C1B-NB	3.67	114.13	110.33
14	G	1140	CLA	C4-C3-C5	3.67	121.59	115.23
14	b	1234	CLA	O2A-C1-C2	3.66	122.20	108.11
14	a	1130	CLA	C1D-ND-C4D	-3.66	103.74	106.31
14	A	1109	CLA	C2B-C1B-NB	3.66	114.12	110.33
14	B	1201	CLA	CHD-C1D-ND	-3.66	119.65	124.80
14	A	1103	CLA	C2B-C1B-NB	3.66	114.12	110.33
14	A	1012	CLA	C1-C2-C3	-3.66	120.20	126.20
14	G	1114	CLA	C1D-ND-C4D	-3.66	103.74	106.31
14	A	1114	CLA	C1D-ND-C4D	-3.66	103.74	106.31
14	H	1234	CLA	O2A-C1-C2	3.66	122.19	108.11
14	H	1208	CLA	CHD-C1D-ND	-3.66	119.66	124.80
14	A	1140	CLA	C4-C3-C5	3.66	121.58	115.23
14	A	1116	CLA	C1-C2-C3	-3.66	120.21	126.20
18	b	4009	BCR	C7-C8-C9	-3.65	120.83	126.23
14	B	1208	CLA	O2A-C1-C2	3.65	122.17	108.11
14	G	1013	CLA	C1-C2-C3	-3.65	120.21	126.20
14	l	1501	CLA	O2A-CGA-CBA	3.65	122.98	111.83
14	H	1201	CLA	CHD-C1D-ND	-3.65	119.66	124.80
15	H	1237	F6C	O2A-CGA-CBA	3.65	122.97	111.83
15	b	1230	F6C	C1C-C2C-C3C	-3.65	102.63	106.82
14	a	1012	CLA	C1-C2-C3	-3.65	120.21	126.20
15	B	1237	F6C	O2A-CGA-CBA	3.65	122.97	111.83
14	a	1108	CLA	CHD-C1D-ND	-3.65	119.66	124.80
14	B	1227	CLA	C2D-C1D-ND	3.65	113.74	110.13
14	b	1211	CLA	CHD-C1D-ND	-3.65	119.67	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	U	1501	CLA	O2A-CGA-CBA	3.65	122.97	111.83
15	H	1230	F6C	C1C-C2C-C3C	-3.65	102.64	106.82
15	B	1230	F6C	C1C-C2C-C3C	-3.65	102.64	106.82
14	H	1234	CLA	C1-C2-C3	-3.65	120.22	126.20
14	B	1211	CLA	CHD-C1D-ND	-3.65	119.67	124.80
14	H	1232	CLA	C2B-C1B-NB	3.65	114.11	110.33
14	A	1119	CLA	C2B-C1B-NB	3.65	114.11	110.33
15	b	1237	F6C	O2A-CGA-CBA	3.65	122.96	111.83
18	A	4007	BCR	C31-C1-C6	-3.65	104.52	110.24
14	G	1109	CLA	CHD-C1D-ND	-3.65	119.67	124.80
15	b	1237	F6C	O2A-C1-C2	3.65	122.14	108.11
14	B	1228	CLA	C2B-C1B-NB	3.65	114.11	110.33
14	H	1208	CLA	O2A-C1-C2	3.64	122.13	108.11
18	H	4009	BCR	C7-C8-C9	-3.64	120.84	126.23
14	B	1208	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	b	1208	CLA	O2A-C1-C2	3.64	122.12	108.11
14	a	1013	CLA	C1-C2-C3	-3.64	120.23	126.20
14	a	1109	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	A	1109	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	L	1501	CLA	O2A-CGA-CBA	3.64	122.94	111.83
15	B	1237	F6C	O2A-C1-C2	3.64	122.12	108.11
18	a	4007	BCR	C31-C1-C6	-3.64	104.54	110.24
14	b	1201	CLA	CHD-C1D-ND	-3.64	119.68	124.80
14	G	1131	CLA	C1D-ND-C4D	-3.64	103.76	106.31
14	A	1123	CLA	O2A-C1-C2	3.64	122.11	108.11
14	W	1701	CLA	C2B-C1B-NB	3.64	114.10	110.33
14	A	1134	CLA	CHD-C1D-ND	-3.64	119.69	124.80
14	G	1119	CLA	C2B-C1B-NB	3.64	114.10	110.33
14	a	1123	CLA	O2A-C1-C2	3.64	122.10	108.11
14	G	1115	CLA	O2A-C1-C2	3.63	122.09	108.11
14	B	1228	CLA	O2A-C1-C2	3.63	122.09	108.11
13	a	1011	CL0	CAA-C2A-C3A	-3.63	103.18	113.00
14	b	1234	CLA	C1-C2-C3	-3.63	120.24	126.20
15	H	1237	F6C	O2A-C1-C2	3.63	122.09	108.11
14	b	1228	CLA	O2A-C1-C2	3.63	122.09	108.11
14	b	1021	CLA	C6-C5-C3	-3.63	104.62	113.47
14	G	1134	CLA	CHD-C1D-ND	-3.63	119.69	124.80
14	B	1212	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	H	1225	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	A	1013	CLA	C1-C2-C3	-3.63	120.25	126.20
18	B	4009	BCR	C7-C8-C9	-3.63	120.87	126.23
14	G	1112	CLA	CHD-C1D-ND	-3.63	119.70	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1021	CLA	C6-C5-C3	-3.63	104.63	113.47
14	H	1228	CLA	C2B-C1B-NB	3.63	114.09	110.33
14	H	1021	CLA	C6-C5-C3	-3.62	104.64	113.47
13	G	1011	CL0	CAA-C2A-C3A	-3.62	103.20	113.00
13	A	1011	CL0	CAA-C2A-C3A	-3.62	103.20	113.00
14	G	1123	CLA	O2A-C1-C2	3.62	122.05	108.11
14	a	1112	CLA	CHD-C1D-ND	-3.62	119.70	124.80
14	a	1115	CLA	O2A-C1-C2	3.62	122.05	108.11
14	H	1022	CLA	CMC-C2C-C1C	3.62	130.70	125.03
14	A	1130	CLA	O2A-CGA-CBA	3.62	122.88	111.83
14	A	1115	CLA	O2A-C1-C2	3.62	122.05	108.11
14	a	1101	CLA	C2B-C1B-NB	3.62	114.08	110.33
14	A	1133	CLA	CHD-C1D-ND	-3.62	119.71	124.80
14	G	1102	CLA	C1D-ND-C4D	-3.62	103.77	106.31
14	A	1131	CLA	C1D-ND-C4D	-3.62	103.77	106.31
14	H	1228	CLA	O2A-C1-C2	3.62	122.03	108.11
14	a	1118	CLA	C2B-C1B-NB	3.62	114.08	110.33
14	b	1227	CLA	C2D-C1D-ND	3.62	113.71	110.13
14	B	1234	CLA	C1-C2-C3	-3.62	120.27	126.20
18	G	4007	BCR	C31-C1-C6	-3.62	104.57	110.24
14	A	1103	CLA	O2D-CGD-O1D	-3.62	116.81	123.85
14	a	1103	CLA	O2D-CGD-O1D	-3.61	116.81	123.85
14	K	1401	CLA	C2B-C1B-NB	3.61	114.07	110.33
14	B	1022	CLA	CMC-C2C-C1C	3.61	130.68	125.03
14	A	1110	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	k	1401	CLA	C2B-C1B-NB	3.61	114.07	110.33
14	G	1130	CLA	O2A-CGA-CBA	3.61	122.84	111.83
14	a	1131	CLA	C1D-ND-C4D	-3.61	103.78	106.31
14	A	1137	CLA	CHD-C1D-ND	-3.61	119.72	124.80
14	H	1216	CLA	O2A-C1-C2	3.61	121.99	108.11
14	a	1130	CLA	O2A-CGA-CBA	3.61	122.83	111.83
14	B	1216	CLA	O2A-C1-C2	3.61	121.99	108.11
14	b	1216	CLA	O2A-C1-C2	3.61	121.98	108.11
14	G	1103	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
14	a	1137	CLA	CHD-C1D-ND	-3.60	119.73	124.80
14	T	1401	CLA	CHD-C1D-ND	-3.60	119.73	124.80
15	B	1238	F6C	C4A-NA-C1A	3.60	108.84	106.31
14	B	1021	CLA	O2A-CGA-CBA	3.60	122.82	111.83
14	a	1119	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	B	1225	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	b	1022	CLA	CMC-C2C-C1C	3.60	130.66	125.03
14	B	1232	CLA	C2B-C1B-NB	3.60	114.06	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1110	CLA	CHD-C1D-ND	-3.60	119.74	124.80
14	k	1401	CLA	CHD-C1D-ND	-3.60	119.74	124.80
14	H	1021	CLA	O2A-CGA-CBA	3.60	122.81	111.83
14	b	1232	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	b	1021	CLA	O2A-CGA-CBA	3.60	122.80	111.83
14	a	1133	CLA	CHD-C1D-ND	-3.60	119.74	124.80
14	G	1110	CLA	CHD-C1D-ND	-3.60	119.74	124.80
14	H	1227	CLA	C2D-C1D-ND	3.60	113.69	110.13
14	U	1501	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	A	1118	CLA	C2B-C1B-NB	3.60	114.06	110.33
14	G	1133	CLA	CHD-C1D-ND	-3.60	119.74	124.80
14	G	1012	CLA	C1D-ND-C4D	-3.59	103.79	106.31
14	A	1130	CLA	C1D-ND-C4D	-3.59	103.79	106.31
14	G	1118	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	G	1101	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	T	1401	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	A	1112	CLA	CHD-C1D-ND	-3.59	119.75	124.80
14	A	1122	CLA	CHD-C1D-ND	-3.59	119.75	124.80
14	B	1221	CLA	C2B-C1B-NB	3.59	114.05	110.33
14	G	1135	CLA	C4D-C3D-CAD	3.59	112.00	108.11
14	a	1134	CLA	CHD-C1D-ND	-3.59	119.76	124.80
14	A	1110	CLA	C2B-C1B-NB	3.58	114.04	110.33
15	H	1237	F6C	C4-C3-C5	3.58	121.44	115.23
14	B	1206	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	A	1101	CLA	C2B-C1B-NB	3.58	114.04	110.33
14	A	1135	CLA	O2A-CGA-CBA	3.58	122.74	111.83
14	H	1221	CLA	C2B-C1B-NB	3.58	114.03	110.33
14	B	1236	CLA	C2B-C1B-NB	3.58	114.03	110.33
14	a	1122	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	G	1137	CLA	CHD-C1D-ND	-3.58	119.77	124.80
14	G	1140	CLA	C2B-C1B-NB	3.57	114.03	110.33
14	a	1119	CLA	C1D-ND-C4D	-3.57	103.80	106.31
14	a	1135	CLA	O2A-CGA-CBA	3.57	122.73	111.83
14	H	1219	CLA	CHD-C1D-ND	-3.57	119.77	124.80
14	G	1119	CLA	C1D-ND-C4D	-3.57	103.81	106.31
18	H	4005	BCR	C34-C9-C10	-3.57	117.03	122.82
14	G	1122	CLA	CHD-C1D-ND	-3.57	119.78	124.80
15	B	1237	F6C	C4-C3-C5	3.57	121.42	115.23
14	a	1135	CLA	C4D-C3D-CAD	3.57	111.98	108.11
14	H	1206	CLA	CHD-C1D-ND	-3.57	119.78	124.80
14	G	1127	CLA	O2A-C1-C2	3.57	121.83	108.11
14	G	1102	CLA	O2D-CGD-O1D	-3.57	116.91	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1022	CLA	C4-C3-C5	3.56	121.42	115.23
14	b	1225	CLA	C2B-C1B-NB	3.56	114.02	110.33
18	R	4020	BCR	C7-C8-C9	-3.56	120.96	126.23
14	A	1127	CLA	O2A-C1-C2	3.56	121.82	108.11
14	L	1501	CLA	C2B-C1B-NB	3.56	114.02	110.33
14	B	1022	CLA	C4-C3-C5	3.56	121.41	115.23
14	B	1216	CLA	CHD-C1D-ND	-3.56	119.79	124.80
14	b	1219	CLA	CHD-C1D-ND	-3.56	119.79	124.80
14	G	1135	CLA	O2A-CGA-CBA	3.56	122.69	111.83
15	b	1237	F6C	C4-C3-C5	3.56	121.40	115.23
14	B	1219	CLA	CHD-C1D-ND	-3.56	119.80	124.80
14	L	1502	CLA	O2A-CGA-CBA	3.56	122.68	111.83
15	H	1230	F6C	C3A-C4A-NA	3.56	113.65	110.13
14	H	1022	CLA	C4-C3-C5	3.56	121.40	115.23
14	K	1401	CLA	CHD-C1D-ND	-3.56	119.80	124.80
14	G	1101	CLA	CHD-C1D-ND	-3.56	119.80	124.80
14	A	1012	CLA	C1D-ND-C4D	-3.55	103.82	106.31
14	G	1117	CLA	C1-C2-C3	-3.55	120.37	126.20
14	U	1502	CLA	O2A-CGA-CBA	3.55	122.67	111.83
14	a	1127	CLA	O2A-C1-C2	3.55	121.78	108.11
14	a	1104	CLA	C2B-C1B-NB	3.55	114.01	110.33
14	A	1104	CLA	C2B-C1B-NB	3.55	114.01	110.33
14	B	1219	CLA	CAC-C3C-C4C	3.55	129.41	124.79
15	b	1207	F6C	CHA-C4D-ND	3.55	136.45	133.05
18	I	4020	BCR	C7-C8-C9	-3.55	120.98	126.23
14	H	1202	CLA	C2B-C1B-NB	3.55	114.01	110.33
14	a	1101	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	b	1233	CLA	CHD-C1D-ND	-3.55	119.81	124.80
14	l	1502	CLA	O2A-CGA-CBA	3.55	122.65	111.83
14	a	1110	CLA	C2B-C1B-NB	3.54	114.00	110.33
15	B	1230	F6C	C3A-C4A-NA	3.54	113.63	110.13
14	A	1135	CLA	C4D-C3D-CAD	3.54	111.95	108.11
14	b	1219	CLA	CAC-C3C-C4C	3.54	129.40	124.79
14	a	1138	CLA	CED-O2D-CGD	3.54	123.95	115.92
14	A	1140	CLA	C2B-C1B-NB	3.54	114.00	110.33
14	b	1206	CLA	CHD-C1D-ND	-3.54	119.82	124.80
14	A	1102	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
18	b	4005	BCR	C34-C9-C10	-3.54	117.09	122.82
14	B	1022	CLA	C2B-C1B-NB	3.54	113.99	110.33
18	i	4020	BCR	C7-C8-C9	-3.53	121.01	126.23
14	H	1236	CLA	C2B-C1B-NB	3.53	113.99	110.33
14	a	1102	CLA	O2D-CGD-O1D	-3.53	116.97	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1104	CLA	C2B-C1B-NB	3.53	113.99	110.33
14	a	1140	CLA	C2B-C1B-NB	3.53	113.99	110.33
14	A	1117	CLA	C1-C2-C3	-3.53	120.41	126.20
14	a	1117	CLA	C1-C2-C3	-3.53	120.41	126.20
14	b	1236	CLA	C2B-C1B-NB	3.53	113.99	110.33
16	a	2001	PQN	C14-C13-C15	3.53	121.35	115.23
14	H	1233	CLA	CHD-C1D-ND	-3.53	119.84	124.80
14	H	1220	CLA	CHD-C1D-ND	-3.53	119.84	124.80
14	H	1219	CLA	CAC-C3C-C4C	3.53	129.38	124.79
15	B	1207	F6C	CHA-C4D-ND	3.53	136.42	133.05
14	b	1221	CLA	C2B-C1B-NB	3.53	113.98	110.33
15	b	1230	F6C	C3A-C4A-NA	3.52	113.61	110.13
14	A	1117	CLA	O2A-CGA-CBA	3.52	122.57	111.83
14	a	1117	CLA	O2A-CGA-CBA	3.52	122.57	111.83
14	a	1102	CLA	C1-C2-C3	-3.52	120.43	126.20
15	H	1207	F6C	CHA-C4D-ND	3.52	136.42	133.05
14	l	1503	CLA	C1-C2-C3	-3.52	120.43	126.20
14	B	1220	CLA	CHD-C1D-ND	-3.52	119.85	124.80
14	G	1117	CLA	O2A-CGA-CBA	3.52	122.57	111.83
14	A	1138	CLA	CED-O2D-CGD	3.52	123.90	115.92
14	G	1110	CLA	C2B-C1B-NB	3.52	113.97	110.33
14	l	1501	CLA	C2B-C1B-NB	3.52	113.97	110.33
14	L	1503	CLA	C1-C2-C3	-3.52	120.43	126.20
14	A	1101	CLA	CHD-C1D-ND	-3.52	119.85	124.80
14	U	1503	CLA	C1-C2-C3	-3.52	120.43	126.20
14	G	1131	CLA	C1-C2-C3	-3.52	120.43	126.20
15	b	1238	F6C	C4A-NA-C1A	3.52	108.78	106.31
18	B	4005	BCR	C34-C9-C10	-3.52	117.12	122.82
14	B	1202	CLA	C4-C3-C5	3.52	121.33	115.23
15	H	1238	F6C	C4A-NA-C1A	3.51	108.78	106.31
14	b	1220	CLA	CHD-C1D-ND	-3.51	119.86	124.80
14	a	1125	CLA	C2B-C1B-NB	3.51	113.97	110.33
14	G	1138	CLA	CED-O2D-CGD	3.51	123.88	115.92
14	b	1202	CLA	C4-C3-C5	3.51	121.32	115.23
14	H	1202	CLA	C4-C3-C5	3.51	121.32	115.23
18	B	4010	BCR	C36-C18-C17	-3.51	117.13	122.82
14	G	1102	CLA	C1-C2-C3	-3.51	120.45	126.20
14	U	1502	CLA	C2B-C1B-NB	3.51	113.97	110.33
14	a	1120	CLA	C2B-C1B-NB	3.51	113.97	110.33
14	B	1213	CLA	CHD-C1D-ND	-3.51	119.86	124.80
14	H	1022	CLA	C2B-C1B-NB	3.51	113.96	110.33
14	G	1120	CLA	CHD-C1D-ND	-3.51	119.87	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1213	CLA	CHD-C1D-ND	-3.51	119.87	124.80
16	A	2001	PQN	C14-C13-C15	3.51	121.32	115.23
14	a	1122	CLA	O2A-C1-C2	3.51	121.61	108.11
18	B	4016	BCR	C7-C8-C9	-3.51	121.05	126.23
14	A	1103	CLA	CHD-C1D-ND	-3.51	119.87	124.80
14	H	1216	CLA	CHD-C1D-ND	-3.50	119.87	124.80
16	G	2001	PQN	C14-C13-C15	3.50	121.31	115.23
14	b	1216	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	a	1120	CLA	CHD-C1D-ND	-3.50	119.87	124.80
14	b	1022	CLA	C2B-C1B-NB	3.50	113.96	110.33
14	b	1239	CLA	CHD-C1D-ND	-3.50	119.88	124.80
14	b	1210	CLA	O2A-CGA-CBA	3.50	122.51	111.83
14	A	1122	CLA	O2A-C1-C2	3.50	121.58	108.11
14	b	1202	CLA	C2B-C1B-NB	3.50	113.95	110.33
14	A	1119	CLA	C1D-ND-C4D	-3.50	103.86	106.31
18	b	4016	BCR	C7-C8-C9	-3.50	121.06	126.23
14	A	1102	CLA	C1-C2-C3	-3.50	120.47	126.20
14	l	1502	CLA	C2B-C1B-NB	3.50	113.95	110.33
14	L	1502	CLA	C2B-C1B-NB	3.50	113.95	110.33
14	b	1213	CLA	CHD-C1D-ND	-3.50	119.88	124.80
14	B	1202	CLA	C2B-C1B-NB	3.50	113.95	110.33
14	B	1210	CLA	O2A-CGA-CBA	3.49	122.49	111.83
14	G	1126	CLA	CHD-C1D-ND	-3.49	119.88	124.80
14	A	1120	CLA	CHD-C1D-ND	-3.49	119.88	124.80
18	b	4010	BCR	C36-C18-C17	-3.49	117.16	122.82
14	b	1227	CLA	C2B-C1B-NB	3.49	113.95	110.33
14	a	1117	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	A	1131	CLA	C1-C2-C3	-3.49	120.47	126.20
14	B	1239	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	a	1119	CLA	C1-O2A-CGA	3.49	125.10	116.65
14	G	1103	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	G	1117	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	a	1103	CLA	CHD-C1D-ND	-3.49	119.89	124.80
14	H	1208	CLA	C1-C2-C3	-3.49	120.48	126.20
18	B	4004	BCR	C19-C18-C17	3.49	124.50	119.01
14	B	1227	CLA	C2B-C1B-NB	3.49	113.94	110.33
18	H	4010	BCR	C36-C18-C17	-3.49	117.17	122.82
18	H	4016	BCR	C7-C8-C9	-3.49	121.08	126.23
14	G	1122	CLA	O2A-C1-C2	3.49	121.53	108.11
14	B	1233	CLA	CHD-C1D-ND	-3.49	119.90	124.80
18	b	4004	BCR	C19-C18-C17	3.49	124.49	119.01
14	H	1210	CLA	O2A-CGA-CBA	3.49	122.46	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1239	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	A	1126	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	a	1126	CLA	CHD-C1D-ND	-3.48	119.90	124.80
14	a	1131	CLA	C1-C2-C3	-3.48	120.50	126.20
14	B	1203	CLA	C2B-C1B-NB	3.48	113.94	110.33
14	b	1202	CLA	CHD-C1D-ND	-3.48	119.91	124.80
14	A	1119	CLA	C1-O2A-CGA	3.48	125.07	116.65
14	G	1119	CLA	C1-O2A-CGA	3.48	125.07	116.65
14	G	1104	CLA	O2A-C1-C2	3.47	121.48	108.11
14	A	1104	CLA	O2A-C1-C2	3.47	121.48	108.11
14	H	1202	CLA	CHD-C1D-ND	-3.47	119.91	124.80
14	H	1227	CLA	C2B-C1B-NB	3.47	113.93	110.33
14	H	1201	CLA	O2A-C1-C2	3.47	121.47	108.11
14	b	1208	CLA	C1-C2-C3	-3.47	120.51	126.20
14	A	1125	CLA	C2B-C1B-NB	3.47	113.93	110.33
14	b	1201	CLA	O2A-C1-C2	3.47	121.47	108.11
14	A	1117	CLA	CHD-C1D-ND	-3.47	119.92	124.80
14	b	1203	CLA	C2B-C1B-NB	3.47	113.92	110.33
14	B	1201	CLA	O2A-C1-C2	3.47	121.45	108.11
14	a	1104	CLA	O2A-C1-C2	3.47	121.45	108.11
14	B	1202	CLA	CHD-C1D-ND	-3.46	119.93	124.80
14	B	1224	CLA	O1D-CGD-CBD	-3.46	117.69	124.52
15	G	1121	F6C	C4A-NA-C1A	3.46	108.74	106.31
18	L	4022	BCR	C15-C14-C13	-3.46	122.43	127.28
14	H	1224	CLA	O1D-CGD-CBD	-3.46	117.70	124.52
14	G	1125	CLA	C2B-C1B-NB	3.46	113.91	110.33
14	A	1138	CLA	CHD-C1D-ND	-3.46	119.94	124.80
14	B	1233	CLA	O2A-CGA-CBA	3.45	124.92	114.00
14	a	1117	CLA	C1D-ND-C4D	-3.45	103.89	106.31
14	A	1013	CLA	CMB-C2B-C3B	3.45	134.67	126.55
14	G	1129	CLA	O2A-C1-C2	3.45	121.40	108.11
14	H	1203	CLA	C2B-C1B-NB	3.45	113.91	110.33
18	H	4004	BCR	C19-C18-C17	3.45	124.44	119.01
18	b	4017	BCR	C33-C5-C6	-3.45	120.72	124.48
13	G	1011	CL0	O2D-CGD-O1D	-3.45	117.13	123.85
14	b	1203	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	A	1117	CLA	O2A-C1-C2	3.45	121.38	108.11
14	B	1208	CLA	C1-C2-C3	-3.45	120.55	126.20
14	b	1233	CLA	O2A-CGA-CBA	3.45	124.89	114.00
14	B	1214	CLA	CHD-C1D-ND	-3.45	119.95	124.80
14	a	1117	CLA	O2A-C1-C2	3.45	121.38	108.11
14	G	1013	CLA	CMB-C2B-C3B	3.45	134.66	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1233	CLA	O2A-CGA-CBA	3.45	124.89	114.00
14	B	1218	CLA	C2B-C1B-NB	3.45	113.90	110.33
13	A	1011	CL0	O2D-CGD-O1D	-3.45	117.14	123.85
18	B	4013	BCR	C28-C27-C26	-3.45	107.91	114.06
18	b	4013	BCR	C28-C27-C26	-3.44	107.91	114.06
14	a	1113	CLA	CHD-C1D-ND	-3.44	119.95	124.80
18	H	4017	BCR	C33-C5-C6	-3.44	120.73	124.48
14	G	1120	CLA	C2B-C1B-NB	3.44	113.90	110.33
14	G	1117	CLA	C1D-ND-C4D	-3.44	103.90	106.31
14	A	1120	CLA	C2B-C1B-NB	3.44	113.90	110.33
14	b	1214	CLA	C1D-ND-C4D	-3.44	103.90	106.31
18	l	4022	BCR	C15-C14-C13	-3.44	122.45	127.28
14	B	1223	CLA	O2A-C1-C2	3.44	121.35	108.11
14	H	1203	CLA	CHD-C1D-ND	-3.44	119.96	124.80
14	a	1129	CLA	O2A-C1-C2	3.44	121.35	108.11
14	a	1013	CLA	CMB-C2B-C3B	3.44	134.64	126.55
14	A	1129	CLA	O2A-C1-C2	3.44	121.34	108.11
14	H	1214	CLA	CHD-C1D-ND	-3.44	119.96	124.80
14	H	1021	CLA	C1-C2-C3	-3.44	120.56	126.20
14	H	1202	CLA	CMB-C2B-C1B	3.44	130.65	125.42
14	a	1125	CLA	C3C-C4C-NC	3.44	114.83	110.43
14	b	1224	CLA	O1D-CGD-CBD	-3.44	117.74	124.52
14	G	1117	CLA	O2A-C1-C2	3.43	121.33	108.11
15	b	1238	F6C	CMA-C3A-C4A	-3.43	118.68	124.73
14	B	1214	CLA	C1D-ND-C4D	-3.43	103.90	106.31
14	a	1114	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	A	1114	CLA	CHD-C1D-ND	-3.43	119.97	124.80
14	b	1223	CLA	O2A-C1-C2	3.43	121.31	108.11
14	A	1125	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
14	B	1023	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
14	A	1111	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
15	H	1238	F6C	CMA-C3A-C4A	-3.43	118.69	124.73
14	G	1138	CLA	CHD-C1D-ND	-3.43	119.98	124.80
14	a	1140	CLA	CHD-C1D-ND	-3.43	119.98	124.80
13	a	1011	CL0	O2D-CGD-O1D	-3.43	117.18	123.85
14	b	1202	CLA	CMB-C2B-C1B	3.43	130.64	125.42
14	A	1125	CLA	C3C-C4C-NC	3.43	114.82	110.43
14	H	1223	CLA	O2A-C1-C2	3.43	121.29	108.11
14	A	1140	CLA	CHD-C1D-ND	-3.43	119.98	124.80
14	B	1202	CLA	CMB-C2B-C1B	3.42	130.63	125.42
18	H	4013	BCR	C28-C27-C26	-3.42	107.95	114.06
14	b	1021	CLA	C1-C2-C3	-3.42	120.59	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1140	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	A	1113	CLA	CHD-C1D-ND	-3.42	119.99	124.80
15	B	1238	F6C	CMA-C3A-C4A	-3.42	118.70	124.73
14	H	1214	CLA	C1D-ND-C4D	-3.42	103.91	106.31
14	G	1013	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	B	1203	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	b	1214	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	G	1111	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
14	G	1114	CLA	CHD-C1D-ND	-3.42	119.99	124.80
14	G	1119	CLA	CHD-C1D-ND	-3.42	119.99	124.80
18	A	4002	BCR	C28-C27-C26	-3.42	107.96	114.06
18	a	4002	BCR	C28-C27-C26	-3.42	107.97	114.06
14	B	1209	CLA	O2A-CGA-CBA	3.42	124.79	114.00
14	a	1111	CLA	O2D-CGD-O1D	-3.41	117.20	123.85
18	B	4017	BCR	C33-C5-C6	-3.41	120.76	124.48
14	B	1021	CLA	C1-C2-C3	-3.41	120.61	126.20
14	A	1112	CLA	O2A-C1-C2	3.41	121.24	108.11
18	U	4022	BCR	C15-C14-C13	-3.41	122.49	127.28
14	G	1112	CLA	O2A-C1-C2	3.41	121.23	108.11
14	H	1209	CLA	O2A-CGA-CBA	3.41	124.77	114.00
14	b	1232	CLA	CHD-C1D-ND	-3.41	120.01	124.80
14	G	1125	CLA	C3C-C4C-NC	3.41	114.79	110.43
14	b	1023	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
14	H	1023	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
15	a	1121	F6C	C4A-NA-C1A	3.40	108.70	106.31
14	a	1013	CLA	CHD-C1D-ND	-3.40	120.01	124.80
14	a	1112	CLA	O2A-C1-C2	3.40	121.20	108.11
18	G	4001	BCR	C24-C23-C22	-3.40	121.20	126.23
14	b	1234	CLA	C2B-C1B-NB	3.40	113.85	110.33
14	A	1013	CLA	CHD-C1D-ND	-3.40	120.02	124.80
18	A	4007	BCR	C3-C4-C5	-3.40	107.99	114.06
14	a	1111	CLA	CHD-C1D-ND	-3.40	120.02	124.80
14	b	1223	CLA	O2D-CGD-O1D	-3.40	117.23	123.85
14	b	1206	CLA	C1D-ND-C4D	-3.40	103.93	106.31
18	a	4003	BCR	C27-C26-C25	-3.40	118.11	122.70
18	a	4002	BCR	C33-C5-C6	-3.40	120.78	124.48
14	a	1138	CLA	CHD-C1D-ND	-3.40	120.02	124.80
14	A	1111	CLA	CHD-C1D-ND	-3.40	120.02	124.80
18	G	4002	BCR	C33-C5-C6	-3.40	120.78	124.48
14	B	1223	CLA	O2D-CGD-O1D	-3.40	117.24	123.85
14	H	1218	CLA	C2B-C1B-NB	3.40	113.85	110.33
14	a	1102	CLA	CHD-C1D-ND	-3.39	120.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1232	CLA	CHD-C1D-ND	-3.39	120.03	124.80
14	a	1129	CLA	C1-C2-C3	-3.39	121.27	126.76
18	G	4002	BCR	C28-C27-C26	-3.39	108.01	114.06
14	A	1119	CLA	CMC-C2C-C3C	3.39	135.31	126.15
18	a	4001	BCR	C24-C23-C22	-3.39	121.22	126.23
14	a	1119	CLA	CMC-C2C-C3C	3.39	135.31	126.15
14	b	1209	CLA	O2A-CGA-CBA	3.39	124.70	114.00
14	b	1218	CLA	C2B-C1B-NB	3.39	113.84	110.33
14	a	1119	CLA	CHD-C1D-ND	-3.39	120.03	124.80
18	G	4007	BCR	C34-C9-C8	3.39	123.26	118.09
18	A	4007	BCR	C34-C9-C8	3.39	123.26	118.09
15	A	1121	F6C	C4A-NA-C1A	3.38	108.69	106.31
14	B	1232	CLA	CHD-C1D-ND	-3.38	120.04	124.80
14	H	1225	CLA	C1-C2-C3	-3.38	120.65	126.20
14	H	1206	CLA	C1D-ND-C4D	-3.38	103.94	106.31
14	b	1205	CLA	O2D-CGD-O1D	-3.38	117.27	123.85
18	G	4007	BCR	C3-C4-C5	-3.38	108.03	114.06
14	B	1206	CLA	C1D-ND-C4D	-3.38	103.94	106.31
18	a	4007	BCR	C3-C4-C5	-3.38	108.03	114.06
18	a	4007	BCR	C34-C9-C8	3.38	123.25	118.09
14	G	1111	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	A	1117	CLA	C1D-ND-C4D	-3.38	103.94	106.31
14	G	1113	CLA	CHD-C1D-ND	-3.38	120.05	124.80
14	B	1205	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
14	a	1137	CLA	C1-C2-C3	-3.38	121.30	126.76
18	A	4001	BCR	C24-C23-C22	-3.38	121.24	126.23
18	a	4001	BCR	C3-C4-C5	-3.37	108.04	114.06
18	A	4001	BCR	C3-C4-C5	-3.37	108.04	114.06
14	H	1223	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
14	A	1106	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	H	1205	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
14	a	1101	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
14	a	1125	CLA	C1C-C2C-C3C	-3.37	103.43	106.98
14	b	1231	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	G	1119	CLA	CMC-C2C-C3C	3.37	135.27	126.15
14	G	1125	CLA	C1C-C2C-C3C	-3.37	103.43	106.98
18	G	4001	BCR	C3-C4-C5	-3.37	108.05	114.06
14	G	1137	CLA	C1-C2-C3	-3.37	121.31	126.76
18	A	4002	BCR	C33-C5-C6	-3.37	120.81	124.48
18	A	4003	BCR	C27-C26-C25	-3.37	118.15	122.70
14	A	1137	CLA	C1-C2-C3	-3.37	121.31	126.76
14	G	1102	CLA	CHD-C1D-ND	-3.37	120.06	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1217	CLA	CHD-C1D-ND	-3.37	120.06	124.80
14	H	1231	CLA	CHD-C1D-ND	-3.36	120.07	124.80
14	B	1231	CLA	CHD-C1D-ND	-3.36	120.07	124.80
18	G	4003	BCR	C27-C26-C25	-3.36	118.16	122.70
14	G	1106	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	a	1106	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	A	1102	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	A	1119	CLA	CHD-C1D-ND	-3.36	120.08	124.80
14	A	1129	CLA	C1-C2-C3	-3.35	121.34	126.76
14	B	1022	CLA	OBD-CAD-C3D	-3.35	120.58	128.42
14	A	1101	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
14	G	1129	CLA	C1-C2-C3	-3.35	121.34	126.76
14	b	1225	CLA	C1-C2-C3	-3.35	120.71	126.20
14	a	1137	CLA	O2A-C1-C2	3.35	121.00	108.11
15	B	1238	F6C	CHA-C4D-ND	3.34	136.25	133.05
14	G	1137	CLA	O2A-C1-C2	3.34	120.98	108.11
14	a	1129	CLA	C2B-C1B-NB	3.34	113.79	110.33
14	H	1234	CLA	C2B-C1B-NB	3.34	113.79	110.33
14	A	1137	CLA	O2A-C1-C2	3.34	120.97	108.11
14	b	1201	CLA	C4-C3-C5	3.34	121.03	115.23
14	B	1231	CLA	CMC-C2C-C1C	3.34	130.26	125.03
14	a	1107	CLA	C2B-C1B-NB	3.34	113.79	110.33
14	b	1022	CLA	OBD-CAD-C3D	-3.34	120.61	128.42
14	B	1234	CLA	CHD-C1D-ND	-3.34	120.10	124.80
14	G	1101	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
14	B	1201	CLA	C4-C3-C5	3.34	121.02	115.23
18	A	4011	BCR	C33-C5-C4	3.34	120.71	113.60
14	B	1225	CLA	C1-C2-C3	-3.33	120.73	126.20
14	H	1201	CLA	C4-C3-C5	3.33	121.01	115.23
14	H	1234	CLA	CHD-C1D-ND	-3.33	120.12	124.80
14	A	1107	CLA	O2A-CGA-CBA	3.33	124.52	114.00
14	b	1231	CLA	CMC-C2C-C1C	3.33	130.24	125.03
14	G	1135	CLA	CHD-C1D-ND	-3.33	120.12	124.80
14	A	1107	CLA	C2B-C1B-NB	3.32	113.77	110.33
14	a	1107	CLA	O2A-CGA-CBA	3.32	124.50	114.00
14	G	1107	CLA	C2B-C1B-NB	3.32	113.77	110.33
14	b	1217	CLA	CHD-C1D-ND	-3.32	120.13	124.80
14	H	1022	CLA	OBD-CAD-C3D	-3.32	120.65	128.42
14	G	1107	CLA	O2A-CGA-CBA	3.32	124.49	114.00
14	H	1217	CLA	CHD-C1D-ND	-3.32	120.14	124.80
14	a	1124	CLA	CAA-C2A-C3A	-3.32	104.04	113.00
14	A	1124	CLA	CAA-C2A-C3A	-3.31	104.05	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	L	1503	CLA	CHD-C1D-ND	-3.31	120.14	124.80
14	A	1135	CLA	CHD-C1D-ND	-3.31	120.14	124.80
14	A	1138	CLA	O2A-CGA-CBA	3.31	121.93	111.83
14	H	1233	CLA	C2B-C1B-NB	3.31	113.76	110.33
18	a	4011	BCR	C33-C5-C4	3.31	120.65	113.60
14	a	1138	CLA	O2A-CGA-CBA	3.31	121.92	111.83
20	a	5005	LMG	O8-C28-C29	3.31	121.92	111.83
14	A	1129	CLA	C2B-C1B-NB	3.31	113.76	110.33
14	H	1231	CLA	CMC-C2C-C1C	3.31	130.20	125.03
14	b	1239	CLA	O2A-C1-C2	3.31	120.83	108.11
14	G	1124	CLA	CAA-C2A-C3A	-3.30	104.07	113.00
20	A	5005	LMG	O8-C28-C29	3.30	121.91	111.83
14	B	1239	CLA	O2A-C1-C2	3.30	120.82	108.11
14	G	1138	CLA	O2A-CGA-CBA	3.30	121.91	111.83
14	H	1235	CLA	C1-O2A-CGA	3.30	124.65	116.65
14	a	1126	CLA	O2A-C1-C2	3.30	120.81	108.11
14	b	1227	CLA	O2A-CGA-CBA	3.30	124.43	114.00
14	b	1234	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	A	1130	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
14	B	1206	CLA	O2A-CGA-CBA	3.30	124.42	114.00
14	A	1115	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
20	G	5005	LMG	O8-C28-C29	3.30	121.89	111.83
14	G	1126	CLA	O2A-C1-C2	3.30	120.80	108.11
14	G	1130	CLA	CAA-C2A-C3A	-3.30	104.09	113.00
14	B	1216	CLA	C4-C3-C5	3.30	120.95	115.23
14	B	1235	CLA	C1-O2A-CGA	3.30	124.63	116.65
14	B	1234	CLA	C2B-C1B-NB	3.30	113.75	110.33
18	G	4011	BCR	C33-C5-C4	3.30	120.63	113.60
14	U	1503	CLA	CHD-C1D-ND	-3.30	120.16	124.80
14	H	1239	CLA	O2A-C1-C2	3.30	120.79	108.11
14	b	1233	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	H	1209	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
14	B	1209	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
15	b	1238	F6C	CHA-C4D-ND	3.29	136.20	133.05
14	a	1115	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
14	a	1128	CLA	C3B-C2B-C1B	-3.29	103.29	107.17
14	b	1206	CLA	O2A-CGA-CBA	3.29	124.40	114.00
14	B	1227	CLA	CHD-C1D-ND	-3.29	120.17	124.80
14	B	1233	CLA	C2B-C1B-NB	3.29	113.74	110.33
14	A	1122	CLA	C4-C3-C5	3.29	120.94	115.23
14	a	1130	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
14	b	1235	CLA	C1-O2A-CGA	3.29	124.61	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1126	CLA	O2A-C1-C2	3.29	120.76	108.11
14	H	1227	CLA	O2A-CGA-CBA	3.29	124.38	114.00
14	b	1209	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
14	H	1206	CLA	O2A-CGA-CBA	3.28	124.37	114.00
14	H	1217	CLA	C2B-C1B-NB	3.28	113.73	110.33
14	H	1216	CLA	C4-C3-C5	3.28	120.92	115.23
14	a	1135	CLA	CHD-C1D-ND	-3.28	120.18	124.80
18	a	4007	BCR	C15-C14-C13	-3.28	122.68	127.28
14	A	1126	CLA	C1-C2-C3	-3.28	120.82	126.20
14	G	1115	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
14	B	1227	CLA	O2A-CGA-CBA	3.28	124.36	114.00
14	G	1114	CLA	O2A-CGA-CBA	3.28	124.36	114.00
14	b	1023	CLA	CHD-C1D-ND	-3.28	120.19	124.80
14	a	1127	CLA	C2B-C1B-NB	3.28	113.72	110.33
14	A	1114	CLA	O2A-CGA-CBA	3.28	124.35	114.00
14	G	1126	CLA	C1-C2-C3	-3.28	120.83	126.20
14	B	1224	CLA	CHD-C1D-ND	-3.27	120.19	124.80
14	W	1701	CLA	C4-C3-C5	3.27	120.91	115.23
18	H	4004	BCR	C38-C26-C27	3.27	120.58	113.60
14	A	1128	CLA	C3B-C2B-C1B	-3.27	103.31	107.17
14	K	1401	CLA	O2A-CGA-CBA	3.27	124.34	114.00
14	H	1228	CLA	C1-C2-C3	-3.27	120.84	126.20
14	k	1401	CLA	O2A-CGA-CBA	3.27	124.34	114.00
14	a	1114	CLA	O2A-CGA-CBA	3.27	124.34	114.00
15	H	1230	F6C	O2A-CGA-CBA	3.27	124.34	114.00
14	H	1232	CLA	O2A-CGA-CBA	3.27	124.33	114.00
18	G	4008	BCR	C35-C13-C12	3.27	123.08	118.09
14	H	1226	CLA	O2A-C1-C2	3.27	120.69	108.11
14	B	1022	CLA	C3C-C4C-NC	3.27	114.62	110.43
14	B	1232	CLA	O2A-CGA-CBA	3.27	124.33	114.00
14	A	1127	CLA	C2B-C1B-NB	3.27	113.72	110.33
18	G	4011	BCR	C34-C9-C10	-3.27	117.52	122.82
14	H	1227	CLA	CHD-C1D-ND	-3.27	120.20	124.80
14	b	1022	CLA	C3C-C4C-NC	3.27	114.61	110.43
14	G	1122	CLA	C4-C3-C5	3.27	120.90	115.23
14	H	1218	CLA	C3C-C4C-NC	3.26	114.61	110.43
14	T	1401	CLA	O2A-CGA-CBA	3.26	124.31	114.00
14	a	1122	CLA	C4-C3-C5	3.26	120.89	115.23
18	H	4005	BCR	C38-C26-C27	3.26	120.56	113.60
15	H	1238	F6C	CHA-C4D-ND	3.26	136.17	133.05
14	a	1108	CLA	O2A-CGA-CBA	3.26	124.31	114.00
14	a	1125	CLA	C4C-C3C-C2C	-3.26	102.14	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1108	CLA	O2A-CGA-CBA	3.26	124.30	114.00
14	b	1227	CLA	CHD-C1D-ND	-3.26	120.21	124.80
14	G	1013	CLA	CMC-C2C-C1C	3.26	130.13	125.03
18	A	4002	BCR	C36-C18-C17	-3.26	117.54	122.82
15	B	1230	F6C	O2A-CGA-CBA	3.26	124.29	114.00
14	b	1232	CLA	O2A-CGA-CBA	3.26	124.29	114.00
18	A	4007	BCR	C15-C14-C13	-3.26	122.71	127.28
18	B	4005	BCR	C38-C26-C27	3.26	120.54	113.60
19	a	5001	LHG	O8-C23-C24	3.26	121.76	111.83
14	a	1126	CLA	C1-C2-C3	-3.26	120.86	126.20
14	a	1118	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	l	1503	CLA	CHD-C1D-ND	-3.26	120.22	124.80
14	B	1218	CLA	C3C-C4C-NC	3.26	114.60	110.43
14	b	1216	CLA	C4-C3-C5	3.26	120.88	115.23
14	b	1226	CLA	O2A-C1-C2	3.25	120.63	108.11
14	G	1120	CLA	O2A-CGA-CBA	3.25	124.28	114.00
15	b	1230	F6C	O2A-CGA-CBA	3.25	124.28	114.00
18	A	4008	BCR	C35-C13-C12	3.25	123.06	118.09
14	A	1108	CLA	O2A-CGA-CBA	3.25	124.28	114.00
14	G	1123	CLA	CMA-C3A-C4A	3.25	120.52	111.77
18	R	4020	BCR	C15-C14-C13	-3.25	122.72	127.28
14	B	1220	CLA	CAA-C2A-C3A	-3.25	104.21	113.00
18	a	4011	BCR	C34-C9-C10	-3.25	117.55	122.82
18	a	4008	BCR	C35-C13-C12	3.25	123.06	118.09
14	b	1224	CLA	CHD-C1D-ND	-3.25	120.23	124.80
19	A	5001	LHG	O8-C23-C24	3.25	121.75	111.83
14	x	1701	CLA	C4-C3-C5	3.25	120.87	115.23
14	a	1123	CLA	CMA-C3A-C4A	3.25	120.51	111.77
14	B	1226	CLA	O2A-C1-C2	3.25	120.62	108.11
14	a	1013	CLA	CMC-C2C-C1C	3.25	130.11	125.03
18	b	4004	BCR	C38-C26-C27	3.25	120.53	113.60
14	H	1220	CLA	CAA-C2A-C3A	-3.25	104.22	113.00
14	G	1129	CLA	C2B-C1B-NB	3.25	113.69	110.33
14	A	1120	CLA	O2A-CGA-CBA	3.25	124.26	114.00
14	B	1217	CLA	C2B-C1B-NB	3.25	113.69	110.33
14	X	1701	CLA	C4-C3-C5	3.25	120.86	115.23
14	a	1120	CLA	O2A-CGA-CBA	3.25	124.26	114.00
14	B	1212	CLA	O2A-CGA-CBA	3.25	124.25	114.00
18	I	4020	BCR	C15-C14-C13	-3.25	122.73	127.28
18	A	4011	BCR	C34-C9-C10	-3.24	117.56	122.82
18	G	4007	BCR	C15-C14-C13	-3.24	122.73	127.28
14	H	1022	CLA	C3C-C4C-NC	3.24	114.59	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1236	CLA	O2A-CGA-CBA	3.24	124.25	114.00
18	G	4008	BCR	C33-C5-C6	-3.24	120.94	124.48
18	G	4002	BCR	C36-C18-C17	-3.24	117.56	122.82
14	b	1220	CLA	CAA-C2A-C3A	-3.24	104.24	113.00
19	G	5001	LHG	O8-C23-C24	3.24	121.72	111.83
14	G	1128	CLA	C3B-C2B-C1B	-3.24	103.35	107.17
18	A	4008	BCR	C33-C5-C6	-3.24	120.95	124.48
14	A	1123	CLA	CMA-C3A-C4A	3.24	120.48	111.77
14	H	1212	CLA	O2A-CGA-CBA	3.24	124.23	114.00
14	b	1218	CLA	C3C-C4C-NC	3.24	114.58	110.43
14	A	1139	CLA	C2B-C1B-NB	3.24	113.68	110.33
14	b	1228	CLA	C1-C2-C3	-3.24	120.89	126.20
14	b	1236	CLA	O2A-CGA-CBA	3.24	124.23	114.00
14	b	1212	CLA	O2A-CGA-CBA	3.24	124.22	114.00
14	G	1101	CLA	O2A-CGA-CBA	3.23	124.22	114.00
14	G	1122	CLA	CAC-C3C-C4C	3.23	129.00	124.79
14	B	1216	CLA	O2A-CGA-CBA	3.23	121.69	111.83
14	H	1023	CLA	CHD-C1D-ND	-3.23	120.25	124.80
14	a	1133	CLA	C2B-C1B-NB	3.23	113.68	110.33
14	a	1139	CLA	C2B-C1B-NB	3.23	113.68	110.33
14	G	1135	CLA	C2B-C1B-NB	3.23	113.68	110.33
14	G	1139	CLA	C2B-C1B-NB	3.23	113.68	110.33
18	B	4004	BCR	C38-C26-C27	3.23	120.49	113.60
14	b	1216	CLA	O2A-CGA-CBA	3.23	121.69	111.83
14	b	1235	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
14	A	1118	CLA	CHD-C1D-ND	-3.23	120.25	124.80
14	G	1125	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
14	B	1228	CLA	C1-C2-C3	-3.23	120.90	126.20
18	b	4005	BCR	C38-C26-C27	3.23	120.48	113.60
18	i	4020	BCR	C15-C14-C13	-3.23	122.75	127.28
14	B	1236	CLA	O2A-CGA-CBA	3.23	124.20	114.00
14	B	1227	CLA	CMD-C2D-C3D	-3.23	120.28	127.69
14	b	1204	CLA	C1-C2-C3	-3.23	120.91	126.20
14	b	1217	CLA	C2B-C1B-NB	3.23	113.67	110.33
14	B	1023	CLA	CHD-C1D-ND	-3.23	120.26	124.80
14	a	1110	CLA	O2A-CGA-CBA	3.23	124.20	114.00
14	A	1013	CLA	CMC-C2C-C1C	3.23	130.08	125.03
14	G	1127	CLA	C2B-C1B-NB	3.23	113.67	110.33
14	B	1212	CLA	CHD-C1D-ND	-3.23	120.26	124.80
14	a	1113	CLA	O2A-CGA-CBA	3.23	124.19	114.00
14	H	1227	CLA	CMD-C2D-C3D	-3.22	120.30	127.69
18	a	4002	BCR	C36-C18-C17	-3.22	117.59	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1227	CLA	CMD-C2D-C3D	-3.22	120.30	127.69
14	H	1222	CLA	CAA-C2A-C3A	-3.22	104.29	113.00
14	b	1212	CLA	CHD-C1D-ND	-3.22	120.27	124.80
14	A	1125	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
14	B	1222	CLA	CAA-C2A-C3A	-3.22	104.30	113.00
15	a	1121	F6C	CHB-C4A-C3A	-3.22	118.79	125.49
14	B	1222	CLA	C1-C2-C3	-3.22	120.92	126.20
14	b	1222	CLA	CAA-C2A-C3A	-3.22	104.30	113.00
14	H	1216	CLA	O2A-CGA-CBA	3.22	121.64	111.83
14	H	1224	CLA	CHD-C1D-ND	-3.22	120.28	124.80
14	b	1221	CLA	C1-C2-C3	-3.22	120.93	126.20
14	a	1101	CLA	O2A-CGA-CBA	3.22	124.16	114.00
14	H	1235	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
14	A	1113	CLA	O2A-CGA-CBA	3.22	124.16	114.00
14	A	1135	CLA	CMD-C2D-C3D	-3.22	120.32	127.69
15	A	1121	F6C	CHB-C4A-C3A	-3.21	118.80	125.49
20	H	5002	LMG	C8-O7-C10	-3.21	110.11	117.80
14	U	1503	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	G	1113	CLA	O2A-CGA-CBA	3.21	124.15	114.00
14	B	1235	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	a	1135	CLA	CMD-C2D-C3D	-3.21	120.33	127.69
14	H	1204	CLA	C1-C2-C3	-3.21	120.94	126.20
14	B	1221	CLA	C1-C2-C3	-3.21	120.94	126.20
14	B	1022	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
14	a	1135	CLA	C2B-C1B-NB	3.21	113.65	110.33
14	G	1110	CLA	O2A-CGA-CBA	3.21	124.14	114.00
18	B	4006	BCR	C3-C4-C5	-3.21	108.33	114.06
14	H	1212	CLA	CHD-C1D-ND	-3.21	120.29	124.80
14	A	1101	CLA	O2A-CGA-CBA	3.21	124.13	114.00
14	G	1140	CLA	O2A-C1-C2	3.21	120.45	108.11
14	A	1110	CLA	O2A-CGA-CBA	3.21	124.13	114.00
14	H	1022	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
14	B	1231	CLA	C2B-C1B-NB	3.21	113.65	110.33
14	l	1503	CLA	C2B-C1B-NB	3.21	113.65	110.33
14	A	1133	CLA	C2B-C1B-NB	3.21	113.65	110.33
14	a	1140	CLA	O2A-C1-C2	3.21	120.44	108.11
14	A	1140	CLA	O2A-C1-C2	3.20	120.44	108.11
14	H	1222	CLA	C1-C2-C3	-3.20	120.95	126.20
14	b	1222	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	G	1012	CLA	C2B-C1B-NB	3.20	113.65	110.33
18	a	4008	BCR	C33-C5-C6	-3.20	120.99	124.48
18	H	4006	BCR	C3-C4-C5	-3.20	108.35	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1221	CLA	C1-C2-C3	-3.20	120.95	126.20
14	G	1118	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	B	1222	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
15	a	1121	F6C	O2A-CGA-CBA	3.20	124.11	114.00
14	b	1215	CLA	O2A-C1-C2	3.20	120.42	108.11
14	B	1204	CLA	C1-C2-C3	-3.20	120.95	126.20
18	b	4006	BCR	C3-C4-C5	-3.20	108.35	114.06
13	a	1011	CL0	O2A-C1-C2	3.20	120.42	108.11
15	G	1121	F6C	CHB-C4A-C3A	-3.20	118.83	125.49
15	H	1237	F6C	CHD-C1D-ND	-3.20	119.49	124.31
14	A	1129	CLA	CHD-C1D-ND	-3.20	120.30	124.80
14	a	1105	CLA	O2A-CGA-CBA	3.20	124.10	114.00
14	l	1503	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
14	G	1135	CLA	CMD-C2D-C3D	-3.20	120.36	127.69
14	a	1107	CLA	CHD-C1D-ND	-3.20	120.31	124.80
14	G	1138	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
14	H	1222	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
14	H	1022	CLA	CMB-C2B-C1B	3.20	130.28	125.42
14	B	1022	CLA	CMB-C2B-C1B	3.19	130.28	125.42
15	G	1121	F6C	O2A-CGA-CBA	3.19	124.09	114.00
14	b	1231	CLA	C2B-C1B-NB	3.19	113.64	110.33
14	a	1130	CLA	OBD-CAD-C3D	-3.19	120.95	128.42
14	G	1133	CLA	C2B-C1B-NB	3.19	113.64	110.33
14	H	1231	CLA	C2B-C1B-NB	3.19	113.64	110.33
14	b	1022	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
13	A	1011	CL0	O2A-C1-C2	3.19	120.39	108.11
14	a	1128	CLA	CHD-C1D-ND	-3.19	120.31	124.80
14	B	1221	CLA	CAA-C2A-C3A	-3.19	104.38	113.00
14	a	1139	CLA	O2A-CGA-CBA	3.19	124.08	114.00
14	H	1215	CLA	O2A-C1-C2	3.19	120.38	108.11
14	B	1215	CLA	O2A-C1-C2	3.19	120.38	108.11
14	b	1222	CLA	C1-C2-C3	-3.19	120.97	126.20
14	A	1012	CLA	C2B-C1B-NB	3.19	113.63	110.33
14	A	1110	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
14	A	1139	CLA	O2A-CGA-CBA	3.19	124.06	114.00
14	A	1106	CLA	C1-C2-C3	-3.18	120.98	126.20
13	G	1011	CL0	O2A-C1-C2	3.18	120.36	108.11
14	A	1105	CLA	O2A-CGA-CBA	3.18	124.06	114.00
14	A	1122	CLA	CAC-C3C-C4C	3.18	128.93	124.79
14	G	1139	CLA	O2A-CGA-CBA	3.18	124.06	114.00
14	A	1135	CLA	C2B-C1B-NB	3.18	113.62	110.33
14	G	1105	CLA	O2A-CGA-CBA	3.18	124.05	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1107	CLA	CHD-C1D-ND	-3.18	120.33	124.80
14	L	1503	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
14	H	1221	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
14	G	1129	CLA	CHD-C1D-ND	-3.18	120.33	124.80
20	B	5002	LMG	C8-O7-C10	-3.18	110.19	117.80
14	b	1222	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
18	a	4003	BCR	C33-C5-C6	-3.18	121.02	124.48
14	a	1129	CLA	CHD-C1D-ND	-3.18	120.33	124.80
14	b	1022	CLA	CMB-C2B-C1B	3.18	130.25	125.42
14	G	1107	CLA	CHD-C1D-ND	-3.18	120.33	124.80
15	A	1121	F6C	O2A-CGA-CBA	3.17	124.03	114.00
14	G	1130	CLA	OBD-CAD-C3D	-3.17	121.00	128.42
14	b	1221	CLA	CAA-C2A-C3A	-3.17	104.42	113.00
18	U	4022	BCR	C33-C5-C4	3.17	120.36	113.60
20	b	5002	LMG	C8-O7-C10	-3.17	110.20	117.80
14	a	1122	CLA	CAC-C3C-C4C	3.17	128.91	124.79
15	B	1237	F6C	CHD-C1D-ND	-3.17	119.54	124.31
14	a	1106	CLA	C1-C2-C3	-3.17	121.01	126.20
14	L	1503	CLA	C2B-C1B-NB	3.17	113.61	110.33
15	b	1237	F6C	CHD-C1D-ND	-3.17	119.54	124.31
14	a	1134	CLA	O2A-CGA-CBA	3.17	124.01	114.00
14	H	1222	CLA	CHD-C1D-ND	-3.17	120.34	124.80
14	a	1110	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	G	1134	CLA	O2A-CGA-CBA	3.17	124.01	114.00
14	A	1130	CLA	OBD-CAD-C3D	-3.17	121.01	128.42
14	G	1110	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	A	1134	CLA	O2A-CGA-CBA	3.16	124.00	114.00
14	a	1138	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
14	U	1502	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
14	A	1138	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
18	G	4003	BCR	C33-C5-C6	-3.16	121.03	124.48
18	A	4003	BCR	C3-C4-C5	-3.16	108.42	114.06
18	a	4003	BCR	C3-C4-C5	-3.16	108.42	114.06
14	G	1132	CLA	CAA-C2A-C3A	-3.16	104.46	113.00
14	a	1012	CLA	C2B-C1B-NB	3.16	113.60	110.33
14	B	1222	CLA	CHD-C1D-ND	-3.16	120.35	124.80
18	l	4022	BCR	C33-C5-C4	3.16	120.33	113.60
14	G	1106	CLA	C1-C2-C3	-3.16	121.02	126.20
14	l	1502	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
18	L	4022	BCR	C33-C5-C4	3.16	120.33	113.60
15	b	1230	F6C	C3C-C4C-NC	3.16	113.78	110.32
14	A	1126	CLA	CAA-C2A-C3A	-3.16	104.47	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4003	BCR	C33-C5-C6	-3.16	121.04	124.48
14	A	1132	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
18	G	4003	BCR	C3-C4-C5	-3.16	108.43	114.06
14	L	1502	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
18	U	4019	BCR	C4-C5-C6	-3.15	118.44	122.70
14	a	1132	CLA	CAA-C2A-C3A	-3.15	104.48	113.00
14	X	1701	CLA	CHD-C1D-ND	-3.15	120.36	124.80
18	a	4008	BCR	C34-C9-C10	-3.15	117.71	122.82
15	b	1230	F6C	O1D-CGD-CBD	-3.15	118.30	124.52
14	A	1128	CLA	CHD-C1D-ND	-3.15	120.37	124.80
18	B	4010	BCR	C19-C18-C17	3.15	123.96	119.01
14	x	1701	CLA	CAC-C3C-C4C	3.15	128.88	124.79
14	H	1233	CLA	CMB-C2B-C1B	3.15	130.21	125.42
14	x	1701	CLA	CHD-C1D-ND	-3.14	120.38	124.80
14	W	1701	CLA	CAC-C3C-C4C	3.14	128.88	124.79
15	H	1230	F6C	O1D-CGD-CBD	-3.14	118.32	124.52
14	A	1135	CLA	C1-C2-C3	-3.14	121.05	126.20
14	G	1126	CLA	CAA-C2A-C3A	-3.14	104.51	113.00
14	a	1126	CLA	CAA-C2A-C3A	-3.14	104.51	113.00
18	A	4008	BCR	C34-C9-C10	-3.14	117.73	122.82
14	a	1107	CLA	CMB-C2B-C1B	3.13	130.19	125.42
14	G	1128	CLA	CHD-C1D-ND	-3.13	120.39	124.80
14	W	1701	CLA	CHD-C1D-ND	-3.13	120.39	124.80
15	B	1230	F6C	O1D-CGD-CBD	-3.13	118.34	124.52
14	H	1215	CLA	C4-C3-C5	3.13	120.66	115.23
14	U	1503	CLA	C2B-C1B-NB	3.13	113.57	110.33
14	b	1214	CLA	CMB-C2B-C1B	3.13	130.18	125.42
18	b	4010	BCR	C19-C18-C17	3.13	123.93	119.01
15	B	1207	F6C	C4-C3-C2	-3.13	115.60	123.63
14	b	1210	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
14	a	1128	CLA	C1D-ND-C4D	-3.13	104.12	106.31
14	G	1135	CLA	C1-C2-C3	-3.13	121.08	126.20
14	H	1210	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
18	l	4019	BCR	C4-C5-C6	-3.12	118.48	122.70
18	L	4019	BCR	C4-C5-C6	-3.12	118.48	122.70
14	B	1215	CLA	C4-C3-C5	3.12	120.65	115.23
14	a	1139	CLA	CHD-C1D-ND	-3.12	120.41	124.80
14	H	1214	CLA	CMB-C2B-C1B	3.12	130.17	125.42
14	A	1107	CLA	CMB-C2B-C1B	3.12	130.17	125.42
14	B	1210	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
14	G	1107	CLA	CMB-C2B-C1B	3.12	130.17	125.42
14	X	1701	CLA	CAC-C3C-C4C	3.12	128.84	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1207	F6C	C4-C3-C2	-3.12	115.62	123.63
14	a	1109	CLA	C4-C3-C5	3.12	120.64	115.23
14	A	1139	CLA	CHD-C1D-ND	-3.11	120.42	124.80
14	B	1023	CLA	CAA-C2A-C3A	-3.11	104.59	113.00
14	b	1233	CLA	CMB-C2B-C1B	3.11	130.16	125.42
14	b	1215	CLA	C4-C3-C5	3.11	120.63	115.23
14	G	1139	CLA	CHD-C1D-ND	-3.11	120.42	124.80
14	B	1214	CLA	CMB-C2B-C1B	3.11	130.16	125.42
14	B	1218	CLA	O2A-CGA-CBA	3.11	123.83	114.00
15	H	1230	F6C	C3C-C4C-NC	3.11	113.73	110.32
18	G	4008	BCR	C34-C9-C10	-3.11	117.78	122.82
14	B	1233	CLA	CMB-C2B-C1B	3.11	130.15	125.42
18	G	4011	BCR	C28-C27-C26	-3.11	108.52	114.06
18	H	4010	BCR	C19-C18-C17	3.10	123.89	119.01
14	G	1123	CLA	C2B-C1B-NB	3.10	113.55	110.33
14	a	1106	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	a	1135	CLA	C1-C2-C3	-3.10	121.11	126.20
14	b	1218	CLA	O2A-CGA-CBA	3.10	123.80	114.00
15	H	1207	F6C	C4-C3-C2	-3.10	115.66	123.63
14	H	1218	CLA	O2A-CGA-CBA	3.10	123.80	114.00
14	a	1128	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
14	H	1023	CLA	CAA-C2A-C3A	-3.10	104.63	113.00
18	a	4011	BCR	C28-C27-C26	-3.10	108.54	114.06
14	G	1109	CLA	C4-C3-C5	3.09	120.60	115.23
14	b	1023	CLA	CAA-C2A-C3A	-3.09	104.64	113.00
15	H	1238	F6C	C3C-C4C-NC	3.09	113.71	110.32
14	B	1228	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
14	b	1219	CLA	O2A-CGA-CBA	3.09	123.76	114.00
14	a	1123	CLA	C2B-C1B-NB	3.09	113.53	110.33
14	A	1109	CLA	C4-C3-C5	3.09	120.59	115.23
15	G	1121	F6C	CHA-C4D-ND	3.09	136.00	133.05
14	A	1106	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	B	1219	CLA	O2A-CGA-CBA	3.09	123.76	114.00
14	a	1122	CLA	C1-C2-C3	-3.09	121.14	126.20
15	B	1230	F6C	C3C-C4C-NC	3.09	113.70	110.32
14	b	1226	CLA	C4-C3-C5	3.08	120.58	115.23
18	A	4011	BCR	C28-C27-C26	-3.08	108.56	114.06
14	A	1130	CLA	CMB-C2B-C3B	3.08	133.80	126.55
14	H	1204	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
14	a	1136	CLA	C4-C3-C5	3.08	120.58	115.23
18	I	4018	BCR	C38-C26-C27	3.08	120.16	113.60
14	H	1223	CLA	CHD-C1D-ND	-3.08	120.47	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1228	CLA	CAA-C2A-C3A	-3.08	104.68	113.00
14	G	1122	CLA	C1-C2-C3	-3.08	121.15	126.20
14	b	1228	CLA	CAA-C2A-C3A	-3.08	104.69	113.00
14	G	1130	CLA	CMB-C2B-C3B	3.08	133.78	126.55
14	H	1023	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
14	b	1226	CLA	C2B-C1B-NB	3.08	113.52	110.33
14	a	1140	CLA	CMC-C2C-C1C	3.07	129.84	125.03
14	a	1118	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	A	1128	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
14	H	1219	CLA	O2A-CGA-CBA	3.07	123.71	114.00
18	i	4018	BCR	C38-C26-C27	3.07	120.15	113.60
14	B	1239	CLA	CMC-C2C-C3C	3.07	134.46	126.15
14	H	1226	CLA	C4-C3-C5	3.07	120.56	115.23
14	B	1226	CLA	C4-C3-C5	3.07	120.56	115.23
14	B	1023	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
14	B	1227	CLA	C4D-C3D-CAD	3.07	111.44	108.11
14	b	1202	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	G	1123	CLA	C1-C2-C3	-3.07	121.17	126.20
14	A	1118	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	a	1012	CLA	C6-C5-C3	-3.07	106.00	113.47
14	A	1122	CLA	C1-C2-C3	-3.07	121.17	126.20
20	B	5002	LMG	O8-C28-C29	3.07	121.19	111.83
14	G	1140	CLA	CMC-C2C-C1C	3.07	129.83	125.03
14	A	1140	CLA	CMC-C2C-C1C	3.07	129.83	125.03
14	b	1023	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
14	A	1130	CLA	O2A-C1-C2	3.07	119.91	108.11
14	G	1012	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	A	1123	CLA	C2B-C1B-NB	3.06	113.50	110.33
14	G	1128	CLA	C1D-ND-C4D	-3.06	104.16	106.31
18	b	4004	BCR	C2-C1-C6	3.06	114.89	110.44
14	b	1239	CLA	CMC-C2C-C3C	3.06	134.44	126.15
14	A	1119	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
14	G	1106	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	H	1239	CLA	CMC-C2C-C3C	3.06	134.43	126.15
14	G	1128	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
14	G	1130	CLA	O2A-C1-C2	3.06	119.89	108.11
14	a	1130	CLA	O2A-C1-C2	3.06	119.88	108.11
18	R	4018	BCR	C38-C26-C27	3.06	120.12	113.60
20	H	5002	LMG	O8-C28-C29	3.06	121.16	111.83
14	a	1123	CLA	C1-C2-C3	-3.06	121.19	126.20
14	L	1501	CLA	CHD-C1D-ND	-3.06	120.50	124.80
14	a	1130	CLA	CMB-C2B-C3B	3.06	133.74	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1136	CLA	C4-C3-C5	3.06	120.53	115.23
14	l	1501	CLA	CHD-C1D-ND	-3.06	120.50	124.80
14	G	1118	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	B	1223	CLA	CHD-C1D-ND	-3.06	120.50	124.80
15	H	1237	F6C	C4A-C3A-C2A	-3.06	102.44	106.97
14	A	1012	CLA	C6-C5-C3	-3.05	106.03	113.47
14	H	1227	CLA	C4D-C3D-CAD	3.05	111.42	108.11
15	B	1237	F6C	C4A-C3A-C2A	-3.05	102.44	106.97
14	b	1223	CLA	CHD-C1D-ND	-3.05	120.50	124.80
18	l	4022	BCR	C3-C4-C5	-3.05	108.61	114.06
15	b	1237	F6C	C4A-C3A-C2A	-3.05	102.44	106.97
14	G	1113	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
18	B	4004	BCR	C2-C1-C6	3.05	114.87	110.44
14	a	1119	CLA	CHC-C1C-C2C	-3.05	118.28	126.95
14	a	1105	CLA	CAA-C2A-C3A	-3.05	104.76	113.00
14	G	1119	CLA	CHC-C1C-C2C	-3.05	118.28	126.95
14	B	1204	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
14	U	1501	CLA	CHD-C1D-ND	-3.05	120.51	124.80
14	G	1012	CLA	C6-C5-C3	-3.05	106.04	113.47
18	U	4022	BCR	C3-C4-C5	-3.05	108.62	114.06
15	a	1121	F6C	CHA-C4D-ND	3.04	135.96	133.05
14	k	1401	CLA	CMA-C3A-C4A	3.04	119.95	111.77
14	K	1401	CLA	CMA-C3A-C4A	3.04	119.95	111.77
14	U	1502	CLA	CMC-C2C-C1C	3.04	129.79	125.03
14	G	1136	CLA	C4-C3-C5	3.04	120.51	115.23
14	A	1105	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
14	a	1012	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	H	1226	CLA	C2B-C1B-NB	3.04	113.48	110.33
20	b	5002	LMG	O8-C28-C29	3.04	121.10	111.83
18	a	4001	BCR	C38-C26-C25	-3.04	121.17	124.48
18	L	4022	BCR	C3-C4-C5	-3.04	108.64	114.06
14	G	1105	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
15	G	1121	F6C	CHD-C1D-ND	-3.04	119.73	124.31
14	T	1401	CLA	CMA-C3A-C4A	3.04	119.94	111.77
14	H	1202	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	b	1021	CLA	C2B-C1B-NB	3.04	113.47	110.33
14	B	1202	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	b	1204	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
18	H	4004	BCR	C2-C1-C6	3.03	114.84	110.44
14	a	1109	CLA	C4D-C3D-CAD	3.03	111.40	108.11
14	a	1139	CLA	C4D-C3D-CAD	3.03	111.40	108.11
15	b	1238	F6C	C3C-C4C-NC	3.03	113.64	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1012	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
18	i	4020	BCR	C3-C4-C5	-3.03	108.65	114.06
14	b	1204	CLA	C6-C5-C3	-3.03	106.08	113.47
15	A	1121	F6C	CHA-C4D-ND	3.03	135.95	133.05
15	B	1207	F6C	OMB-CMB-C2B	-3.03	118.78	125.62
14	b	1227	CLA	C4D-C3D-CAD	3.03	111.40	108.11
14	B	1204	CLA	C6-C5-C3	-3.03	106.09	113.47
15	b	1207	F6C	OMB-CMB-C2B	-3.03	118.79	125.62
15	B	1238	F6C	C3C-C4C-NC	3.03	113.64	110.32
14	a	1136	CLA	O2A-C1-C2	3.03	119.75	108.11
14	H	1204	CLA	C6-C5-C3	-3.02	106.10	113.47
14	G	1136	CLA	O2A-C1-C2	3.02	119.75	108.11
14	a	1109	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
14	B	1021	CLA	C2B-C1B-NB	3.02	113.46	110.33
14	L	1502	CLA	CMC-C2C-C1C	3.02	129.76	125.03
14	G	1109	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
14	l	1502	CLA	CMC-C2C-C1C	3.02	129.76	125.03
14	G	1124	CLA	CAA-C2A-C1A	-3.02	102.07	111.97
18	G	4002	BCR	C38-C26-C27	3.02	120.03	113.60
14	H	1204	CLA	C3D-C4D-ND	3.02	114.89	109.99
14	A	1123	CLA	C1-C2-C3	-3.02	121.25	126.20
14	a	1119	CLA	O2A-CGA-CBA	3.02	121.03	111.83
14	A	1124	CLA	CAA-C2A-C1A	-3.02	102.09	111.97
14	A	1136	CLA	O2A-C1-C2	3.02	119.71	108.11
14	A	1128	CLA	C1D-ND-C4D	-3.01	104.20	106.31
15	H	1207	F6C	OMB-CMB-C2B	-3.01	118.82	125.62
14	A	1119	CLA	O2A-CGA-CBA	3.01	121.02	111.83
14	B	1021	CLA	CHD-C1D-ND	-3.01	120.57	124.80
14	b	1239	CLA	C3C-C4C-NC	3.01	114.29	110.43
18	A	4002	BCR	C38-C26-C27	3.01	120.01	113.60
14	b	1211	CLA	O2A-CGA-CBA	3.01	121.01	111.83
14	B	1226	CLA	C2B-C1B-NB	3.01	113.45	110.33
18	I	4020	BCR	C3-C4-C5	-3.01	108.69	114.06
14	B	1219	CLA	O1D-CGD-CBD	-3.01	118.59	124.52
15	b	1237	F6C	CHA-C4D-ND	3.01	135.93	133.05
14	b	1021	CLA	CHD-C1D-ND	-3.01	120.57	124.80
14	A	1139	CLA	C4D-C3D-CAD	3.01	111.37	108.11
14	H	1021	CLA	CHD-C1D-ND	-3.01	120.57	124.80
14	a	1124	CLA	CAA-C2A-C1A	-3.01	102.13	111.97
14	A	1109	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	b	1219	CLA	O1D-CGD-CBD	-3.00	118.60	124.52
14	B	1204	CLA	C3D-C4D-ND	3.00	114.87	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1219	CLA	O1D-CGD-CBD	-3.00	118.60	124.52
14	a	1113	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	G	1119	CLA	O2A-CGA-CBA	3.00	120.99	111.83
18	a	4002	BCR	C38-C26-C27	3.00	119.99	113.60
18	b	4006	BCR	C38-C26-C25	-3.00	121.21	124.48
18	G	4001	BCR	C38-C26-C25	-3.00	121.21	124.48
14	A	1113	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
14	H	1239	CLA	C3C-C4C-NC	3.00	114.27	110.43
14	G	1125	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
18	R	4020	BCR	C3-C4-C5	-2.99	108.72	114.06
14	H	1211	CLA	O2A-CGA-CBA	2.99	120.96	111.83
14	b	1204	CLA	C3D-C4D-ND	2.99	114.85	109.99
14	B	1223	CLA	C3C-C4C-NC	2.99	114.26	110.43
14	A	1125	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	B	1211	CLA	O2A-CGA-CBA	2.99	120.95	111.83
14	a	1125	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	A	1011	CL0	CMA-C3A-C4A	-2.99	108.17	114.61
14	A	1109	CLA	C4D-C3D-CAD	2.99	111.35	108.11
14	H	1223	CLA	C3C-C4C-NC	2.99	114.26	110.43
15	a	1121	F6C	CHD-C1D-ND	-2.99	119.81	124.31
14	a	1136	CLA	CMA-C3A-C4A	2.99	119.80	111.77
15	H	1237	F6C	CHA-C4D-ND	2.99	135.91	133.05
15	B	1237	F6C	CHA-C4D-ND	2.99	135.91	133.05
14	G	1139	CLA	C4D-C3D-CAD	2.99	111.35	108.11
14	H	1229	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
15	A	1121	F6C	CHD-C1D-ND	-2.98	119.82	124.31
13	a	1011	CL0	CMA-C3A-C4A	-2.98	108.19	114.61
13	G	1011	CL0	CMA-C3A-C4A	-2.98	108.19	114.61
14	a	1128	CLA	C4-C3-C5	2.98	120.40	115.23
14	B	1022	CLA	CHD-C1D-ND	-2.98	120.61	124.80
14	b	1229	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	G	1136	CLA	CMA-C3A-C4A	2.98	119.78	111.77
14	B	1201	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	G	1128	CLA	C4-C3-C5	2.98	120.39	115.23
14	H	1211	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
14	B	1215	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
14	a	1106	CLA	C4-C3-C5	2.97	120.39	115.23
14	A	1115	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	A	1012	CLA	CAA-C2A-C3A	-2.97	104.96	113.00
14	a	1136	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	b	1225	CLA	CMB-C2B-C3B	2.97	133.54	126.55
14	B	1229	CLA	O2D-CGD-O1D	-2.97	118.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1109	CLA	C1-C2-C3	-2.97	121.33	126.20
14	A	1136	CLA	CMA-C3A-C4A	2.97	119.76	111.77
14	a	1012	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
14	G	1012	CLA	CAA-C2A-C3A	-2.97	104.97	113.00
14	a	1115	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	H	1022	CLA	CHD-C1D-ND	-2.97	120.62	124.80
14	a	1109	CLA	C1-C2-C3	-2.97	121.33	126.20
18	A	4001	BCR	C38-C26-C25	-2.97	121.24	124.48
14	G	1115	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	a	1111	CLA	CAC-C3C-C4C	2.97	128.65	124.79
18	b	4016	BCR	C30-C25-C26	-2.97	118.58	122.64
14	b	1201	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	B	1211	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
18	B	4006	BCR	C34-C9-C10	-2.97	118.01	122.82
14	B	1239	CLA	C3C-C4C-NC	2.97	114.23	110.43
14	H	1214	CLA	C2B-C1B-NB	2.97	113.40	110.33
14	B	1235	CLA	CAA-C2A-C3A	-2.96	104.99	113.00
18	B	4006	BCR	C38-C26-C25	-2.96	121.25	124.48
14	H	1235	CLA	CAA-C2A-C3A	-2.96	104.99	113.00
14	H	1021	CLA	C2B-C1B-NB	2.96	113.40	110.33
18	m	4021	BCR	C19-C18-C17	2.96	123.67	119.01
18	H	4006	BCR	C34-C9-C10	-2.96	118.02	122.82
18	B	4016	BCR	C30-C25-C26	-2.96	118.59	122.64
14	b	1214	CLA	C2B-C1B-NB	2.96	113.40	110.33
14	G	1106	CLA	C4-C3-C5	2.96	120.36	115.23
14	A	1128	CLA	C4-C3-C5	2.96	120.36	115.23
14	b	1229	CLA	C3D-C4D-ND	2.96	114.79	109.99
14	A	1136	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	H	1201	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	G	1109	CLA	C4D-C3D-CAD	2.95	111.31	108.11
14	B	1210	CLA	C1-O2A-CGA	2.95	123.80	116.65
14	b	1211	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
18	V	4021	BCR	C19-C18-C17	2.95	123.65	119.01
18	b	4006	BCR	C34-C9-C10	-2.95	118.03	122.82
18	M	4021	BCR	C19-C18-C17	2.95	123.65	119.01
14	b	1215	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	G	1109	CLA	C1-C2-C3	-2.95	121.37	126.20
14	A	1111	CLA	CAC-C3C-C4C	2.95	128.62	124.79
14	G	1136	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
18	H	4016	BCR	C30-C25-C26	-2.95	118.61	122.64
14	B	1226	CLA	C1D-ND-C4D	-2.95	104.25	106.31
18	B	4014	BCR	C34-C9-C10	-2.94	118.05	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1225	CLA	CMB-C2B-C3B	2.94	133.48	126.55
14	a	1116	CLA	CMC-C2C-C1C	2.94	129.63	125.03
14	b	1022	CLA	CHD-C1D-ND	-2.94	120.66	124.80
14	A	1106	CLA	C4-C3-C5	2.94	120.34	115.23
18	U	4019	BCR	C24-C25-C26	-2.94	114.78	121.56
14	b	1223	CLA	C3C-C4C-NC	2.94	114.20	110.43
14	b	1210	CLA	C1-O2A-CGA	2.94	123.77	116.65
18	l	4019	BCR	C24-C25-C26	-2.94	114.78	121.56
18	b	4009	BCR	C33-C5-C6	-2.94	121.27	124.48
14	B	1218	CLA	CMC-C2C-C1C	2.94	129.63	125.03
14	B	1229	CLA	C3D-C4D-ND	2.94	114.77	109.99
14	H	1219	CLA	CMB-C2B-C1B	2.94	129.90	125.42
14	A	1113	CLA	CMA-C3A-C4A	2.94	119.67	111.77
14	b	1216	CLA	CED-O2D-CGD	2.94	122.58	115.92
18	H	4014	BCR	C34-C9-C10	-2.94	118.06	122.82
15	H	1237	F6C	CMA-C3A-C2A	-2.94	118.21	126.15
14	G	1140	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
14	A	1140	CLA	O2D-CGD-O1D	-2.94	118.14	123.85
14	B	1225	CLA	CMB-C2B-C3B	2.93	133.45	126.55
14	b	1235	CLA	CAA-C2A-C3A	-2.93	105.07	113.00
18	H	4006	BCR	C38-C26-C25	-2.93	121.28	124.48
14	B	1232	CLA	C4D-C3D-CAD	2.93	111.29	108.11
14	G	1113	CLA	CMA-C3A-C4A	2.93	119.66	111.77
14	B	1214	CLA	C2B-C1B-NB	2.93	113.37	110.33
14	b	1217	CLA	CMC-C2C-C1C	2.93	129.62	125.03
14	A	1115	CLA	CMC-C2C-C1C	2.93	129.62	125.03
18	b	4004	BCR	C36-C18-C17	-2.93	118.07	122.82
14	a	1130	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	H	1205	CLA	CHD-C1D-ND	-2.93	120.68	124.80
14	B	1205	CLA	CHD-C1D-ND	-2.93	120.68	124.80
14	B	1022	CLA	C1-C2-C3	-2.93	121.40	126.20
14	B	1226	CLA	C1-C2-C3	-2.93	121.40	126.20
14	b	1203	CLA	CMC-C2C-C1C	2.93	129.61	125.03
14	a	1127	CLA	C3C-C4C-NC	2.93	114.18	110.43
14	A	1118	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
14	l	1502	CLA	C3D-C4D-ND	2.93	114.75	109.99
14	H	1210	CLA	C1-O2A-CGA	2.93	123.74	116.65
14	H	1023	CLA	C4-C3-C5	2.93	120.31	115.23
15	B	1238	F6C	OMB-CMB-C2B	-2.93	119.02	125.62
14	a	1140	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
14	A	1116	CLA	CMC-C2C-C1C	2.93	129.61	125.03
14	H	1022	CLA	C1-C2-C3	-2.92	121.41	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	B	1237	F6C	CMA-C3A-C2A	-2.92	118.24	126.15
14	H	1215	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	b	1022	CLA	C1-C2-C3	-2.92	121.41	126.20
14	H	1216	CLA	CED-O2D-CGD	2.92	122.55	115.92
18	L	4019	BCR	C24-C25-C26	-2.92	114.82	121.56
14	B	1217	CLA	CMC-C2C-C1C	2.92	129.60	125.03
14	b	1213	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
14	a	1113	CLA	CMA-C3A-C4A	2.92	119.62	111.77
18	H	4004	BCR	C36-C18-C17	-2.92	118.08	122.82
14	H	1213	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	G	1011	CL0	C4D-ND-C1D	-2.92	103.00	105.22
14	G	1111	CLA	CAC-C3C-C4C	2.92	128.59	124.79
18	B	4004	BCR	C36-C18-C17	-2.92	118.09	122.82
14	G	1116	CLA	CMC-C2C-C1C	2.92	129.59	125.03
14	B	1213	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
15	b	1237	F6C	CMA-C3A-C2A	-2.92	118.26	126.15
14	G	1118	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
14	G	1130	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	A	1130	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	b	1226	CLA	C1-C2-C3	-2.92	121.42	126.20
14	a	1118	CLA	CAA-C2A-C3A	-2.92	105.12	113.00
15	b	1238	F6C	OMB-CMB-C2B	-2.91	119.04	125.62
14	b	1232	CLA	C4D-C3D-CAD	2.91	111.27	108.11
14	a	1115	CLA	CMC-C2C-C1C	2.91	129.59	125.03
18	b	4014	BCR	C34-C9-C10	-2.91	118.10	122.82
14	G	1115	CLA	CMC-C2C-C1C	2.91	129.59	125.03
18	B	4009	BCR	C33-C5-C6	-2.91	121.31	124.48
15	H	1238	F6C	OMB-CMB-C2B	-2.91	119.05	125.62
14	B	1210	CLA	C4-C3-C5	2.91	120.28	115.23
14	H	1217	CLA	CMC-C2C-C1C	2.91	129.58	125.03
14	b	1218	CLA	CMC-C2C-C1C	2.91	129.58	125.03
14	b	1021	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	H	1210	CLA	C4-C3-C5	2.91	120.28	115.23
19	H	5004	LHG	O8-C23-C24	2.91	120.71	111.83
14	b	1205	CLA	CHD-C1D-ND	-2.91	120.71	124.80
14	B	1205	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
14	B	1023	CLA	C4-C3-C5	2.91	120.28	115.23
18	A	4001	BCR	C36-C18-C17	-2.91	118.10	122.82
15	H	1238	F6C	C3D-C4D-ND	2.91	114.72	109.93
14	H	1205	CLA	CAA-C2A-C3A	-2.91	105.14	113.00
14	G	1127	CLA	C3C-C4C-NC	2.91	114.15	110.43
14	B	1236	CLA	C3D-C4D-ND	2.91	114.71	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	a	1011	CL0	C4D-ND-C1D	-2.91	103.01	105.22
14	H	1226	CLA	C1-C2-C3	-2.91	121.44	126.20
14	B	1220	CLA	C2B-C1B-NB	2.91	113.34	110.33
14	H	1226	CLA	C1D-ND-C4D	-2.91	104.27	106.31
14	H	1236	CLA	C3D-C4D-ND	2.91	114.71	109.99
19	B	5004	LHG	O8-C23-C24	2.90	120.69	111.83
20	l	5007	LMG	O8-C28-C29	2.90	120.69	111.83
14	b	1023	CLA	C4-C3-C5	2.90	120.27	115.23
14	H	1229	CLA	C3D-C4D-ND	2.90	114.71	109.99
20	U	5007	LMG	O8-C28-C29	2.90	120.69	111.83
18	b	4017	BCR	C34-C9-C10	-2.90	118.11	122.82
19	b	5004	LHG	O8-C23-C24	2.90	120.68	111.83
14	a	1109	CLA	CMA-C3A-C4A	2.90	119.56	111.77
14	B	1216	CLA	CED-O2D-CGD	2.90	122.49	115.92
18	H	4009	BCR	C33-C5-C6	-2.90	121.32	124.48
14	H	1203	CLA	CMC-C2C-C1C	2.90	129.56	125.03
14	a	1120	CLA	OBD-CAD-C3D	-2.90	121.64	128.42
18	H	4017	BCR	C34-C9-C10	-2.90	118.12	122.82
14	B	1234	CLA	C3C-C4C-NC	2.90	114.14	110.43
14	B	1021	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	B	1203	CLA	CMC-C2C-C1C	2.89	129.56	125.03
15	b	1238	F6C	C3D-C4D-ND	2.89	114.69	109.93
20	L	5007	LMG	O8-C28-C29	2.89	120.66	111.83
14	H	1221	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	A	1127	CLA	C3C-C4C-NC	2.89	114.14	110.43
14	b	1205	CLA	CAA-C2A-C3A	-2.89	105.18	113.00
14	b	1219	CLA	CMB-C2B-C1B	2.89	129.82	125.42
14	b	1236	CLA	C3D-C4D-ND	2.89	114.69	109.99
14	B	1221	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	G	1118	CLA	C4D-C3D-CAD	2.89	111.25	108.11
14	H	1218	CLA	CMC-C2C-C1C	2.89	129.55	125.03
14	H	1211	CLA	C3D-C4D-ND	2.89	114.68	109.99
15	B	1238	F6C	C3D-C4D-ND	2.89	114.69	109.93
14	H	1213	CLA	CMC-C2C-C1C	2.89	129.55	125.03
14	U	1502	CLA	C3D-C4D-ND	2.89	114.68	109.99
18	A	4008	BCR	C34-C9-C8	2.89	122.50	118.09
14	L	1502	CLA	C3D-C4D-ND	2.89	114.68	109.99
14	H	1021	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
15	b	1230	F6C	CAC-C3C-C4C	2.89	128.88	124.91
14	H	1234	CLA	C3C-C4C-NC	2.89	114.13	110.43
14	a	1129	CLA	C4D-C3D-CAD	2.89	111.24	108.11
14	L	1503	CLA	C3D-C4D-ND	2.89	114.68	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4008	BCR	C34-C9-C8	2.88	122.49	118.09
14	b	1210	CLA	C4-C3-C5	2.88	120.23	115.23
14	H	1236	CLA	CMB-C2B-C1B	2.88	129.81	125.42
14	b	1220	CLA	C2B-C1B-NB	2.88	113.31	110.33
14	B	1219	CLA	CMB-C2B-C1B	2.88	129.81	125.42
14	A	1123	CLA	CHD-C1D-ND	-2.88	120.75	124.80
14	G	1109	CLA	CMA-C3A-C4A	2.88	119.51	111.77
14	U	1503	CLA	C3D-C4D-ND	2.88	114.67	109.99
14	A	1109	CLA	CMA-C3A-C4A	2.88	119.51	111.77
14	H	1232	CLA	C4D-C3D-CAD	2.88	111.23	108.11
18	G	4008	BCR	C34-C9-C8	2.88	122.48	118.09
18	B	4017	BCR	C34-C9-C10	-2.88	118.15	122.82
14	H	1220	CLA	C2B-C1B-NB	2.88	113.31	110.33
14	A	1120	CLA	OBD-CAD-C3D	-2.88	121.69	128.42
14	b	1226	CLA	CMB-C2B-C3B	2.88	133.31	126.55
14	G	1135	CLA	C4-C3-C5	2.87	120.22	115.23
14	a	1013	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
14	A	1135	CLA	C4-C3-C5	2.87	120.22	115.23
14	B	1226	CLA	CMB-C2B-C3B	2.87	133.31	126.55
14	G	1120	CLA	OBD-CAD-C3D	-2.87	121.70	128.42
14	X	1701	CLA	CMC-C2C-C1C	2.87	129.52	125.03
14	B	1236	CLA	CMB-C2B-C1B	2.87	129.79	125.42
14	b	1221	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	G	1136	CLA	C1-C2-C3	-2.87	121.50	126.20
14	A	1013	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	H	1226	CLA	CMB-C2B-C3B	2.87	133.30	126.55
14	A	1136	CLA	C1-C2-C3	-2.87	121.50	126.20
14	G	1123	CLA	CHD-C1D-ND	-2.87	120.77	124.80
14	W	1701	CLA	CMC-C2C-C1C	2.87	129.51	125.03
14	G	1013	CLA	C3D-C4D-ND	2.87	114.65	109.99
14	G	1131	CLA	CMC-C2C-C1C	2.87	129.51	125.03
14	a	1136	CLA	C1-C2-C3	-2.87	121.50	126.20
14	a	1118	CLA	C4-C3-C5	2.87	120.20	115.23
14	G	1128	CLA	CMB-C2B-C3B	2.87	133.29	126.55
14	G	1118	CLA	C4-C3-C5	2.86	120.20	115.23
14	G	1135	CLA	O2A-C1-C2	2.86	119.13	108.11
14	a	1118	CLA	C4D-C3D-CAD	2.86	111.22	108.11
18	G	4001	BCR	C36-C18-C17	-2.86	118.18	122.82
14	a	1135	CLA	C4-C3-C5	2.86	120.20	115.23
14	H	1236	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
18	a	4001	BCR	C36-C18-C17	-2.86	118.18	122.82
14	a	1135	CLA	O2A-C1-C2	2.86	119.12	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1234	CLA	C3C-C4C-NC	2.86	114.09	110.43
14	A	1118	CLA	C4D-C3D-CAD	2.86	111.21	108.11
21	A	6002	LMT	C1'-O5'-C5'	-2.86	108.14	113.72
14	x	1701	CLA	CMC-C2C-C1C	2.86	129.50	125.03
14	a	1128	CLA	CMB-C2B-C3B	2.86	133.27	126.55
14	A	1135	CLA	O2A-C1-C2	2.86	119.11	108.11
14	b	1236	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
21	G	6002	LMT	C1'-O5'-C5'	-2.86	108.14	113.72
14	B	1211	CLA	C3D-C4D-ND	2.86	114.63	109.99
14	a	1114	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
14	B	1236	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
14	G	1013	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
14	G	1124	CLA	C3D-C4D-ND	2.86	114.63	109.99
14	b	1211	CLA	C3D-C4D-ND	2.86	114.63	109.99
15	B	1238	F6C	CMA-C3A-C2A	-2.86	118.42	126.15
14	A	1128	CLA	CMB-C2B-C3B	2.86	133.27	126.55
14	b	1226	CLA	C1D-ND-C4D	-2.85	104.31	106.31
14	a	1131	CLA	CMC-C2C-C1C	2.85	129.50	125.03
15	H	1237	F6C	CHB-C4A-C3A	-2.85	119.55	125.49
14	b	1213	CLA	CMC-C2C-C1C	2.85	129.49	125.03
14	G	1123	CLA	C3C-C4C-NC	2.85	114.09	110.43
14	H	1226	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
14	l	1503	CLA	C3D-C4D-ND	2.85	114.62	109.99
14	B	1228	CLA	C3D-C4D-ND	2.85	114.62	109.99
14	a	1123	CLA	CHD-C1D-ND	-2.85	120.79	124.80
14	a	1124	CLA	C3D-C4D-ND	2.85	114.62	109.99
14	b	1226	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
18	b	4010	BCR	C34-C9-C8	2.85	122.44	118.09
14	A	1106	CLA	O2A-C1-C2	2.85	119.08	108.11
14	b	1233	CLA	CMA-C3A-C4A	2.85	119.44	111.77
14	A	1118	CLA	C4-C3-C5	2.85	120.18	115.23
14	A	1131	CLA	CMC-C2C-C1C	2.85	129.49	125.03
15	B	1237	F6C	CHB-C4A-C3A	-2.85	119.56	125.49
14	a	1105	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
15	b	1238	F6C	CMA-C3A-C2A	-2.85	118.44	126.15
14	a	1013	CLA	C3D-C4D-ND	2.85	114.62	109.99
14	b	1236	CLA	CMB-C2B-C1B	2.85	129.76	125.42
14	A	1123	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
15	H	1238	F6C	CMA-C3A-C2A	-2.85	118.45	126.15
14	a	1106	CLA	O2A-C1-C2	2.85	119.07	108.11
14	B	1233	CLA	CMA-C3A-C4A	2.85	119.43	111.77
14	H	1218	CLA	CMA-C3A-C4A	2.85	119.42	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1218	CLA	CMA-C3A-C4A	2.85	119.42	111.77
14	A	1105	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
14	G	1129	CLA	C4D-C3D-CAD	2.85	111.20	108.11
15	H	1230	F6C	CAC-C3C-C4C	2.85	128.83	124.91
14	G	1106	CLA	O2A-C1-C2	2.85	119.06	108.11
15	b	1237	F6C	CHB-C4A-C3A	-2.84	119.57	125.49
14	l	1501	CLA	C1-C2-C3	-2.84	121.54	126.20
14	G	1138	CLA	CMC-C2C-C1C	2.84	129.48	125.03
14	b	1239	CLA	C4-C3-C5	2.84	120.16	115.23
14	a	1127	CLA	CHD-C1D-ND	-2.84	120.80	124.80
14	G	1104	CLA	C3D-C4D-ND	2.84	114.61	109.99
14	A	1013	CLA	C3D-C4D-ND	2.84	114.61	109.99
14	H	1233	CLA	CMA-C3A-C4A	2.84	119.41	111.77
14	B	1213	CLA	CMC-C2C-C1C	2.84	129.47	125.03
21	a	6002	LMT	C1'-O5'-C5'	-2.84	108.17	113.72
20	R	5006	LMG	C8-O7-C10	-2.84	111.00	117.80
14	A	1124	CLA	C3D-C4D-ND	2.84	114.60	109.99
14	a	1012	CLA	CMC-C2C-C1C	2.84	129.47	125.03
14	b	1218	CLA	CMA-C3A-C4A	2.84	119.40	111.77
14	H	1239	CLA	C4-C3-C5	2.84	120.15	115.23
14	A	1114	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
14	G	1114	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
14	G	1129	CLA	CAA-C2A-C3A	-2.83	105.34	113.00
14	H	1222	CLA	C4-C3-C5	2.83	120.15	115.23
14	B	1239	CLA	C4-C3-C5	2.83	120.15	115.23
14	A	1104	CLA	C3D-C4D-ND	2.83	114.59	109.99
14	B	1222	CLA	C4-C3-C5	2.83	120.15	115.23
15	B	1230	F6C	O2D-CGD-O1D	-2.83	118.33	123.85
14	G	1123	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	B	1226	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
20	I	5006	LMG	C8-O7-C10	-2.83	111.02	117.80
14	a	1123	CLA	C3C-C4C-NC	2.83	114.06	110.43
14	G	1119	CLA	CED-O2D-CGD	2.83	122.33	115.92
14	K	1401	CLA	CMC-C2C-C1C	2.83	129.45	125.03
20	i	5006	LMG	C8-O7-C10	-2.83	111.03	117.80
14	G	1105	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
14	A	1123	CLA	C3C-C4C-NC	2.83	114.05	110.43
14	H	1214	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
15	H	1230	F6C	O2D-CGD-O1D	-2.82	118.35	123.85
14	a	1122	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
14	G	1012	CLA	CMC-C2C-C1C	2.82	129.44	125.03
14	B	1221	CLA	CHD-C1D-ND	-2.82	120.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1228	CLA	C3D-C4D-ND	2.82	114.57	109.99
14	A	1138	CLA	CMC-C2C-C1C	2.82	129.44	125.03
13	A	1011	CL0	C4D-ND-C1D	-2.82	103.08	105.22
18	H	4010	BCR	C34-C9-C8	2.82	122.39	118.09
14	L	1501	CLA	C1-C2-C3	-2.82	121.58	126.20
14	a	1129	CLA	CAA-C2A-C3A	-2.82	105.39	113.00
15	B	1230	F6C	CAC-C3C-C4C	2.82	128.79	124.91
14	H	1228	CLA	C3D-C4D-ND	2.82	114.56	109.99
14	b	1221	CLA	CHD-C1D-ND	-2.82	120.84	124.80
14	b	1214	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
14	A	1127	CLA	CHD-C1D-ND	-2.82	120.84	124.80
15	b	1230	F6C	O2D-CGD-O1D	-2.82	118.37	123.85
14	H	1235	CLA	C3D-C4D-ND	2.82	114.56	109.99
14	T	1401	CLA	CMC-C2C-C1C	2.81	129.43	125.03
14	A	1122	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
14	a	1111	CLA	CAA-C2A-C3A	-2.81	105.39	113.00
14	a	1138	CLA	CMC-C2C-C1C	2.81	129.43	125.03
15	b	1238	F6C	CHA-C1A-C2A	-2.81	122.84	130.41
14	H	1021	CLA	C3D-C4D-ND	2.81	114.56	109.99
14	a	1123	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
14	A	1012	CLA	CMC-C2C-C1C	2.81	129.43	125.03
14	A	1129	CLA	C4D-C3D-CAD	2.81	111.16	108.11
14	A	1119	CLA	CED-O2D-CGD	2.81	122.29	115.92
18	b	4005	BCR	C28-C27-C26	-2.81	109.04	114.06
14	A	1129	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
15	B	1238	F6C	CHA-C1A-C2A	-2.81	122.85	130.41
14	b	1222	CLA	C4-C3-C5	2.81	120.11	115.23
14	H	1222	CLA	CAA-C2A-C1A	-2.81	102.77	111.97
14	b	1222	CLA	CAA-C2A-C1A	-2.81	102.77	111.97
14	a	1105	CLA	C3D-C4D-ND	2.81	114.55	109.99
14	U	1501	CLA	C1-C2-C3	-2.81	121.60	126.20
14	A	1108	CLA	CAA-C2A-C3A	-2.81	105.41	113.00
14	b	1222	CLA	C3C-C4C-NC	2.81	114.03	110.43
14	G	1127	CLA	CHD-C1D-ND	-2.81	120.85	124.80
14	a	1119	CLA	CED-O2D-CGD	2.80	122.28	115.92
15	b	1207	F6C	C1-O2A-CGA	2.80	123.44	116.65
18	A	4011	BCR	C31-C1-C6	-2.80	105.85	110.24
14	A	1102	CLA	CMB-C2B-C3B	2.80	133.14	126.55
15	H	1238	F6C	CHA-C1A-C2A	-2.80	122.87	130.41
14	a	1104	CLA	C3D-C4D-ND	2.80	114.54	109.99
14	B	1214	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	B	1222	CLA	CAA-C2A-C1A	-2.80	102.80	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4010	BCR	C38-C26-C25	-2.80	121.43	124.48
18	B	4010	BCR	C34-C9-C8	2.80	122.36	118.09
14	b	1021	CLA	C4-C3-C5	2.80	120.08	115.23
14	B	1021	CLA	C4-C3-C5	2.80	120.08	115.23
14	H	1222	CLA	C3C-C4C-NC	2.80	114.01	110.43
14	B	1222	CLA	C3C-C4C-NC	2.80	114.01	110.43
14	H	1221	CLA	CHD-C1D-ND	-2.80	120.87	124.80
18	I	4020	BCR	C34-C9-C8	2.79	122.36	118.09
18	B	4010	BCR	C38-C26-C25	-2.79	121.44	124.48
15	B	1207	F6C	C1-O2A-CGA	2.79	123.41	116.65
14	k	1401	CLA	CMC-C2C-C1C	2.79	129.40	125.03
14	G	1136	CLA	C3D-C4D-ND	2.79	114.53	109.99
14	G	1111	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
18	a	4011	BCR	C31-C1-C6	-2.79	105.86	110.24
14	a	1140	CLA	C3C-C4C-NC	2.79	114.01	110.43
14	A	1111	CLA	CAA-C2A-C3A	-2.79	105.45	113.00
14	b	1232	CLA	CMA-C3A-C4A	2.79	119.28	111.77
14	G	1108	CLA	CAA-C2A-C3A	-2.79	105.46	113.00
14	H	1021	CLA	C4-C3-C5	2.79	120.07	115.23
18	b	4010	BCR	C34-C9-C10	-2.79	118.30	122.82
14	a	1102	CLA	CMB-C2B-C3B	2.79	133.11	126.55
14	a	1108	CLA	CAA-C2A-C3A	-2.79	105.46	113.00
14	B	1231	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
14	b	1229	CLA	C4D-C3D-CAD	2.79	111.14	108.11
14	G	1110	CLA	C3D-C4D-ND	2.79	114.52	109.99
14	A	1134	CLA	CMA-C3A-C4A	2.79	119.27	111.77
14	b	1234	CLA	CMB-C2B-C1B	2.79	129.66	125.42
14	H	1227	CLA	C3D-C4D-ND	2.79	114.52	109.99
15	H	1207	F6C	C1-O2A-CGA	2.79	123.40	116.65
14	B	1210	CLA	C3D-C4D-ND	2.79	114.52	109.99
14	B	1235	CLA	C3D-C4D-ND	2.79	114.52	109.99
18	B	4005	BCR	C40-C30-C25	-2.79	105.87	110.24
14	H	1239	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
14	G	1102	CLA	CMB-C2B-C3B	2.78	133.10	126.55
18	i	4020	BCR	C34-C9-C8	2.78	122.34	118.09
14	b	1212	CLA	C3C-C4C-NC	2.78	114.00	110.43
18	i	4018	BCR	C23-C24-C25	-2.78	119.56	127.00
18	H	4005	BCR	C40-C30-C25	-2.78	105.88	110.24
14	b	1209	CLA	CMC-C2C-C1C	2.78	129.38	125.03
14	b	1215	CLA	CMC-C2C-C1C	2.78	129.38	125.03
18	B	4010	BCR	C34-C9-C10	-2.78	118.31	122.82
18	R	4018	BCR	C23-C24-C25	-2.78	119.57	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1239	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	G	1105	CLA	C3D-C4D-ND	2.78	114.51	109.99
14	B	1232	CLA	CMA-C3A-C4A	2.78	119.25	111.77
14	G	1132	CLA	CMB-C2B-C1B	2.78	129.65	125.42
18	H	4005	BCR	C28-C27-C26	-2.78	109.10	114.06
14	H	1232	CLA	CMA-C3A-C4A	2.78	119.24	111.77
18	I	4018	BCR	C23-C24-C25	-2.78	119.58	127.00
14	B	1209	CLA	CMC-C2C-C1C	2.78	129.38	125.03
14	G	1122	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	H	1233	CLA	C3D-C4D-ND	2.78	114.50	109.99
14	a	1110	CLA	C3D-C4D-ND	2.78	114.50	109.99
14	A	1105	CLA	C3D-C4D-ND	2.78	114.50	109.99
18	G	4011	BCR	C31-C1-C6	-2.78	105.89	110.24
15	B	1238	F6C	CHB-C4A-C3A	-2.78	119.71	125.49
18	R	4020	BCR	C34-C9-C8	2.78	122.33	118.09
18	B	4005	BCR	C28-C27-C26	-2.78	109.10	114.06
14	b	1235	CLA	C3D-C4D-ND	2.78	114.50	109.99
18	H	4010	BCR	C33-C5-C6	-2.78	121.45	124.48
19	B	5004	LHG	C5-O7-C7	-2.78	111.15	117.80
18	G	4011	BCR	C1-C6-C5	-2.78	118.84	122.64
14	b	1231	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
14	H	1212	CLA	C3C-C4C-NC	2.78	113.98	110.43
14	B	1212	CLA	C3C-C4C-NC	2.78	113.98	110.43
18	a	4007	BCR	C7-C8-C9	-2.77	122.13	126.23
14	a	1139	CLA	C3C-C4C-NC	2.77	113.98	110.43
18	b	4005	BCR	C40-C30-C25	-2.77	105.89	110.24
18	B	4010	BCR	C33-C5-C6	-2.77	121.46	124.48
18	U	4019	BCR	C33-C5-C4	2.77	119.51	113.60
18	A	4007	BCR	C7-C8-C9	-2.77	122.13	126.23
14	A	1115	CLA	C4-C3-C5	2.77	120.04	115.23
14	H	1215	CLA	CMC-C2C-C1C	2.77	129.37	125.03
14	L	1502	CLA	CMB-C2B-C1B	2.77	129.64	125.42
14	U	1502	CLA	CMB-C2B-C1B	2.77	129.64	125.42
14	a	1136	CLA	C3D-C4D-ND	2.77	114.49	109.99
14	b	1021	CLA	C3D-C4D-ND	2.77	114.49	109.99
14	B	1216	CLA	C3D-C4D-ND	2.77	114.49	109.99
14	H	1234	CLA	CMB-C2B-C1B	2.77	129.64	125.42
14	a	1134	CLA	CMA-C3A-C4A	2.77	119.22	111.77
14	G	1137	CLA	O1D-CGD-CBD	-2.77	119.06	124.52
14	B	1239	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
14	A	1136	CLA	C3D-C4D-ND	2.77	114.48	109.99
15	b	1238	F6C	CHB-C4A-C3A	-2.77	119.73	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1115	CLA	C4-C3-C5	2.77	120.03	115.23
14	G	1134	CLA	CMA-C3A-C4A	2.77	119.20	111.77
18	H	4010	BCR	C34-C9-C10	-2.76	118.34	122.82
14	l	1502	CLA	CMB-C2B-C1B	2.76	129.63	125.42
18	b	4010	BCR	C38-C26-C25	-2.76	121.47	124.48
14	A	1132	CLA	CMB-C2B-C1B	2.76	129.63	125.42
14	B	1021	CLA	C3D-C4D-ND	2.76	114.48	109.99
14	a	1132	CLA	CMB-C2B-C1B	2.76	129.62	125.42
14	b	1023	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	G	1139	CLA	C3C-C4C-NC	2.76	113.97	110.43
14	b	1210	CLA	C3D-C4D-ND	2.76	114.48	109.99
14	B	1204	CLA	CMB-C2B-C1B	2.76	129.62	125.42
18	b	4010	BCR	C33-C5-C6	-2.76	121.47	124.48
14	G	1140	CLA	C3C-C4C-NC	2.76	113.97	110.43
15	A	1121	F6C	CMA-C3A-C2A	-2.76	118.68	126.15
14	B	1023	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	G	1115	CLA	C4-C3-C5	2.76	120.02	115.23
16	b	2002	PQN	C11-C12-C13	-2.76	122.08	126.83
16	B	2002	PQN	C11-C12-C13	-2.76	122.08	126.83
19	b	5004	LHG	C5-O7-C7	-2.76	111.19	117.80
14	b	1227	CLA	C3D-C4D-ND	2.76	114.47	109.99
14	A	1110	CLA	C3D-C4D-ND	2.76	114.47	109.99
14	H	1209	CLA	CMC-C2C-C1C	2.76	129.34	125.03
14	a	1137	CLA	O1D-CGD-CBD	-2.76	119.08	124.52
14	b	1217	CLA	CMB-C2B-C1B	2.76	129.62	125.42
14	A	1139	CLA	C3C-C4C-NC	2.76	113.96	110.43
14	a	1101	CLA	CMB-C2B-C1B	2.76	129.61	125.42
14	A	1140	CLA	C3C-C4C-NC	2.75	113.96	110.43
18	b	4004	BCR	C15-C14-C13	-2.75	123.42	127.28
14	G	1101	CLA	CMB-C2B-C1B	2.75	129.61	125.42
18	b	4014	BCR	C28-C27-C26	-2.75	109.14	114.06
15	G	1121	F6C	CMA-C3A-C2A	-2.75	118.70	126.15
18	L	4019	BCR	C33-C5-C4	2.75	119.47	113.60
14	A	1137	CLA	O1D-CGD-CBD	-2.75	119.09	124.52
15	H	1238	F6C	CHB-C4A-C3A	-2.75	119.76	125.49
18	H	4009	BCR	C3-C4-C5	-2.75	109.15	114.06
14	a	1103	CLA	C4-C3-C5	2.75	120.00	115.23
19	H	5004	LHG	C5-O7-C7	-2.75	111.21	117.80
14	H	1231	CLA	C3D-C4D-ND	2.75	114.46	109.99
14	b	1220	CLA	C3D-C4D-ND	2.75	114.46	109.99
14	b	1204	CLA	CMB-C2B-C1B	2.75	129.61	125.42
14	b	1233	CLA	C3D-C4D-ND	2.75	114.46	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1231	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	B	1220	CLA	C3D-C4D-ND	2.75	114.46	109.99
14	B	1233	CLA	C3D-C4D-ND	2.75	114.45	109.99
14	b	1231	CLA	C3D-C4D-ND	2.75	114.45	109.99
14	G	1103	CLA	C4-C3-C5	2.75	120.00	115.23
14	b	1216	CLA	C3D-C4D-ND	2.75	114.45	109.99
14	a	1129	CLA	C3D-C4D-ND	2.75	114.45	109.99
16	H	2002	PQN	C11-C12-C13	-2.75	122.10	126.83
18	a	4011	BCR	C1-C6-C5	-2.74	118.89	122.64
14	a	1101	CLA	C3D-C4D-ND	2.74	114.45	109.99
18	H	4004	BCR	C15-C14-C13	-2.74	123.43	127.28
18	H	4014	BCR	C28-C27-C26	-2.74	109.16	114.06
14	A	1126	CLA	C4-C3-C5	2.74	119.99	115.23
14	G	1126	CLA	C3D-C4D-ND	2.74	114.44	109.99
14	B	1205	CLA	C3C-C4C-NC	2.74	113.94	110.43
14	H	1216	CLA	C3D-C4D-ND	2.74	114.44	109.99
14	B	1215	CLA	CMC-C2C-C1C	2.74	129.31	125.03
14	a	1126	CLA	C4-C3-C5	2.74	119.98	115.23
15	H	1237	F6C	C3D-C4D-ND	2.74	114.44	109.93
14	A	1139	CLA	CAA-C2A-C3A	-2.74	105.60	113.00
14	H	1210	CLA	C3D-C4D-ND	2.74	114.44	109.99
14	G	1126	CLA	C4-C3-C5	2.74	119.98	115.23
14	a	1138	CLA	C4-C3-C5	2.74	119.98	115.23
18	l	4019	BCR	C33-C5-C4	2.74	119.43	113.60
18	B	4006	BCR	C28-C27-C26	-2.74	109.17	114.06
14	H	1217	CLA	CMB-C2B-C1B	2.74	129.59	125.42
14	B	1234	CLA	CMB-C2B-C1B	2.74	129.59	125.42
14	B	1227	CLA	C3D-C4D-ND	2.74	114.44	109.99
15	B	1238	F6C	CHD-C1D-ND	-2.74	120.19	124.31
18	A	4011	BCR	C1-C6-C5	-2.74	118.90	122.64
14	H	1023	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	B	1217	CLA	CMB-C2B-C1B	2.74	129.59	125.42
14	A	1138	CLA	C4-C3-C5	2.74	119.98	115.23
14	B	1224	CLA	C3C-C4C-NC	2.74	113.94	110.43
14	A	1103	CLA	C4-C3-C5	2.74	119.98	115.23
14	A	1132	CLA	C3D-C4D-ND	2.74	114.43	109.99
15	a	1121	F6C	CMA-C3A-C2A	-2.74	118.75	126.15
15	B	1230	F6C	C3D-C4D-ND	2.74	114.44	109.93
15	B	1237	F6C	C3D-C4D-ND	2.74	114.44	109.93
14	a	1139	CLA	CAA-C2A-C3A	-2.73	105.61	113.00
15	B	1237	F6C	CHA-C1A-C2A	-2.73	123.06	130.41
15	b	1238	F6C	CHD-C1D-ND	-2.73	120.19	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1220	CLA	C3D-C4D-ND	2.73	114.43	109.99
18	b	4009	BCR	C3-C4-C5	-2.73	109.18	114.06
18	B	4014	BCR	C28-C27-C26	-2.73	109.18	114.06
14	G	1138	CLA	C4-C3-C5	2.73	119.97	115.23
14	H	1228	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
14	b	1209	CLA	C3D-C4D-ND	2.73	114.43	109.99
18	G	4007	BCR	C7-C8-C9	-2.73	122.19	126.23
14	a	1125	CLA	CAC-C3C-C4C	2.73	128.34	124.79
18	H	4006	BCR	C28-C27-C26	-2.73	109.19	114.06
14	A	1101	CLA	CMB-C2B-C1B	2.73	129.57	125.42
14	A	1125	CLA	CAC-C3C-C4C	2.73	128.34	124.79
14	A	1101	CLA	C3D-C4D-ND	2.73	114.42	109.99
14	A	1126	CLA	C3D-C4D-ND	2.73	114.42	109.99
14	G	1101	CLA	C3D-C4D-ND	2.73	114.42	109.99
15	b	1230	F6C	C3D-C4D-ND	2.73	114.42	109.93
14	H	1204	CLA	CMB-C2B-C1B	2.73	129.57	125.42
14	H	1208	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
14	G	1139	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
14	a	1109	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	a	1012	CLA	OBD-CAD-C3D	-2.72	122.05	128.42
14	H	1205	CLA	C3C-C4C-NC	2.72	113.92	110.43
14	B	1229	CLA	C4D-C3D-CAD	2.72	111.06	108.11
14	a	1132	CLA	C3D-C4D-ND	2.72	114.41	109.99
18	B	4009	BCR	C3-C4-C5	-2.72	109.20	114.06
14	A	1012	CLA	OBD-CAD-C3D	-2.72	122.05	128.42
14	G	1012	CLA	OBD-CAD-C3D	-2.72	122.05	128.42
14	B	1225	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
14	B	1209	CLA	C3D-C4D-ND	2.72	114.41	109.99
18	I	4018	BCR	C33-C5-C4	2.72	119.40	113.60
14	B	1231	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	G	1129	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	A	1134	CLA	C3D-C4D-ND	2.72	114.41	109.99
14	B	1208	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
18	b	4006	BCR	C28-C27-C26	-2.72	109.21	114.06
14	A	1102	CLA	C1-O2A-CGA	2.72	123.23	116.65
15	G	1121	F6C	C3D-C4D-ND	2.72	114.41	109.93
14	b	1208	CLA	CAA-C2A-C3A	-2.72	105.66	113.00
14	B	1225	CLA	CHD-C1D-ND	-2.72	120.98	124.80
14	A	1109	CLA	C3D-C4D-ND	2.72	114.40	109.99
18	b	4004	BCR	C33-C5-C6	-2.72	121.52	124.48
14	A	1140	CLA	C1-C2-C3	-2.72	121.75	126.20
14	H	1218	CLA	O2D-CGD-O1D	-2.72	118.56	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1217	CLA	C4-C3-C5	2.72	119.94	115.23
14	B	1228	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
15	H	1237	F6C	O2D-CGD-O1D	-2.72	118.56	123.85
15	B	1237	F6C	O2D-CGD-O1D	-2.72	118.56	123.85
14	U	1501	CLA	O2A-C1-C2	2.71	118.56	108.11
14	l	1501	CLA	O2A-C1-C2	2.71	118.56	108.11
14	a	1139	CLA	C3D-C4D-ND	2.71	114.40	109.99
15	b	1237	F6C	CHA-C1A-C2A	-2.71	123.11	130.41
14	a	1140	CLA	C1-C2-C3	-2.71	121.75	126.20
14	B	1217	CLA	C3C-C4C-NC	2.71	113.91	110.43
14	H	1220	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
15	a	1121	F6C	C3D-C4D-ND	2.71	114.40	109.93
14	a	1126	CLA	C3D-C4D-ND	2.71	114.39	109.99
14	B	1221	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	L	1501	CLA	O2A-C1-C2	2.71	118.54	108.11
14	H	1209	CLA	C3D-C4D-ND	2.71	114.39	109.99
15	H	1230	F6C	C3D-C4D-ND	2.71	114.39	109.93
14	G	1125	CLA	CAC-C3C-C4C	2.71	128.32	124.79
14	G	1134	CLA	C3D-C4D-ND	2.71	114.39	109.99
14	H	1224	CLA	CMC-C2C-C1C	2.71	129.27	125.03
14	b	1218	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	A	1131	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
18	A	4002	BCR	C3-C4-C5	-2.71	109.22	114.06
18	B	4004	BCR	C15-C14-C13	-2.71	123.48	127.28
15	H	1237	F6C	CHA-C1A-C2A	-2.71	123.13	130.41
14	b	1220	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
18	R	4018	BCR	C33-C5-C4	2.71	119.37	113.60
14	H	1224	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	A	1133	CLA	C4D-C3D-CAD	2.71	111.05	108.11
18	I	4020	BCR	C35-C13-C12	2.71	122.22	118.09
14	B	1220	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
14	b	1217	CLA	C3C-C4C-NC	2.71	113.90	110.43
14	A	1012	CLA	C4-C3-C5	2.71	119.93	115.23
14	A	1101	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
15	B	1238	F6C	CMD-C2D-C3D	-2.71	121.48	127.69
14	A	1127	CLA	CMC-C2C-C1C	2.70	129.26	125.03
14	b	1224	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	a	1118	CLA	C1-C2-C3	-2.70	121.77	126.20
14	a	1104	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
14	B	1218	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	G	1102	CLA	C1-O2A-CGA	2.70	123.19	116.65
18	i	4018	BCR	C33-C5-C4	2.70	119.35	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1224	CLA	CMC-C2C-C1C	2.70	129.25	125.03
14	a	1101	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
15	H	1238	F6C	CMD-C2D-C3D	-2.70	121.50	127.69
14	G	1140	CLA	C1-C2-C3	-2.70	121.77	126.20
15	b	1238	F6C	CMD-C2D-C3D	-2.70	121.50	127.69
18	G	4002	BCR	C3-C4-C5	-2.70	109.24	114.06
14	b	1223	CLA	C6-C5-C3	-2.70	106.89	113.47
14	G	1131	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
18	H	4004	BCR	C27-C26-C25	-2.70	119.06	122.70
14	H	1221	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	H	1221	CLA	CMA-C3A-C4A	2.70	119.02	111.77
14	H	1221	CLA	C4-C3-C5	2.70	119.91	115.23
14	b	1220	CLA	C4-C3-C5	2.70	119.91	115.23
15	b	1237	F6C	O2D-CGD-O1D	-2.70	118.60	123.85
14	U	1501	CLA	C3C-C4C-NC	2.70	113.89	110.43
14	A	1139	CLA	C3D-C4D-ND	2.70	114.37	109.99
14	A	1104	CLA	CAA-C2A-C3A	-2.70	105.71	113.00
14	G	1101	CLA	CAA-C2A-C3A	-2.70	105.72	113.00
14	G	1133	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
18	R	4020	BCR	C35-C13-C12	2.70	122.20	118.09
14	G	1132	CLA	C3D-C4D-ND	2.69	114.37	109.99
14	G	1118	CLA	C1-C2-C3	-2.69	121.78	126.20
14	b	1228	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
14	A	1118	CLA	C1-C2-C3	-2.69	121.78	126.20
14	a	1127	CLA	CMC-C2C-C1C	2.69	129.24	125.03
14	H	1229	CLA	C4D-C3D-CAD	2.69	111.03	108.11
14	B	1221	CLA	CMA-C3A-C4A	2.69	119.01	111.77
14	G	1104	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
14	a	1102	CLA	C1-O2A-CGA	2.69	123.17	116.65
18	H	4004	BCR	C33-C5-C6	-2.69	121.55	124.48
14	a	1131	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
14	b	1225	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
18	B	4004	BCR	C33-C5-C6	-2.69	121.55	124.48
18	a	4002	BCR	C3-C4-C5	-2.69	109.26	114.06
14	A	1129	CLA	C3D-C4D-ND	2.69	114.36	109.99
15	b	1237	F6C	C3D-C4D-ND	2.69	114.36	109.93
14	b	1221	CLA	CMA-C3A-C4A	2.69	119.00	111.77
14	G	1012	CLA	C4-C3-C5	2.69	119.90	115.23
14	G	1106	CLA	CMC-C2C-C1C	2.69	129.24	125.03
14	l	1501	CLA	C3C-C4C-NC	2.69	113.88	110.43
14	l	1502	CLA	CAA-C2A-C3A	-2.69	105.73	113.00
15	b	1237	F6C	C3C-C4C-NC	2.69	113.27	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1134	CLA	C3D-C4D-ND	2.69	114.36	109.99
14	B	1235	CLA	CMC-C2C-C1C	2.69	129.24	125.03
14	H	1223	CLA	C6-C5-C3	-2.69	106.92	113.47
18	B	4004	BCR	C27-C26-C25	-2.69	119.07	122.70
15	H	1238	F6C	CHD-C1D-ND	-2.69	120.26	124.31
14	b	1217	CLA	C4-C3-C5	2.69	119.89	115.23
14	L	1502	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
18	i	4020	BCR	C35-C13-C12	2.69	122.19	118.09
18	b	4004	BCR	C27-C26-C25	-2.69	119.08	122.70
14	a	1110	CLA	CMC-C2C-C1C	2.69	129.23	125.03
14	G	1109	CLA	C3D-C4D-ND	2.68	114.35	109.99
14	b	1225	CLA	CHD-C1D-ND	-2.68	121.03	124.80
14	a	1012	CLA	C4-C3-C5	2.68	119.89	115.23
18	B	4014	BCR	C36-C18-C17	-2.68	118.47	122.82
14	H	1225	CLA	CHD-C1D-ND	-2.68	121.03	124.80
14	B	1223	CLA	C6-C5-C3	-2.68	106.93	113.47
14	b	1221	CLA	C4-C3-C5	2.68	119.89	115.23
15	H	1230	F6C	CHB-C4A-C3A	-2.68	119.91	125.49
14	H	1220	CLA	C4-C3-C5	2.68	119.88	115.23
14	b	1205	CLA	C3C-C4C-NC	2.68	113.87	110.43
15	A	1121	F6C	C3D-C4D-ND	2.68	114.35	109.93
14	H	1239	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
14	b	1214	CLA	CAA-CBA-CGA	-2.68	105.59	113.21
14	H	1217	CLA	C3C-C4C-NC	2.68	113.86	110.43
14	L	1503	CLA	C4-C3-C5	2.68	119.88	115.23
14	A	1102	CLA	CMC-C2C-C1C	2.68	129.22	125.03
14	L	1501	CLA	C3C-C4C-NC	2.68	113.86	110.43
14	U	1502	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
14	B	1214	CLA	CAA-CBA-CGA	-2.68	105.61	113.21
14	a	1120	CLA	CMC-C2C-C1C	2.68	129.22	125.03
14	H	1021	CLA	CBC-CAC-C3C	-2.68	105.16	112.42
15	H	1230	F6C	CHA-C4D-ND	2.68	135.61	133.05
14	B	1217	CLA	C4-C3-C5	2.68	119.88	115.23
14	A	1106	CLA	C3D-C4D-ND	2.68	114.34	109.99
14	b	1224	CLA	CMC-C2C-C1C	2.68	129.22	125.03
14	b	1239	CLA	CAA-CBA-CGA	-2.68	105.61	113.21
14	k	1401	CLA	C3D-C4D-ND	2.68	114.34	109.99
15	H	1237	F6C	C3C-C4C-NC	2.68	113.25	110.32
18	B	4004	BCR	C37-C22-C21	-2.67	118.48	122.82
14	b	1221	CLA	C3C-C4C-NC	2.67	113.86	110.43
18	b	4014	BCR	C36-C18-C17	-2.67	118.49	122.82
14	b	1021	CLA	CBC-CAC-C3C	-2.67	105.17	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1205	CLA	O2A-C1-C2	2.67	118.39	108.11
14	B	1239	CLA	CAA-CBA-CGA	-2.67	105.62	113.21
14	G	1102	CLA	CMC-C2C-C1C	2.67	129.21	125.03
14	G	1110	CLA	CMC-C2C-C1C	2.67	129.21	125.03
15	H	1237	F6C	C3A-C4A-NA	2.67	112.77	110.13
14	b	1235	CLA	CMC-C2C-C1C	2.67	129.21	125.03
15	B	1230	F6C	CHB-C4A-C3A	-2.67	119.93	125.49
14	B	1211	CLA	C4-C3-C5	2.67	119.86	115.23
14	b	1208	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
14	B	1217	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
14	A	1106	CLA	C4D-C3D-CAD	2.67	111.00	108.11
14	a	1102	CLA	CMC-C2C-C1C	2.67	129.21	125.03
14	H	1225	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
15	B	1237	F6C	C3C-C4C-NC	2.67	113.25	110.32
14	U	1503	CLA	C4-C3-C5	2.67	119.86	115.23
14	a	1128	CLA	C2B-C1B-NB	2.67	113.09	110.33
15	b	1230	F6C	CHB-C4A-C3A	-2.67	119.94	125.49
14	H	1228	CLA	CAC-C3C-C4C	2.67	128.26	124.79
14	a	1106	CLA	CMC-C2C-C1C	2.67	129.20	125.03
14	b	1208	CLA	CMC-C2C-C1C	2.67	129.20	125.03
14	U	1503	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
14	b	1235	CLA	CMA-C3A-C4A	2.67	118.94	111.77
14	B	1205	CLA	O2A-C1-C2	2.67	118.37	108.11
14	B	1233	CLA	CMC-C2C-C1C	2.67	129.20	125.03
14	G	1106	CLA	C3D-C4D-ND	2.67	114.32	109.99
14	K	1401	CLA	C3D-C4D-ND	2.67	114.32	109.99
14	H	1205	CLA	O2A-C1-C2	2.67	118.36	108.11
14	l	1503	CLA	C4-C3-C5	2.66	119.85	115.23
14	L	1503	CLA	CAA-C2A-C3A	-2.66	105.80	113.00
20	I	5006	LMG	O8-C28-C29	2.66	119.96	111.83
14	H	1208	CLA	CMC-C2C-C1C	2.66	129.20	125.03
14	A	1106	CLA	CMC-C2C-C1C	2.66	129.20	125.03
14	G	1139	CLA	C3D-C4D-ND	2.66	114.32	109.99
18	b	4004	BCR	C37-C22-C21	-2.66	118.50	122.82
14	G	1127	CLA	CMC-C2C-C1C	2.66	129.20	125.03
18	b	4013	BCR	C3-C4-C5	-2.66	109.31	114.06
14	B	1021	CLA	CBC-CAC-C3C	-2.66	105.20	112.42
14	G	1115	CLA	O1D-CGD-CBD	-2.66	119.27	124.52
14	G	1133	CLA	C4D-C3D-CAD	2.66	111.00	108.11
18	B	4013	BCR	C3-C4-C5	-2.66	109.31	114.06
14	B	1221	CLA	C4-C3-C5	2.66	119.85	115.23
14	T	1401	CLA	C3D-C4D-ND	2.66	114.31	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1208	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	b	1211	CLA	C4-C3-C5	2.66	119.85	115.23
20	i	5006	LMG	O8-C28-C29	2.66	119.95	111.83
18	H	4014	BCR	C36-C18-C17	-2.66	118.51	122.82
14	H	1235	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	H	1208	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	a	1135	CLA	CAC-C3C-C4C	2.66	128.25	124.79
14	H	1233	CLA	C4D-C3D-CAD	2.66	111.00	108.11
14	A	1133	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	H	1214	CLA	CAA-CBA-CGA	-2.66	105.66	113.21
14	H	1235	CLA	CMA-C3A-C4A	2.66	118.92	111.77
16	G	2001	PQN	C11-C12-C13	-2.66	122.25	126.83
14	b	1217	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	H	1201	CLA	CMC-C2C-C1C	2.66	129.19	125.03
14	a	1119	CLA	C3D-C4D-ND	2.66	114.31	109.99
14	H	1221	CLA	CAC-C3C-C4C	2.66	128.25	124.79
14	b	1023	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
14	B	1220	CLA	C4-C3-C5	2.66	119.84	115.23
14	a	1133	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	B	1235	CLA	CMA-C3A-C4A	2.65	118.91	111.77
18	I	4020	BCR	C31-C1-C6	-2.65	106.08	110.24
14	a	1115	CLA	O1D-CGD-CBD	-2.65	119.28	124.52
14	G	1133	CLA	CMC-C2C-C1C	2.65	129.18	125.03
14	A	1110	CLA	CMC-C2C-C1C	2.65	129.18	125.03
18	H	4013	BCR	C3-C4-C5	-2.65	109.33	114.06
15	b	1230	F6C	CHD-C1D-ND	-2.65	120.32	124.31
14	G	1135	CLA	CAC-C3C-C4C	2.65	128.24	124.79
14	b	1228	CLA	CAC-C3C-C4C	2.65	128.24	124.79
15	B	1230	F6C	CHD-C1D-ND	-2.65	120.32	124.31
14	b	1021	CLA	C3C-C4C-NC	2.65	113.83	110.43
14	b	1233	CLA	CMC-C2C-C1C	2.65	129.18	125.03
14	B	1021	CLA	CMC-C2C-C1C	2.65	129.18	125.03
18	R	4020	BCR	C31-C1-C6	-2.65	106.09	110.24
18	H	4004	BCR	C37-C22-C21	-2.65	118.52	122.82
14	B	1213	CLA	C4-C3-C5	2.65	119.83	115.23
14	H	1211	CLA	C4-C3-C5	2.65	119.83	115.23
14	B	1208	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	l	1503	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
14	H	1217	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	H	1023	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
14	A	1119	CLA	C3D-C4D-ND	2.65	114.29	109.99
14	W	1701	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	H	1233	CLA	CMC-C2C-C1C	2.65	129.17	125.03
14	a	1133	CLA	CMC-C2C-C1C	2.65	129.17	125.03
14	A	1120	CLA	CMC-C2C-C1C	2.65	129.17	125.03
14	B	1023	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
14	A	1115	CLA	O1D-CGD-CBD	-2.65	119.30	124.52
14	b	1219	CLA	C3D-C4D-ND	2.65	114.29	109.99
14	b	1208	CLA	C3D-C4D-ND	2.64	114.29	109.99
14	x	1701	CLA	C3C-C4C-NC	2.64	113.82	110.43
14	H	1225	CLA	C3D-C4D-ND	2.64	114.28	109.99
20	R	5006	LMG	O8-C28-C29	2.64	119.89	111.83
14	B	1228	CLA	CAC-C3C-C4C	2.64	128.23	124.79
14	b	1227	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
14	b	1225	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	B	1219	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	H	1208	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	H	1220	CLA	CAC-C3C-C4C	2.64	128.23	124.79
15	b	1230	F6C	CHA-C4D-ND	2.64	135.58	133.05
14	H	1235	CLA	O2A-C1-C2	2.64	118.27	108.11
14	A	1117	CLA	CMA-C3A-C4A	2.64	118.87	111.77
14	a	1114	CLA	CMD-C2D-C3D	-2.64	121.64	127.69
14	B	1208	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	H	1213	CLA	C4-C3-C5	2.64	119.81	115.23
14	a	1127	CLA	C4-C3-C5	2.64	119.81	115.23
14	b	1219	CLA	CMC-C2C-C1C	2.64	129.16	125.03
14	a	1106	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	A	1108	CLA	C3D-C4D-ND	2.64	114.28	109.99
14	H	1227	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
14	a	1113	CLA	OBD-CAD-C3D	-2.64	122.25	128.42
14	b	1213	CLA	C4-C3-C5	2.64	119.81	115.23
14	G	1127	CLA	C4-C3-C5	2.64	119.81	115.23
14	H	1214	CLA	CMC-C2C-C1C	2.64	129.15	125.03
14	b	1215	CLA	CMB-C2B-C1B	2.64	129.43	125.42
14	G	1123	CLA	CMC-C2C-C1C	2.64	129.15	125.03
14	A	1123	CLA	CMC-C2C-C1C	2.64	129.15	125.03
14	G	1117	CLA	CMA-C3A-C4A	2.64	118.86	111.77
14	B	1227	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
18	U	4019	BCR	C8-C7-C6	-2.64	119.96	127.00
14	G	1107	CLA	C3C-C4C-NC	2.64	113.81	110.43
14	b	1233	CLA	C4D-C3D-CAD	2.64	110.97	108.11
14	H	1219	CLA	CMC-C2C-C1C	2.63	129.15	125.03
15	H	1230	F6C	CHD-C1D-ND	-2.63	120.34	124.31
18	L	4019	BCR	C8-C7-C6	-2.63	119.96	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	b	1237	F6C	C3A-C4A-NA	2.63	112.73	110.13
14	B	1221	CLA	CAC-C3C-C4C	2.63	128.22	124.79
14	b	1021	CLA	CMC-C2C-C1C	2.63	129.15	125.03
18	l	4019	BCR	C8-C7-C6	-2.63	119.97	127.00
14	a	1128	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	B	1235	CLA	O2A-C1-C2	2.63	118.23	108.11
14	b	1214	CLA	CMC-C2C-C1C	2.63	129.15	125.03
14	k	1401	CLA	CMB-C2B-C1B	2.63	129.42	125.42
14	G	1119	CLA	C3D-C4D-ND	2.63	114.26	109.99
14	H	1021	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	B	1204	CLA	O2A-C1-C2	2.63	118.22	108.11
14	H	1219	CLA	C3D-C4D-ND	2.63	114.26	109.99
14	a	1133	CLA	C4D-C3D-CAD	2.63	110.96	108.11
16	A	2001	PQN	C11-C12-C13	-2.63	122.30	126.83
14	G	1139	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	b	1235	CLA	O2A-C1-C2	2.63	118.22	108.11
14	G	1106	CLA	C4D-C3D-CAD	2.63	110.96	108.11
14	b	1229	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	a	1117	CLA	CMA-C3A-C4A	2.63	118.83	111.77
14	X	1701	CLA	C3C-C4C-NC	2.63	113.80	110.43
14	H	1229	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	H	1225	CLA	C3C-C4C-NC	2.63	113.79	110.43
14	B	1219	CLA	CMC-C2C-C1C	2.63	129.14	125.03
14	H	1229	CLA	CMA-C3A-C4A	2.63	118.83	111.77
16	a	2001	PQN	C11-C12-C13	-2.62	122.31	126.83
14	a	1128	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
14	b	1221	CLA	CAC-C3C-C4C	2.62	128.21	124.79
14	b	1201	CLA	CMC-C2C-C1C	2.62	129.13	125.03
18	A	4011	BCR	C24-C25-C26	-2.62	115.51	121.56
14	A	1127	CLA	C4-C3-C5	2.62	119.78	115.23
14	G	1128	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
14	G	1126	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
14	b	1233	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	G	1120	CLA	C3D-C4D-ND	2.62	114.25	109.99
18	a	4011	BCR	C24-C25-C26	-2.62	115.52	121.56
14	B	1206	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
14	B	1229	CLA	CMA-C3A-C4A	2.62	118.82	111.77
14	A	1128	CLA	C4B-C3B-C2B	-2.62	104.04	107.30
15	H	1230	F6C	CHA-C1A-C2A	-2.62	123.36	130.41
14	b	1214	CLA	CMA-C3A-C4A	2.62	118.82	111.77
14	G	1118	CLA	C3D-C4D-ND	2.62	114.25	109.99
14	a	1120	CLA	C3D-C4D-ND	2.62	114.25	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1113	CLA	C4D-C3D-CAD	2.62	110.95	108.11
15	B	1230	F6C	CHA-C1A-C2A	-2.62	123.36	130.41
14	B	1202	CLA	O2A-C1-C2	2.62	118.19	108.11
14	G	1120	CLA	CMC-C2C-C1C	2.62	129.13	125.03
14	A	1114	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
14	H	1215	CLA	CMB-C2B-C1B	2.62	129.41	125.42
14	A	1128	CLA	C3C-C4C-NC	2.62	113.79	110.43
14	B	1201	CLA	CMC-C2C-C1C	2.62	129.13	125.03
14	H	1204	CLA	O2A-C1-C2	2.62	118.19	108.11
14	B	1225	CLA	C3C-C4C-NC	2.62	113.78	110.43
14	A	1113	CLA	OBD-CAD-C3D	-2.62	122.30	128.42
14	b	1220	CLA	CAC-C3C-C4C	2.62	128.20	124.79
14	H	1206	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
14	H	1202	CLA	O2A-C1-C2	2.62	118.19	108.11
14	b	1204	CLA	O2A-C1-C2	2.62	118.19	108.11
18	L	4019	BCR	C38-C26-C27	2.62	119.18	113.60
14	b	1202	CLA	O2A-C1-C2	2.62	118.18	108.11
14	A	1105	CLA	CAC-C3C-C4C	2.62	128.20	124.79
14	G	1103	CLA	C3D-C4D-ND	2.62	114.24	109.99
14	B	1225	CLA	C3D-C4D-ND	2.62	114.24	109.99
14	H	1224	CLA	CAA-C2A-C3A	-2.62	105.93	113.00
14	H	1204	CLA	C4D-C3D-CAD	2.62	110.95	108.11
18	G	4011	BCR	C24-C25-C26	-2.62	115.53	121.56
14	B	1021	CLA	C3C-C4C-NC	2.62	113.78	110.43
14	b	1206	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
14	G	1111	CLA	C3D-C4D-ND	2.62	114.24	109.99
14	a	1103	CLA	C3D-C4D-ND	2.62	114.24	109.99
14	G	1114	CLA	CMD-C2D-C3D	-2.62	121.69	127.69
14	B	1210	CLA	O1D-CGD-CBD	-2.62	119.36	124.52
14	B	1214	CLA	CMA-C3A-C4A	2.62	118.80	111.77
14	a	1139	CLA	CMC-C2C-C1C	2.62	129.12	125.03
14	G	1113	CLA	OBD-CAD-C3D	-2.62	122.30	128.42
14	B	1233	CLA	C4D-C3D-CAD	2.61	110.95	108.11
14	a	1108	CLA	C3D-C4D-ND	2.61	114.24	109.99
14	B	1224	CLA	CAA-C2A-C3A	-2.61	105.93	113.00
15	A	1121	F6C	C3C-C4C-NC	2.61	113.19	110.32
14	H	1021	CLA	C3C-C4C-NC	2.61	113.78	110.43
14	a	1118	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	a	1111	CLA	CMC-C2C-C1C	2.61	129.12	125.03
14	H	1214	CLA	CMA-C3A-C4A	2.61	118.79	111.77
14	B	1215	CLA	CMB-C2B-C1B	2.61	129.40	125.42
14	a	1140	CLA	C3D-C4D-ND	2.61	114.23	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1120	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	B	1214	CLA	CMC-C2C-C1C	2.61	129.11	125.03
15	b	1230	F6C	CHA-C1A-C2A	-2.61	123.39	130.41
14	A	1128	CLA	C2B-C1B-NB	2.61	113.03	110.33
14	B	1220	CLA	CAC-C3C-C4C	2.61	128.19	124.79
14	b	1232	CLA	CMD-C2D-C3D	-2.61	121.70	127.69
18	l	4019	BCR	C38-C26-C27	2.61	119.16	113.60
14	b	1224	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
14	A	1133	CLA	CMC-C2C-C1C	2.61	129.11	125.03
14	b	1225	CLA	C3C-C4C-NC	2.61	113.77	110.43
14	A	1139	CLA	CMC-C2C-C1C	2.61	129.11	125.03
18	A	4011	BCR	C30-C25-C24	2.61	122.73	115.65
14	G	1133	CLA	C3D-C4D-ND	2.61	114.23	109.99
18	a	4011	BCR	C30-C25-C24	2.61	122.72	115.65
18	U	4019	BCR	C38-C26-C27	2.61	119.16	113.60
14	A	1133	CLA	C3D-C4D-ND	2.61	114.23	109.99
14	A	1135	CLA	CAC-C3C-C4C	2.61	128.18	124.79
15	B	1230	F6C	CHA-C4D-ND	2.61	135.54	133.05
18	i	4020	BCR	C31-C1-C6	-2.61	106.16	110.24
14	b	1209	CLA	C4D-C3D-CAD	2.61	110.94	108.11
14	H	1201	CLA	O1D-CGD-CBD	-2.61	119.38	124.52
14	H	1233	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
18	G	4011	BCR	C30-C25-C24	2.61	122.72	115.65
14	a	1106	CLA	C4D-C3D-CAD	2.60	110.94	108.11
15	B	1207	F6C	CMC-C2C-C1C	2.60	129.38	125.42
14	H	1210	CLA	CMC-C2C-C1C	2.60	129.10	125.03
14	A	1111	CLA	CMC-C2C-C1C	2.60	129.10	125.03
14	a	1123	CLA	C4D-C3D-CAD	2.60	110.93	108.11
14	a	1107	CLA	C3C-C4C-NC	2.60	113.77	110.43
14	a	1123	CLA	CMC-C2C-C1C	2.60	129.10	125.03
14	b	1229	CLA	CMA-C3A-C4A	2.60	118.77	111.77
14	a	1012	CLA	C3D-C4D-ND	2.60	114.22	109.99
14	B	1233	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
14	H	1232	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
14	B	1209	CLA	CMD-C2D-C3D	-2.60	121.73	127.69
14	H	1023	CLA	CHB-C4A-NA	2.60	128.15	124.40
18	U	4019	BCR	C37-C22-C21	-2.60	118.61	122.82
15	B	1237	F6C	C3A-C4A-NA	2.60	112.70	110.13
14	B	1229	CLA	CMC-C2C-C1C	2.60	129.09	125.03
14	A	1137	CLA	C3D-C4D-ND	2.60	114.21	109.99
14	X	1701	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
18	G	4002	BCR	C7-C8-C9	-2.60	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	W	1701	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
14	B	1232	CLA	CMD-C2D-C3D	-2.60	121.74	127.69
14	A	1106	CLA	O1D-CGD-CBD	-2.60	119.40	124.52
14	A	1013	CLA	C3C-C4C-NC	2.59	113.75	110.43
14	A	1118	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	b	1205	CLA	OBD-CAD-C3D	-2.59	122.35	128.42
14	G	1111	CLA	CMC-C2C-C1C	2.59	129.09	125.03
14	G	1108	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	G	1110	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	b	1222	CLA	C3D-C4D-ND	2.59	114.20	109.99
18	A	4002	BCR	C30-C25-C26	-2.59	119.09	122.64
18	U	4022	BCR	C35-C13-C12	2.59	122.05	118.09
14	B	1210	CLA	CMC-C2C-C1C	2.59	129.08	125.03
14	H	1209	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
14	H	1205	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	a	1110	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	A	1103	CLA	C3D-C4D-ND	2.59	114.20	109.99
14	B	1229	CLA	CMB-C2B-C3B	2.59	132.64	126.55
14	b	1022	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
14	b	1210	CLA	CMC-C2C-C1C	2.59	129.08	125.03
15	A	1121	F6C	OMB-CMB-C2B	-2.59	119.78	125.62
14	A	1113	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	A	1132	CLA	C4D-C3D-CAD	2.59	110.92	108.11
14	H	1229	CLA	CMB-C2B-C3B	2.59	132.64	126.55
14	K	1401	CLA	CMB-C2B-C1B	2.59	129.36	125.42
14	b	1223	CLA	C4-C3-C5	2.59	119.72	115.23
14	G	1106	CLA	O1D-CGD-CBD	-2.59	119.42	124.52
14	G	1112	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
14	T	1401	CLA	CMB-C2B-C1B	2.59	129.36	125.42
14	G	1105	CLA	CAC-C3C-C4C	2.59	128.15	124.79
14	a	1105	CLA	CAC-C3C-C4C	2.59	128.15	124.79
14	b	1229	CLA	CMB-C2B-C3B	2.59	132.63	126.55
14	a	1135	CLA	C3D-C4D-ND	2.59	114.19	109.99
14	a	1127	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	A	1139	CLA	CMB-C2B-C1B	2.58	129.35	125.42
14	b	1209	CLA	CMD-C2D-C3D	-2.58	121.76	127.69
14	b	1201	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
14	A	1134	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
14	B	1234	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
15	B	1207	F6C	C3C-C4C-NC	2.58	113.15	110.32
14	H	1211	CLA	CMC-C2C-C1C	2.58	129.07	125.03
14	G	1139	CLA	CMB-C2B-C1B	2.58	129.35	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1106	CLA	C3C-C4C-NC	2.58	113.74	110.43
15	A	1121	F6C	CHA-C1A-C2A	-2.58	123.47	130.41
15	G	1121	F6C	C3C-C4C-NC	2.58	113.15	110.32
18	A	4002	BCR	C7-C8-C9	-2.58	122.42	126.23
14	B	1023	CLA	CHB-C4A-NA	2.58	128.12	124.40
14	B	1022	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
15	a	1121	F6C	CHA-C1A-C2A	-2.58	123.47	130.41
14	H	1232	CLA	CMC-C2C-C1C	2.58	129.07	125.03
14	A	1110	CLA	C4D-C3D-CAD	2.58	110.91	108.11
14	G	1108	CLA	CMB-C2B-C3B	2.58	132.62	126.55
14	G	1128	CLA	C3C-C4C-NC	2.58	113.74	110.43
14	a	1013	CLA	C3C-C4C-NC	2.58	113.74	110.43
14	a	1129	CLA	C3C-C4C-NC	2.58	113.74	110.43
15	a	1121	F6C	C3C-C4C-NC	2.58	113.15	110.32
14	a	1137	CLA	C3D-C4D-ND	2.58	114.18	109.99
15	b	1207	F6C	CMC-C2C-C1C	2.58	129.35	125.42
14	a	1133	CLA	C3D-C4D-ND	2.58	114.18	109.99
14	a	1106	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
14	B	1223	CLA	CMB-C2B-C3B	2.58	132.62	126.55
14	H	1205	CLA	OBD-CAD-C3D	-2.58	122.39	128.42
14	b	1204	CLA	C1-O2A-CGA	2.58	122.89	116.65
14	B	1205	CLA	C4-C3-C5	2.58	119.70	115.23
14	A	1108	CLA	CMB-C2B-C3B	2.58	132.61	126.55
14	A	1107	CLA	C3C-C4C-NC	2.58	113.73	110.43
14	b	1211	CLA	CMC-C2C-C1C	2.58	129.06	125.03
14	B	1205	CLA	OBD-CAD-C3D	-2.58	122.39	128.42
14	A	1118	CLA	CMC-C2C-C1C	2.58	129.06	125.03
14	H	1210	CLA	O1D-CGD-CBD	-2.58	119.44	124.52
14	b	1214	CLA	OBD-CAD-C3D	-2.58	122.40	128.42
14	H	1231	CLA	C3C-C4C-NC	2.57	113.73	110.43
14	x	1701	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	B	1204	CLA	C4D-C3D-CAD	2.57	110.90	108.11
14	a	1120	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	b	1234	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	H	1022	CLA	CAA-C2A-C3A	-2.57	106.04	113.00
14	G	1140	CLA	C3D-C4D-ND	2.57	114.17	109.99
18	L	4019	BCR	C37-C22-C21	-2.57	118.65	122.82
15	G	1121	F6C	OMB-CMB-C2B	-2.57	119.81	125.62
14	B	1232	CLA	CMC-C2C-C1C	2.57	129.06	125.03
14	b	1223	CLA	CMB-C2B-C3B	2.57	132.60	126.55
15	G	1121	F6C	CHA-C1A-C2A	-2.57	123.49	130.41
14	a	1126	CLA	O1D-CGD-CBD	-2.57	119.44	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1132	CLA	C4D-C3D-CAD	2.57	110.90	108.11
14	A	1126	CLA	O1D-CGD-CBD	-2.57	119.44	124.52
14	B	1201	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
14	A	1106	CLA	CMA-C3A-C4A	2.57	118.68	111.77
14	H	1223	CLA	C4-C3-C5	2.57	119.69	115.23
14	G	1120	CLA	CMA-C3A-C4A	2.57	118.68	111.77
14	G	1118	CLA	CMC-C2C-C1C	2.57	129.05	125.03
18	A	4002	BCR	C15-C14-C13	-2.57	123.67	127.28
14	a	1111	CLA	C3D-C4D-ND	2.57	114.17	109.99
14	A	1120	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
18	l	4022	BCR	C35-C13-C12	2.57	122.01	118.09
14	G	1128	CLA	C2B-C1B-NB	2.57	112.99	110.33
14	b	1232	CLA	CMC-C2C-C1C	2.57	129.05	125.03
14	B	1202	CLA	CMC-C2C-C1C	2.57	129.05	125.03
14	A	1120	CLA	CMA-C3A-C4A	2.57	118.68	111.77
14	a	1113	CLA	C4D-C3D-CAD	2.57	110.90	108.11
14	H	1204	CLA	C1-O2A-CGA	2.57	122.87	116.65
14	a	1108	CLA	CMB-C2B-C3B	2.57	132.59	126.55
14	G	1134	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
14	G	1104	CLA	C4D-C3D-CAD	2.57	110.89	108.11
15	b	1207	F6C	C3C-C4C-NC	2.57	113.13	110.32
14	a	1106	CLA	C3C-C4C-NC	2.57	113.72	110.43
14	G	1131	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	a	1139	CLA	CMB-C2B-C1B	2.57	129.33	125.42
14	b	1213	CLA	CAC-C3C-C4C	2.57	128.13	124.79
14	b	1205	CLA	C4-C3-C5	2.57	119.68	115.23
14	A	1104	CLA	C4D-C3D-CAD	2.57	110.89	108.11
14	B	1209	CLA	C4D-C3D-CAD	2.57	110.89	108.11
18	G	4002	BCR	C30-C25-C26	-2.57	119.13	122.64
14	b	1202	CLA	C3C-C4C-NC	2.57	113.72	110.43
15	B	1238	F6C	CMC-C2C-C1C	2.57	129.33	125.42
14	A	1140	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	B	1217	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	H	1209	CLA	C4D-C3D-CAD	2.57	110.89	108.11
15	H	1207	F6C	CMC-C2C-C1C	2.57	129.33	125.42
14	B	1202	CLA	C3C-C4C-NC	2.57	113.72	110.43
14	H	1223	CLA	CMB-C2B-C3B	2.57	132.59	126.55
14	G	1135	CLA	C3D-C4D-ND	2.57	114.16	109.99
14	a	1106	CLA	CMA-C3A-C4A	2.57	118.67	111.77
14	A	1139	CLA	CMD-C2D-C3D	-2.57	121.81	127.69
14	H	1216	CLA	CMB-C2B-C1B	2.57	129.32	125.42
14	a	1120	CLA	CMA-C3A-C4A	2.57	118.67	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1217	CLA	C3D-C4D-ND	2.56	114.16	109.99
14	b	1210	CLA	O1D-CGD-CBD	-2.56	119.46	124.52
14	A	1135	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	k	1401	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
14	G	1106	CLA	C3C-C4C-NC	2.56	113.71	110.43
14	G	1123	CLA	C4D-C3D-CAD	2.56	110.89	108.11
14	a	1139	CLA	CMD-C2D-C3D	-2.56	121.81	127.69
14	B	1239	CLA	C2B-C1B-NB	2.56	112.98	110.33
14	b	1204	CLA	CAC-C3C-C4C	2.56	128.12	124.79
14	T	1401	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
14	a	1115	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	H	1205	CLA	C4-C3-C5	2.56	119.67	115.23
14	B	1204	CLA	C1-O2A-CGA	2.56	122.85	116.65
14	B	1221	CLA	C3D-C4D-ND	2.56	114.15	109.99
14	B	1214	CLA	OBD-CAD-C3D	-2.56	122.43	128.42
14	A	1132	CLA	CMD-C2D-C3D	-2.56	121.82	127.69
14	b	1213	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
14	G	1139	CLA	CMD-C2D-C3D	-2.56	121.82	127.69
14	A	1127	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
18	l	4019	BCR	C37-C22-C21	-2.56	118.67	122.82
14	b	1023	CLA	CHB-C4A-NA	2.56	128.09	124.40
14	G	1129	CLA	C3C-C4C-NC	2.56	113.71	110.43
14	a	1118	CLA	CMC-C2C-C1C	2.56	129.03	125.03
14	A	1112	CLA	C4-C3-C5	2.56	119.67	115.23
14	G	1116	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	G	1120	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
14	H	1214	CLA	OBD-CAD-C3D	-2.56	122.44	128.42
14	G	1012	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	H	1222	CLA	C3D-C4D-ND	2.56	114.14	109.99
14	b	1204	CLA	C4D-C3D-CAD	2.56	110.88	108.11
15	a	1121	F6C	OMB-CMB-C2B	-2.56	119.85	125.62
14	H	1234	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
18	b	4010	BCR	C28-C27-C26	-2.56	109.50	114.06
14	G	1138	CLA	CMB-C2B-C3B	2.56	132.56	126.55
14	G	1106	CLA	CMA-C3A-C4A	2.55	118.64	111.77
14	A	1112	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
14	A	1129	CLA	C3C-C4C-NC	2.55	113.70	110.43
14	B	1223	CLA	C4-C3-C5	2.55	119.66	115.23
14	A	1111	CLA	C3D-C4D-ND	2.55	114.14	109.99
18	G	4002	BCR	C30-C25-C24	2.55	122.58	115.65
14	b	1216	CLA	CMB-C2B-C1B	2.55	129.31	125.42
14	H	1208	CLA	C4-C3-C5	2.55	119.66	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	a	4002	BCR	C30-C25-C26	-2.55	119.15	122.64
14	H	1202	CLA	C3C-C4C-NC	2.55	113.70	110.43
14	a	1134	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
13	a	1011	CL0	C4-C3-C5	2.55	119.66	115.23
14	b	1217	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	a	1132	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
18	b	4016	BCR	C27-C26-C25	-2.55	119.26	122.70
14	b	1205	CLA	C4D-C3D-CAD	2.55	110.88	108.11
18	H	4016	BCR	C27-C26-C25	-2.55	119.26	122.70
14	B	1216	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	H	1201	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	H	1239	CLA	C4D-C3D-CAD	2.55	110.88	108.11
14	b	1205	CLA	O1D-CGD-CBD	-2.55	119.49	124.52
14	B	1213	CLA	CAC-C3C-C4C	2.55	128.11	124.79
14	A	1131	CLA	CMD-C2D-C3D	-2.55	121.84	127.69
14	A	1123	CLA	C4D-C3D-CAD	2.55	110.87	108.11
18	B	4010	BCR	C28-C27-C26	-2.55	109.51	114.06
14	B	1222	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	1204	CLA	CAC-C3C-C4C	2.55	128.10	124.79
14	A	1116	CLA	C3D-C4D-ND	2.55	114.13	109.99
14	b	1208	CLA	C4-C3-C5	2.55	119.65	115.23
18	a	4002	BCR	C7-C8-C9	-2.55	122.47	126.23
14	U	1503	CLA	CBA-CAA-C2A	-2.55	106.22	113.79
14	A	1129	CLA	CMD-C2D-C3D	-2.55	121.85	127.69
14	b	1212	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	b	1022	CLA	C4D-C3D-CAD	2.55	110.87	108.11
14	a	1126	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
14	a	1112	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
18	a	4008	BCR	C23-C24-C25	-2.54	120.20	127.00
14	G	1137	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	K	1401	CLA	O2D-CGD-O1D	-2.54	118.89	123.85
18	A	4002	BCR	C30-C25-C24	2.54	122.55	115.65
14	a	1138	CLA	CMB-C2B-C3B	2.54	132.53	126.55
14	A	1122	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	a	1112	CLA	C4-C3-C5	2.54	119.64	115.23
14	b	1231	CLA	C3C-C4C-NC	2.54	113.69	110.43
14	B	1231	CLA	C3C-C4C-NC	2.54	113.69	110.43
14	G	1120	CLA	C4D-C3D-CAD	2.54	110.87	108.11
14	a	1122	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	G	1132	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
14	B	1213	CLA	C3C-C4C-NC	2.54	113.69	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1201	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	G	1136	CLA	CAA-C2A-C3A	-2.54	106.13	113.00
18	G	4002	BCR	C15-C14-C13	-2.54	123.71	127.28
14	G	1112	CLA	C4-C3-C5	2.54	119.64	115.23
14	b	1212	CLA	C3D-C4D-ND	2.54	114.12	109.99
14	G	1122	CLA	C3D-C4D-ND	2.54	114.12	109.99
15	H	1238	F6C	CMC-C2C-C1C	2.54	129.29	125.42
14	b	1239	CLA	C4D-C3D-CAD	2.54	110.86	108.11
14	b	1213	CLA	C3C-C4C-NC	2.54	113.68	110.43
14	A	1136	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
14	a	1013	CLA	C4-C3-C5	2.54	119.64	115.23
14	b	1221	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	A	1012	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	H	1213	CLA	CAC-C3C-C4C	2.54	128.09	124.79
18	R	4020	BCR	C33-C5-C6	-2.54	121.71	124.48
14	l	1501	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
14	A	1138	CLA	CMB-C2B-C3B	2.54	132.52	126.55
14	b	1235	CLA	C4-C3-C5	2.54	119.63	115.23
21	G	6002	LMT	O5B-C5B-C4B	2.54	114.27	109.70
14	B	1205	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
14	B	1205	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	H	1220	CLA	CED-O2D-CGD	2.54	121.67	115.92
14	L	1501	CLA	CMC-C2C-C1C	2.54	129.00	125.03
18	L	4022	BCR	C35-C13-C12	2.54	121.96	118.09
14	a	1131	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
14	b	1204	CLA	CAA-C2A-C3A	-2.54	106.14	113.00
18	B	4005	BCR	C31-C1-C6	-2.54	106.27	110.24
14	B	1211	CLA	CMC-C2C-C1C	2.54	129.00	125.03
14	H	1221	CLA	C3D-C4D-ND	2.54	114.11	109.99
14	b	1214	CLA	C3D-C4D-ND	2.54	114.11	109.99
13	A	1011	CL0	C4-C3-C5	2.54	119.63	115.23
14	G	1131	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
14	B	1204	CLA	CAC-C3C-C4C	2.54	128.09	124.79
14	B	1212	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
15	B	1207	F6C	CHD-C1D-ND	-2.54	120.49	124.31
21	A	6002	LMT	O5B-C5B-C4B	2.54	114.27	109.70
14	A	1013	CLA	C4-C3-C5	2.54	119.63	115.23
18	a	4011	BCR	C35-C13-C12	2.54	121.96	118.09
14	H	1212	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
18	H	4010	BCR	C28-C27-C26	-2.54	109.53	114.06
14	l	1503	CLA	CBA-CAA-C2A	-2.54	106.25	113.79
18	B	4016	BCR	C27-C26-C25	-2.54	119.28	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1127	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
14	a	1115	CLA	CBA-CAA-C2A	2.53	121.33	113.79
14	H	1201	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	a	1132	CLA	C4D-C3D-CAD	2.53	110.86	108.11
18	a	4002	BCR	C30-C25-C24	2.53	122.53	115.65
14	a	1124	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
13	G	1011	CL0	C4-C3-C5	2.53	119.63	115.23
14	H	1022	CLA	C4D-C3D-CAD	2.53	110.86	108.11
15	b	1238	F6C	CMC-C2C-C1C	2.53	129.28	125.42
14	A	1131	CLA	C3D-C4D-ND	2.53	114.11	109.99
14	a	1117	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
14	G	1138	CLA	CAC-C3C-C4C	2.53	128.09	124.79
14	A	1138	CLA	CAC-C3C-C4C	2.53	128.09	124.79
14	G	1117	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
18	G	4008	BCR	C23-C24-C25	-2.53	120.23	127.00
14	A	1120	CLA	C3C-C4C-NC	2.53	113.67	110.43
14	b	1211	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
14	B	1239	CLA	C4D-C3D-CAD	2.53	110.86	108.11
14	B	1208	CLA	C4-C3-C5	2.53	119.62	115.23
14	G	1115	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	H	1204	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
14	B	1205	CLA	C4D-C3D-CAD	2.53	110.86	108.11
15	H	1207	F6C	CHD-C1D-ND	-2.53	120.50	124.31
14	l	1501	CLA	CMC-C2C-C1C	2.53	128.99	125.03
14	A	1126	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
14	a	1131	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	A	1130	CLA	C4-C3-C5	2.53	119.62	115.23
15	H	1207	F6C	C3C-C4C-NC	2.53	113.09	110.32
14	L	1503	CLA	CBA-CAA-C2A	-2.53	106.27	113.79
14	a	1123	CLA	C4-C3-C5	2.53	119.62	115.23
14	b	1202	CLA	CMC-C2C-C1C	2.53	128.99	125.03
14	A	1123	CLA	C1-O2A-CGA	2.53	122.77	116.65
14	B	1022	CLA	C4D-C3D-CAD	2.53	110.85	108.11
14	U	1503	CLA	C3C-C4C-NC	2.53	113.67	110.43
18	a	4002	BCR	C15-C14-C13	-2.53	123.73	127.28
14	G	1129	CLA	CMD-C2D-C3D	-2.53	121.89	127.69
14	B	1235	CLA	C4-C3-C5	2.53	119.62	115.23
14	B	1201	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	G	1123	CLA	C4-C3-C5	2.53	119.62	115.23
18	A	4011	BCR	C35-C13-C12	2.53	121.95	118.09
14	B	1212	CLA	C3D-C4D-ND	2.53	114.10	109.99
14	G	1116	CLA	CAA-C2A-C3A	-2.53	106.17	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1235	CLA	C4-C3-C5	2.53	119.61	115.23
14	A	1120	CLA	C4D-C3D-CAD	2.53	110.85	108.11
15	b	1207	F6C	CAC-C3C-C4C	2.53	128.39	124.91
14	H	1216	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
14	B	1201	CLA	CMD-C2D-C3D	-2.53	121.90	127.69
14	B	1204	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
14	b	1216	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
14	H	1205	CLA	O1D-CGD-CBD	-2.53	119.54	124.52
14	B	1213	CLA	O1D-CGD-CBD	-2.53	119.54	124.52
14	a	1136	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
14	H	1212	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	H	1236	CLA	CMC-C2C-C1C	2.52	128.98	125.03
14	A	1117	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
14	G	1127	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	a	1129	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
14	B	1211	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
14	G	1135	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	G	1123	CLA	C1-O2A-CGA	2.52	122.76	116.65
14	U	1501	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
14	A	1124	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
14	A	1123	CLA	C4-C3-C5	2.52	119.61	115.23
14	b	1220	CLA	CED-O2D-CGD	2.52	121.64	115.92
18	H	4005	BCR	C31-C1-C6	-2.52	106.29	110.24
14	H	1201	CLA	CMD-C2D-C3D	-2.52	121.90	127.69
15	b	1230	F6C	CMA-C3A-C4A	-2.52	120.29	124.73
14	a	1120	CLA	C3C-C4C-NC	2.52	113.66	110.43
18	A	4011	BCR	C4-C5-C6	-2.52	119.30	122.70
14	G	1115	CLA	CBA-CAA-C2A	2.52	121.30	113.79
14	A	1116	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
14	A	1115	CLA	C3D-C4D-ND	2.52	114.09	109.99
14	L	1501	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
14	A	1113	CLA	C3D-C4D-ND	2.52	114.08	109.99
18	i	4020	BCR	C33-C5-C6	-2.52	121.73	124.48
18	G	4011	BCR	C35-C13-C12	2.52	121.94	118.09
14	H	1213	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
14	H	1202	CLA	CMC-C2C-C1C	2.52	128.97	125.03
14	A	1116	CLA	C3C-C4C-NC	2.52	113.66	110.43
14	A	1114	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
14	G	1113	CLA	C3D-C4D-ND	2.52	114.08	109.99
15	B	1207	F6C	CAC-C3C-C4C	2.52	128.38	124.91
18	a	4008	BCR	C28-C27-C26	-2.52	109.57	114.06
14	B	1224	CLA	C4-C3-C5	2.52	119.60	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1115	CLA	C4D-C3D-CAD	2.52	110.84	108.11
18	A	4008	BCR	C23-C24-C25	-2.52	120.27	127.00
14	H	1213	CLA	C3C-C4C-NC	2.52	113.65	110.43
18	I	4020	BCR	C33-C5-C6	-2.52	121.74	124.48
14	a	1120	CLA	C4D-C3D-CAD	2.52	110.84	108.11
14	G	1112	CLA	C3D-C4D-ND	2.52	114.08	109.99
14	b	1236	CLA	CMC-C2C-C1C	2.52	128.97	125.03
14	a	1123	CLA	C1-O2A-CGA	2.52	122.74	116.65
14	G	1013	CLA	C3C-C4C-NC	2.52	113.65	110.43
18	b	4005	BCR	C31-C1-C6	-2.52	106.30	110.24
14	B	1214	CLA	C3D-C4D-ND	2.52	114.08	109.99
18	G	4003	BCR	C30-C25-C26	-2.51	119.20	122.64
14	G	1124	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
14	H	1205	CLA	CMC-C2C-C1C	2.51	128.96	125.03
15	b	1207	F6C	CHD-C1D-ND	-2.51	120.53	124.31
14	a	1135	CLA	C3C-C4C-NC	2.51	113.65	110.43
15	H	1230	F6C	CMA-C3A-C4A	-2.51	120.30	124.73
14	G	1013	CLA	C4-C3-C5	2.51	119.59	115.23
14	G	1116	CLA	C3C-C4C-NC	2.51	113.65	110.43
14	B	1214	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	H	1218	CLA	C3D-C4D-ND	2.51	114.07	109.99
15	H	1207	F6C	CAC-C3C-C4C	2.51	128.37	124.91
14	b	1023	CLA	C3D-C4D-ND	2.51	114.07	109.99
14	B	1214	CLA	C4-C3-C5	2.51	119.59	115.23
14	B	1021	CLA	CAA-CBA-CGA	-2.51	106.08	113.21
14	B	1216	CLA	CMB-C2B-C1B	2.51	129.24	125.42
14	A	1115	CLA	CBA-CAA-C2A	2.51	121.27	113.79
21	a	6001	LMT	O5'-C5'-C4'	2.51	114.92	109.72
14	B	1236	CLA	CMC-C2C-C1C	2.51	128.96	125.03
14	G	1107	CLA	C3D-C4D-ND	2.51	114.07	109.99
14	a	1119	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
21	a	6002	LMT	O5B-C5B-C4B	2.51	114.22	109.70
18	G	4008	BCR	C28-C27-C26	-2.51	109.58	114.06
14	H	1239	CLA	C3D-C4D-ND	2.51	114.07	109.99
14	H	1211	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
14	A	1127	CLA	C3D-C4D-ND	2.51	114.06	109.99
14	a	1130	CLA	C4-C3-C5	2.51	119.58	115.23
14	l	1503	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	A	1116	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
14	G	1115	CLA	CMB-C2B-C3B	2.51	132.45	126.55
14	H	1234	CLA	C3D-C4D-ND	2.51	114.06	109.99
14	G	1119	CLA	O2D-CGD-O1D	-2.51	118.97	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1224	CLA	C4-C3-C5	2.51	119.58	115.23
14	G	1106	CLA	CAA-C2A-C1A	-2.51	103.76	111.97
14	a	1137	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
14	L	1503	CLA	C3C-C4C-NC	2.51	113.64	110.43
14	a	1116	CLA	CAA-C2A-C3A	-2.51	106.23	113.00
14	A	1107	CLA	C3D-C4D-ND	2.51	114.06	109.99
14	a	1138	CLA	CAC-C3C-C4C	2.51	128.05	124.79
14	a	1117	CLA	CAA-C2A-C1A	-2.51	103.76	111.97
14	a	1140	CLA	C4D-C3D-CAD	2.51	110.83	108.11
14	a	1127	CLA	C3D-C4D-ND	2.50	114.06	109.99
14	H	1021	CLA	CAA-CBA-CGA	-2.50	106.10	113.21
14	G	1120	CLA	C3C-C4C-NC	2.50	113.64	110.43
14	a	1115	CLA	CMB-C2B-C3B	2.50	132.44	126.55
14	a	1101	CLA	CMA-C3A-C4A	2.50	118.50	111.77
18	B	4005	BCR	C37-C22-C21	-2.50	118.76	122.82
14	G	1117	CLA	CAA-C2A-C1A	-2.50	103.77	111.97
14	a	1138	CLA	CAA-C2A-C3A	-2.50	106.23	113.00
18	a	4011	BCR	C4-C5-C6	-2.50	119.32	122.70
14	G	1130	CLA	C4-C3-C5	2.50	119.57	115.23
18	A	4008	BCR	C28-C27-C26	-2.50	109.59	114.06
14	b	1201	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	G	1126	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
14	B	1023	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	a	1114	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
14	A	1113	CLA	C3C-C4C-NC	2.50	113.64	110.43
14	G	1114	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
14	A	1107	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	G	1116	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
15	A	1121	F6C	O2D-CGD-O1D	-2.50	118.98	123.85
14	b	1021	CLA	CAA-CBA-CGA	-2.50	106.11	113.21
14	b	1201	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
14	a	1116	CLA	C3C-C4C-NC	2.50	113.63	110.43
14	G	1137	CLA	CAA-CBA-CGA	-2.50	106.11	113.21
14	B	1213	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	B	1218	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	H	1239	CLA	C2B-C1B-NB	2.50	112.92	110.33
14	a	1107	CLA	C3D-C4D-ND	2.50	114.05	109.99
18	G	4007	BCR	C23-C24-C25	-2.50	120.33	127.00
14	a	1113	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
14	A	1117	CLA	CAA-C2A-C1A	-2.50	103.79	111.97
15	a	1121	F6C	O2D-CGD-O1D	-2.50	118.99	123.85
14	A	1102	CLA	C3D-C4D-ND	2.50	114.05	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1104	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	U	1501	CLA	CMC-C2C-C1C	2.50	128.94	125.03
14	b	1224	CLA	C3D-C4D-ND	2.50	114.05	109.99
14	G	1103	CLA	CAC-C3C-C4C	2.50	128.04	124.79
14	b	1213	CLA	C4D-C3D-CAD	2.50	110.82	108.11
14	a	1113	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	A	1138	CLA	CAA-C2A-C3A	-2.49	106.26	113.00
18	a	4003	BCR	C30-C25-C26	-2.49	119.23	122.64
14	a	1106	CLA	CAA-C2A-C1A	-2.49	103.80	111.97
14	H	1214	CLA	C6-C5-C3	-2.49	107.39	113.47
14	a	1116	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	A	1106	CLA	CAA-C2A-C1A	-2.49	103.80	111.97
14	H	1214	CLA	C4-C3-C5	2.49	119.56	115.23
18	A	4003	BCR	C30-C25-C26	-2.49	119.23	122.64
18	l	4022	BCR	C19-C18-C17	2.49	122.93	119.01
14	A	1115	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	G	1138	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	a	1102	CLA	C3D-C4D-ND	2.49	114.04	109.99
21	G	6001	LMT	O5'-C5'-C4'	2.49	114.88	109.72
14	a	1114	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	A	1115	CLA	CMB-C2B-C3B	2.49	132.41	126.55
14	H	1202	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	H	1214	CLA	C3D-C4D-ND	2.49	114.04	109.99
14	G	1107	CLA	CMC-C2C-C1C	2.49	128.93	125.03
14	A	1113	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
14	a	1103	CLA	CAC-C3C-C4C	2.49	128.03	124.79
15	B	1230	F6C	CMA-C3A-C4A	-2.49	120.34	124.73
14	G	1113	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
14	A	1119	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
14	H	1205	CLA	C3D-C4D-ND	2.49	114.03	109.99
14	A	1137	CLA	CAA-CBA-CGA	-2.49	106.14	113.21
14	a	1131	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
14	H	1023	CLA	C3D-C4D-ND	2.49	114.03	109.99
14	a	1116	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
14	B	1220	CLA	CED-O2D-CGD	2.49	121.56	115.92
18	G	4011	BCR	C4-C5-C6	-2.49	119.34	122.70
14	a	1130	CLA	C1-O2A-CGA	2.49	122.67	116.65
14	b	1239	CLA	C2B-C1B-NB	2.49	112.91	110.33
14	A	1101	CLA	CMA-C3A-C4A	2.49	118.46	111.77
18	U	4022	BCR	C19-C18-C17	2.49	122.92	119.01
14	G	1113	CLA	C3C-C4C-NC	2.49	113.62	110.43
18	A	4007	BCR	C23-C24-C25	-2.49	120.36	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1130	CLA	C1-O2A-CGA	2.49	122.67	116.65
14	A	1101	CLA	CMC-C2C-C1C	2.49	128.92	125.03
14	b	1214	CLA	C6-C5-C3	-2.49	107.41	113.47
21	A	6001	LMT	O5'-C5'-C4'	2.49	114.86	109.72
14	A	1116	CLA	C4-C3-C5	2.49	119.54	115.23
14	G	1101	CLA	CMA-C3A-C4A	2.49	118.45	111.77
14	G	1125	CLA	C4D-C3D-CAD	2.49	110.81	108.11
14	U	1501	CLA	C3D-C4D-ND	2.48	114.03	109.99
18	A	4002	BCR	C23-C24-C25	-2.48	120.36	127.00
14	G	1138	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
14	b	1231	CLA	C4D-C3D-CAD	2.48	110.80	108.11
18	b	4005	BCR	C37-C22-C21	-2.48	118.79	122.82
14	B	1239	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	b	1212	CLA	CMC-C2C-C1C	2.48	128.91	125.03
18	G	4002	BCR	C23-C24-C25	-2.48	120.36	127.00
14	B	1214	CLA	C6-C5-C3	-2.48	107.42	113.47
14	b	1218	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	A	1138	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	B	1224	CLA	C3D-C4D-ND	2.48	114.02	109.99
15	G	1121	F6C	O2D-CGD-O1D	-2.48	119.02	123.85
14	H	1212	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	A	1130	CLA	C1-O2A-CGA	2.48	122.66	116.65
14	B	1202	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	L	1501	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	G	1126	CLA	C4D-C3D-CAD	2.48	110.80	108.11
14	b	1214	CLA	C4-C3-C5	2.48	119.53	115.23
14	b	1202	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	B	1239	CLA	CMB-C2B-C1B	2.48	129.20	125.42
18	a	4002	BCR	C23-C24-C25	-2.48	120.37	127.00
14	A	1103	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
14	A	1103	CLA	CAC-C3C-C4C	2.48	128.02	124.79
14	H	1224	CLA	C3D-C4D-ND	2.48	114.02	109.99
14	b	1225	CLA	CMC-C2C-C1C	2.48	128.91	125.03
14	T	1401	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
14	A	1140	CLA	C4D-C3D-CAD	2.48	110.80	108.11
14	B	1201	CLA	C4D-C3D-CAD	2.48	110.80	108.11
14	b	1234	CLA	C3D-C4D-ND	2.48	114.01	109.99
14	l	1501	CLA	C3D-C4D-ND	2.48	114.01	109.99
18	H	4013	BCR	C34-C9-C10	-2.48	118.81	122.82
14	A	1120	CLA	CMB-C2B-C1B	2.47	129.19	125.42
14	B	1236	CLA	C3C-C4C-NC	2.47	113.60	110.43
14	b	1229	CLA	CAA-C2A-C1A	-2.47	103.87	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1224	CLA	C4-C3-C5	2.47	119.52	115.23
18	a	4007	BCR	C23-C24-C25	-2.47	120.39	127.00
14	a	1138	CLA	C3D-C4D-ND	2.47	114.01	109.99
14	B	1225	CLA	CMC-C2C-C1C	2.47	128.90	125.03
14	a	1122	CLA	CAA-C2A-C3A	-2.47	106.32	113.00
14	G	1140	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	a	1104	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
14	b	1223	CLA	OBD-CAD-C3D	-2.47	122.64	128.42
14	a	1134	CLA	CMC-C2C-C1C	2.47	128.90	125.03
14	a	1120	CLA	CMB-C2B-C1B	2.47	129.18	125.42
14	G	1115	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	H	1213	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	a	1126	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	k	1401	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
14	b	1239	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	A	1112	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	H	1223	CLA	OBD-CAD-C3D	-2.47	122.64	128.42
14	a	1107	CLA	CMC-C2C-C1C	2.47	128.90	125.03
14	H	1206	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
14	G	1102	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	a	1134	CLA	CMB-C2B-C3B	2.47	132.36	126.55
14	G	1103	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	G	1116	CLA	C4-C3-C5	2.47	119.51	115.23
14	a	1116	CLA	C4-C3-C5	2.47	119.51	115.23
14	B	1203	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
14	B	1234	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	K	1401	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
14	H	1214	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	A	1111	CLA	C3C-C4C-NC	2.47	113.59	110.43
14	G	1101	CLA	CMC-C2C-C1C	2.47	128.89	125.03
14	L	1502	CLA	C4-C3-C5	2.47	119.51	115.23
14	A	1104	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
14	A	1122	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
14	x	1701	CLA	C4D-C3D-CAD	2.47	110.79	108.11
14	b	1215	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	b	1202	CLA	CAC-C3C-C4C	2.47	128.00	124.79
14	G	1114	CLA	C3D-C4D-ND	2.47	114.00	109.99
14	a	1101	CLA	CMC-C2C-C1C	2.47	128.89	125.03
18	H	4009	BCR	C38-C26-C27	2.47	118.85	113.60
14	a	1113	CLA	C3C-C4C-NC	2.47	113.59	110.43
14	l	1502	CLA	C4-C3-C5	2.47	119.51	115.23
14	H	1231	CLA	C4D-C3D-CAD	2.47	110.78	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1105	CLA	CMC-C2C-C1C	2.47	128.89	125.03
14	H	1234	CLA	C4-C3-C5	2.47	119.51	115.23
14	H	1229	CLA	CAA-C2A-C1A	-2.47	103.90	111.97
14	B	1229	CLA	CAA-C2A-C1A	-2.47	103.90	111.97
18	U	4019	BCR	C34-C9-C8	2.46	121.85	118.09
18	L	4019	BCR	C34-C9-C8	2.46	121.85	118.09
14	a	1126	CLA	C3C-C4C-NC	2.46	113.59	110.43
18	L	4022	BCR	C19-C18-C17	2.46	122.89	119.01
14	G	1134	CLA	CMC-C2C-C1C	2.46	128.88	125.03
14	B	1206	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
14	b	1232	CLA	C3D-C4D-ND	2.46	113.99	109.99
14	b	1227	CLA	CMA-C3A-C4A	2.46	118.39	111.77
14	B	1234	CLA	C4-C3-C5	2.46	119.50	115.23
14	b	1205	CLA	C3D-C4D-ND	2.46	113.99	109.99
14	b	1210	CLA	CMB-C2B-C3B	2.46	132.34	126.55
18	H	4005	BCR	C37-C22-C21	-2.46	118.83	122.82
18	B	4013	BCR	C34-C9-C10	-2.46	118.83	122.82
14	b	1206	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
14	G	1134	CLA	CMB-C2B-C3B	2.46	132.34	126.55
14	W	1701	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	B	1210	CLA	CMB-C2B-C3B	2.46	132.33	126.55
14	B	1203	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	b	1206	CLA	C3D-C4D-ND	2.46	113.98	109.99
18	R	4018	BCR	C2-C1-C6	2.46	114.01	110.44
14	b	1215	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
14	H	1227	CLA	CMA-C3A-C4A	2.46	118.38	111.77
14	B	1223	CLA	C4D-C3D-CAD	2.46	110.78	108.11
14	A	1105	CLA	CMC-C2C-C1C	2.46	128.87	125.03
14	T	1401	CLA	CAC-C3C-C4C	2.46	127.99	124.79
14	a	1104	CLA	C4-C3-C5	2.46	119.49	115.23
14	A	1135	CLA	C3C-C4C-NC	2.46	113.58	110.43
14	H	1210	CLA	CMB-C2B-C3B	2.46	132.33	126.55
14	B	1231	CLA	C4D-C3D-CAD	2.46	110.77	108.11
14	G	1131	CLA	O1D-CGD-CBD	-2.46	119.67	124.52
14	A	1109	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
14	G	1104	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
14	b	1214	CLA	C4D-C3D-CAD	2.46	110.77	108.11
14	G	1122	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
14	G	1126	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	U	1502	CLA	C4-C3-C5	2.45	119.49	115.23
14	b	1234	CLA	C4-C3-C5	2.45	119.49	115.23
18	b	4013	BCR	C34-C9-C10	-2.45	118.84	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1239	CLA	CMB-C2B-C1B	2.45	129.16	125.42
14	A	1114	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	a	1112	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	X	1701	CLA	C4D-C3D-CAD	2.45	110.77	108.11
14	H	1206	CLA	C3D-C4D-ND	2.45	113.97	109.99
18	I	4018	BCR	C2-C1-C6	2.45	114.00	110.44
14	a	1103	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
14	b	1236	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	A	1131	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
14	B	1212	CLA	CMC-C2C-C1C	2.45	128.87	125.03
14	H	1235	CLA	CMB-C2B-C3B	2.45	132.31	126.55
14	b	1218	CLA	CMB-C2B-C3B	2.45	132.31	126.55
14	H	1203	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
14	B	1202	CLA	CAC-C3C-C4C	2.45	127.98	124.79
14	A	1126	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	H	1218	CLA	CMB-C2B-C3B	2.45	132.31	126.55
14	A	1134	CLA	CMB-C2B-C3B	2.45	132.31	126.55
14	H	1202	CLA	CAC-C3C-C4C	2.45	127.98	124.79
14	k	1401	CLA	CAC-C3C-C4C	2.45	127.98	124.79
14	B	1205	CLA	C3D-C4D-ND	2.45	113.97	109.99
14	B	1215	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
14	T	1401	CLA	C3C-C4C-NC	2.45	113.57	110.43
14	G	1120	CLA	CMB-C2B-C1B	2.45	129.15	125.42
14	b	1227	CLA	CAC-C3C-C4C	2.45	127.97	124.79
14	H	1239	CLA	CMB-C2B-C1B	2.45	129.14	125.42
14	B	1231	CLA	CMB-C2B-C1B	2.45	129.14	125.42
14	B	1218	CLA	CMB-C2B-C3B	2.45	132.30	126.55
14	H	1215	CLA	CAA-C2A-C3A	-2.45	106.39	113.00
14	B	1232	CLA	C3D-C4D-ND	2.44	113.96	109.99
14	B	1213	CLA	CMA-C3A-C4A	2.44	118.34	111.77
14	b	1235	CLA	CMB-C2B-C3B	2.44	132.30	126.55
14	B	1227	CLA	CMA-C3A-C4A	2.44	118.34	111.77
15	b	1238	F6C	C6-C7-C8	-2.44	107.84	115.97
18	G	4007	BCR	C29-C30-C25	-2.44	106.89	110.44
18	B	4009	BCR	C38-C26-C27	2.44	118.80	113.60
14	A	1013	CLA	CHB-C1B-C2B	-2.44	120.34	127.43
14	G	1132	CLA	CMA-C3A-C4A	2.44	118.33	111.77
14	H	1231	CLA	C4-C3-C5	2.44	119.47	115.23
14	B	1215	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	G	1012	CLA	C3C-C4C-NC	2.44	113.56	110.43
14	H	1213	CLA	CMA-C3A-C4A	2.44	118.33	111.77
14	B	1235	CLA	CMB-C2B-C3B	2.44	132.29	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1022	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	A	1110	CLA	C3C-C4C-NC	2.44	113.56	110.43
14	b	1213	CLA	CMA-C3A-C4A	2.44	118.33	111.77
14	a	1013	CLA	CHB-C1B-C2B	-2.44	120.35	127.43
18	b	4009	BCR	C38-C26-C27	2.44	118.80	113.60
14	a	1123	CLA	C3D-C4D-ND	2.44	113.95	109.99
18	i	4018	BCR	C2-C1-C6	2.44	113.98	110.44
14	b	1223	CLA	C4D-C3D-CAD	2.44	110.75	108.11
14	a	1132	CLA	CMA-C3A-C4A	2.44	118.32	111.77
14	A	1132	CLA	CMA-C3A-C4A	2.44	118.32	111.77
14	B	1206	CLA	C3D-C4D-ND	2.44	113.95	109.99
18	i	4018	BCR	C37-C22-C21	-2.44	118.87	122.82
14	G	1109	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
14	K	1401	CLA	CAC-C3C-C4C	2.44	127.96	124.79
14	H	1231	CLA	CMB-C2B-C1B	2.44	129.13	125.42
14	A	1116	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
14	H	1215	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	b	1022	CLA	C3D-C4D-ND	2.44	113.95	109.99
14	B	1223	CLA	OBD-CAD-C3D	-2.44	122.72	128.42
14	H	1225	CLA	CMC-C2C-C1C	2.44	128.84	125.03
14	A	1134	CLA	CMC-C2C-C1C	2.44	128.84	125.03
15	H	1238	F6C	C6-C7-C8	-2.44	107.87	115.97
14	A	1126	CLA	C4D-C3D-CAD	2.44	110.75	108.11
14	b	1231	CLA	CMB-C2B-C1B	2.44	129.13	125.42
18	l	4019	BCR	C34-C9-C8	2.44	121.81	118.09
14	G	1104	CLA	C4-C3-C5	2.43	119.45	115.23
14	A	1113	CLA	CMC-C2C-C1C	2.43	128.84	125.03
18	a	4007	BCR	C29-C30-C25	-2.43	106.90	110.44
14	A	1104	CLA	C4-C3-C5	2.43	119.45	115.23
14	a	1105	CLA	CMC-C2C-C1C	2.43	128.84	125.03
14	b	1215	CLA	C1-O2A-CGA	2.43	122.54	116.65
14	G	1123	CLA	C3D-C4D-ND	2.43	113.94	109.99
14	H	1215	CLA	C1-O2A-CGA	2.43	122.54	116.65
14	H	1220	CLA	C3C-C4C-NC	2.43	113.55	110.43
15	B	1238	F6C	C6-C7-C8	-2.43	107.88	115.97
18	G	4007	BCR	C34-C9-C10	-2.43	118.88	122.82
14	a	1109	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
14	a	1116	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
14	b	1220	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	A	1133	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
14	a	1134	CLA	O1D-CGD-CBD	-2.43	119.72	124.52
14	H	1223	CLA	C4D-C3D-CAD	2.43	110.74	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1217	CLA	CMA-C3A-C4A	2.43	118.30	111.77
14	H	1203	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	b	1203	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
13	A	1011	CL0	CMC-C2C-C1C	2.43	129.10	124.73
14	G	1110	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	G	1115	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	a	1125	CLA	C4D-C3D-CAD	2.43	110.74	108.11
14	b	1222	CLA	CMB-C2B-C3B	2.43	132.26	126.55
14	b	1231	CLA	C4-C3-C5	2.43	119.44	115.23
14	G	1124	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
18	H	4014	BCR	C35-C13-C12	2.43	121.79	118.09
14	H	1223	CLA	CMC-C2C-C1C	2.43	128.82	125.03
14	A	1123	CLA	C3D-C4D-ND	2.43	113.93	109.99
14	A	1105	CLA	CMD-C2D-C3D	-2.43	122.13	127.69
14	b	1203	CLA	C3C-C4C-NC	2.43	113.54	110.43
14	G	1111	CLA	C4D-C3D-CAD	2.43	110.74	108.11
18	a	4001	BCR	C34-C9-C10	-2.43	118.89	122.82
14	a	1118	CLA	C3C-C4C-NC	2.42	113.54	110.43
13	a	1011	CL0	CMC-C2C-C1C	2.42	129.10	124.73
14	G	1013	CLA	CHB-C1B-C2B	-2.42	120.39	127.43
14	H	1022	CLA	C3D-C4D-ND	2.42	113.93	109.99
14	L	1503	CLA	CMB-C2B-C1B	2.42	129.11	125.42
14	a	1012	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	H	1226	CLA	C3D-C4D-ND	2.42	113.92	109.99
18	B	4014	BCR	C35-C13-C12	2.42	121.79	118.09
14	a	1134	CLA	CMD-C2D-C3D	-2.42	122.13	127.69
14	H	1236	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	B	1215	CLA	C1-O2A-CGA	2.42	122.51	116.65
18	A	4001	BCR	C34-C9-C10	-2.42	118.89	122.82
14	H	1222	CLA	CMB-C2B-C3B	2.42	132.25	126.55
14	a	1111	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	H	1220	CLA	CAA-CBA-CGA	-2.42	106.33	113.21
14	G	1105	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
14	a	1105	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
14	B	1222	CLA	CMB-C2B-C3B	2.42	132.24	126.55
18	R	4018	BCR	C37-C22-C21	-2.42	118.89	122.82
14	G	1111	CLA	C3C-C4C-NC	2.42	113.53	110.43
18	a	4007	BCR	C8-C7-C6	-2.42	120.53	127.00
14	A	1012	CLA	C3C-C4C-NC	2.42	113.53	110.43
14	b	1223	CLA	CMC-C2C-C1C	2.42	128.81	125.03
14	B	1220	CLA	CAA-CBA-CGA	-2.42	106.34	113.21
14	G	1107	CLA	C4D-C3D-CAD	2.42	110.73	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	G	5001	LHG	C5-O7-C7	-2.42	112.01	117.80
14	a	1113	CLA	CMC-C2C-C1C	2.42	128.81	125.03
18	b	4014	BCR	C35-C13-C12	2.42	121.78	118.09
19	A	5001	LHG	C5-O7-C7	-2.42	112.01	117.80
13	G	1011	CL0	CMC-C2C-C1C	2.42	129.09	124.73
14	B	1223	CLA	CMC-C2C-C1C	2.42	128.81	125.03
14	K	1401	CLA	C3C-C4C-NC	2.42	113.53	110.43
18	A	4007	BCR	C8-C7-C6	-2.42	120.54	127.00
14	A	1134	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
14	k	1401	CLA	C4D-C3D-CAD	2.42	110.73	108.11
14	H	1232	CLA	C3D-C4D-ND	2.42	113.92	109.99
14	G	1113	CLA	CMC-C2C-C1C	2.42	128.81	125.03
16	A	2001	PQN	C11-C3-C2	-2.42	120.75	124.89
14	A	1134	CLA	O1D-CGD-CBD	-2.42	119.75	124.52
14	A	1107	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
14	G	1112	CLA	C1-C2-C3	-2.42	122.24	126.20
14	a	1112	CLA	C1-C2-C3	-2.42	122.24	126.20
19	a	5001	LHG	C5-O7-C7	-2.42	112.02	117.80
18	G	4001	BCR	C34-C9-C10	-2.41	118.90	122.82
14	B	1201	CLA	CMB-C2B-C3B	2.41	132.23	126.55
14	a	1115	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	H	1213	CLA	C3D-C4D-ND	2.41	113.91	109.99
14	B	1226	CLA	C3D-C4D-ND	2.41	113.91	109.99
14	B	1217	CLA	CMA-C3A-C4A	2.41	118.26	111.77
14	A	1125	CLA	C4D-C3D-CAD	2.41	110.73	108.11
14	A	1117	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
14	H	1227	CLA	CAC-C3C-C4C	2.41	127.93	124.79
14	G	1117	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
14	a	1134	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	a	1124	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
14	a	1133	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
14	U	1503	CLA	CMB-C2B-C1B	2.41	129.09	125.42
18	I	4018	BCR	C37-C22-C21	-2.41	118.91	122.82
14	G	1134	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
14	G	1134	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
14	a	1107	CLA	CAA-C2A-C3A	-2.41	106.48	113.00
14	a	1110	CLA	C3C-C4C-NC	2.41	113.52	110.43
14	B	1231	CLA	C4-C3-C5	2.41	119.41	115.23
18	A	4007	BCR	C29-C30-C25	-2.41	106.94	110.44
14	l	1503	CLA	CMB-C2B-C1B	2.41	129.09	125.42
14	A	1115	CLA	C3C-C4C-NC	2.41	113.51	110.43
14	b	1220	CLA	CAA-CBA-CGA	-2.41	106.37	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	H	4005	BCR	C23-C24-C25	-2.41	120.57	127.00
14	H	1217	CLA	CMA-C3A-C4A	2.41	118.24	111.77
14	a	1117	CLA	CHC-C1C-C2C	-2.41	120.11	126.95
18	A	4001	BCR	C2-C1-C6	2.41	113.93	110.44
14	A	1116	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
18	G	4007	BCR	C8-C7-C6	-2.40	120.58	127.00
14	G	1133	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
14	k	1401	CLA	C3C-C4C-NC	2.40	113.51	110.43
14	b	1209	CLA	CMB-C2B-C1B	2.40	129.08	125.42
14	a	1130	CLA	CMC-C2C-C1C	2.40	128.79	125.03
14	A	1107	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
14	B	1213	CLA	C3D-C4D-ND	2.40	113.89	109.99
16	G	2001	PQN	C11-C3-C2	-2.40	120.77	124.89
14	A	1124	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
14	A	1139	CLA	CMA-C3A-C4A	2.40	118.23	111.77
14	A	1107	CLA	C4D-C3D-CAD	2.40	110.71	108.11
18	G	4001	BCR	C2-C1-C6	2.40	113.93	110.44
14	B	1220	CLA	C3C-C4C-NC	2.40	113.51	110.43
14	G	1109	CLA	C1-O2A-CGA	2.40	122.46	116.65
14	G	1129	CLA	CMC-C2C-C1C	2.40	128.79	125.03
14	a	1107	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
14	G	1128	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
14	B	1227	CLA	CAC-C3C-C4C	2.40	127.91	124.79
14	a	1107	CLA	C4D-C3D-CAD	2.40	110.71	108.11
14	G	1107	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
14	b	1226	CLA	C3D-C4D-ND	2.40	113.89	109.99
14	G	1124	CLA	C4D-C3D-CAD	2.40	110.71	108.11
14	H	1201	CLA	CMB-C2B-C3B	2.40	132.19	126.55
14	G	1116	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
14	a	1116	CLA	O1D-CGD-CBD	-2.40	119.79	124.52
18	A	4007	BCR	C34-C9-C10	-2.40	118.93	122.82
18	R	4018	BCR	C31-C1-C6	-2.40	106.48	110.24
14	b	1213	CLA	C3D-C4D-ND	2.40	113.88	109.99
14	b	1236	CLA	CAA-C2A-C3A	-2.40	106.53	113.00
18	a	4007	BCR	C34-C9-C10	-2.40	118.94	122.82
14	G	1127	CLA	CMA-C3A-C4A	2.39	118.21	111.77
14	a	1109	CLA	C1-O2A-CGA	2.39	122.44	116.65
18	b	4006	BCR	C15-C14-C13	-2.39	123.92	127.28
14	b	1231	CLA	CAC-C3C-C4C	2.39	127.90	124.79
14	H	1208	CLA	C3C-C4C-NC	2.39	113.50	110.43
18	a	4001	BCR	C2-C1-C6	2.39	113.92	110.44
14	G	1116	CLA	O1D-CGD-CBD	-2.39	119.80	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1107	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
18	b	4005	BCR	C23-C24-C25	-2.39	120.61	127.00
18	B	4006	BCR	C15-C14-C13	-2.39	123.92	127.28
14	a	1133	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
14	B	1236	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
14	G	1139	CLA	CMA-C3A-C4A	2.39	118.20	111.77
18	a	4001	BCR	C33-C5-C6	-2.39	121.88	124.48
20	B	5002	LMG	O7-C10-O9	-2.39	118.12	123.70
18	I	4018	BCR	C31-C1-C6	-2.39	106.50	110.24
20	b	5002	LMG	O7-C10-O9	-2.39	118.12	123.70
14	H	1211	CLA	C4D-C3D-CAD	2.39	110.70	108.11
14	b	1201	CLA	CMB-C2B-C3B	2.39	132.17	126.55
18	G	4002	BCR	C8-C7-C6	-2.39	120.62	127.00
14	A	1128	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
14	A	1112	CLA	C1-C2-C3	-2.39	122.29	126.20
14	G	1134	CLA	C3C-C4C-NC	2.39	113.49	110.43
14	G	1137	CLA	CMC-C2C-C1C	2.39	128.76	125.03
14	A	1129	CLA	CMC-C2C-C1C	2.39	128.76	125.03
14	A	1134	CLA	C4D-C3D-CAD	2.39	110.70	108.11
14	K	1401	CLA	C4D-C3D-CAD	2.39	110.70	108.11
15	a	1121	F6C	CBC-CAC-C3C	-2.39	105.95	112.42
14	H	1236	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
14	b	1204	CLA	C6-C7-C8	-2.38	108.04	115.97
14	A	1132	CLA	O1D-CGD-CBD	-2.38	119.81	124.52
18	H	4006	BCR	C15-C14-C13	-2.38	123.93	127.28
14	a	1127	CLA	CMA-C3A-C4A	2.38	118.18	111.77
14	A	1109	CLA	C1-O2A-CGA	2.38	122.42	116.65
14	B	1209	CLA	CMB-C2B-C1B	2.38	129.05	125.42
14	A	1137	CLA	CMC-C2C-C1C	2.38	128.76	125.03
18	i	4018	BCR	C31-C1-C6	-2.38	106.51	110.24
14	b	1222	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	G	1137	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
14	T	1401	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	a	1137	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
14	a	1118	CLA	CMB-C2B-C1B	2.38	129.04	125.42
14	H	1204	CLA	C6-C7-C8	-2.38	108.06	115.97
18	B	4009	BCR	C37-C22-C21	-2.38	118.96	122.82
14	a	1137	CLA	CMB-C2B-C3B	2.38	132.15	126.55
14	a	1124	CLA	C4D-C3D-CAD	2.38	110.69	108.11
14	a	1128	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
14	a	1130	CLA	C3D-C4D-ND	2.38	113.85	109.99
14	A	1105	CLA	CMA-C3A-C4A	2.38	118.16	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1137	CLA	CMB-C2B-C3B	2.38	132.14	126.55
16	a	2001	PQN	C11-C3-C2	-2.38	120.81	124.89
18	H	4009	BCR	C37-C22-C21	-2.38	118.97	122.82
14	A	1118	CLA	C3C-C4C-NC	2.38	113.47	110.43
18	B	4005	BCR	C23-C24-C25	-2.38	120.65	127.00
14	G	1138	CLA	O2A-C1-C2	2.38	117.25	108.11
14	A	1127	CLA	CMA-C3A-C4A	2.38	118.16	111.77
14	a	1118	CLA	C1-O2A-CGA	2.38	122.40	116.65
18	G	4001	BCR	C33-C5-C6	-2.38	121.89	124.48
14	G	1118	CLA	C3C-C4C-NC	2.38	113.47	110.43
14	G	1118	CLA	C1-O2A-CGA	2.37	122.40	116.65
14	B	1204	CLA	C6-C7-C8	-2.37	108.07	115.97
18	b	4014	BCR	C19-C18-C17	2.37	122.74	119.01
15	A	1121	F6C	CBC-CAC-C3C	-2.37	105.98	112.42
14	G	1102	CLA	C4D-C3D-CAD	2.37	110.68	108.11
21	G	6001	LMT	O5'-C5'-C6'	2.37	112.32	106.44
21	a	6001	LMT	O5'-C5'-C6'	2.37	112.32	106.44
14	A	1137	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
18	b	4009	BCR	C37-C22-C21	-2.37	118.97	122.82
14	a	1139	CLA	CMA-C3A-C4A	2.37	118.15	111.77
18	H	4017	BCR	C23-C24-C25	-2.37	120.66	127.00
14	G	1137	CLA	CMB-C2B-C3B	2.37	132.13	126.55
14	a	1111	CLA	CMB-C2B-C3B	2.37	132.13	126.55
14	G	1133	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
14	a	1138	CLA	O2A-C1-C2	2.37	117.23	108.11
14	A	1102	CLA	C4D-C3D-CAD	2.37	110.68	108.11
14	B	1211	CLA	C4D-C3D-CAD	2.37	110.68	108.11
21	A	6001	LMT	O5'-C5'-C6'	2.37	112.31	106.44
14	A	1111	CLA	CMB-C2B-C3B	2.37	132.13	126.55
14	A	1133	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
14	H	1234	CLA	C4C-C3C-C2C	-2.37	103.44	106.89
18	b	4017	BCR	C23-C24-C25	-2.37	120.67	127.00
14	b	1021	CLA	O2A-C1-C2	2.37	117.22	108.11
14	a	1137	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	G	1105	CLA	CMA-C3A-C4A	2.37	118.14	111.77
14	B	1208	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	H	1231	CLA	CAC-C3C-C4C	2.37	127.87	124.79
18	H	4014	BCR	C19-C18-C17	2.37	122.73	119.01
18	B	4017	BCR	C23-C24-C25	-2.37	120.68	127.00
14	A	1134	CLA	C3C-C4C-NC	2.37	113.46	110.43
14	B	1231	CLA	CAC-C3C-C4C	2.37	127.87	124.79
14	G	1130	CLA	CMC-C2C-C1C	2.37	128.73	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1130	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
18	a	4002	BCR	C8-C7-C6	-2.37	120.68	127.00
14	A	1118	CLA	CMB-C2B-C1B	2.36	129.02	125.42
14	H	1021	CLA	O2A-C1-C2	2.36	117.20	108.11
15	G	1121	F6C	CBC-CAC-C3C	-2.36	106.01	112.42
14	B	1021	CLA	O2A-C1-C2	2.36	117.20	108.11
14	b	1204	CLA	CMC-C2C-C1C	2.36	128.73	125.03
14	a	1119	CLA	CHB-C4A-NA	2.36	127.81	124.40
14	a	1111	CLA	C4D-C3D-CAD	2.36	110.67	108.11
14	W	1701	CLA	C3D-C4D-ND	2.36	113.83	109.99
14	G	1118	CLA	CMB-C2B-C1B	2.36	129.01	125.42
14	B	1234	CLA	C4C-C3C-C2C	-2.36	103.45	106.89
18	l	4022	BCR	C37-C22-C21	-2.36	118.99	122.82
14	a	1013	CLA	CHB-C4A-NA	2.36	127.81	124.40
14	A	1013	CLA	CHB-C4A-NA	2.36	127.81	124.40
14	A	1138	CLA	O2A-C1-C2	2.36	117.19	108.11
18	B	4014	BCR	C19-C18-C17	2.36	122.72	119.01
18	B	4014	BCR	C15-C14-C13	-2.36	123.97	127.28
14	G	1130	CLA	C3D-C4D-ND	2.36	113.82	109.99
14	H	1209	CLA	CMB-C2B-C1B	2.36	129.01	125.42
14	H	1213	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
14	A	1130	CLA	CMC-C2C-C1C	2.36	128.72	125.03
14	A	1118	CLA	C1-O2A-CGA	2.36	122.36	116.65
14	B	1203	CLA	C4-C3-C5	2.36	119.32	115.23
14	H	1232	CLA	C3C-C4C-NC	2.36	113.45	110.43
14	a	1105	CLA	CMA-C3A-C4A	2.36	118.11	111.77
14	a	1132	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
14	A	1119	CLA	CHB-C4A-NA	2.36	127.80	124.40
14	G	1136	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
14	a	1114	CLA	C4D-C3D-CAD	2.36	110.67	108.11
14	H	1227	CLA	O1D-CGD-CBD	-2.36	119.87	124.52
14	G	1130	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
20	H	5002	LMG	O7-C10-O9	-2.36	118.20	123.70
14	a	1136	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
14	H	1203	CLA	C4-C3-C5	2.35	119.31	115.23
14	A	1124	CLA	C4D-C3D-CAD	2.35	110.66	108.11
14	X	1701	CLA	C3D-C4D-ND	2.35	113.81	109.99
14	A	1131	CLA	CMB-C2B-C1B	2.35	129.00	125.42
14	a	1129	CLA	CMC-C2C-C1C	2.35	128.71	125.03
14	b	1208	CLA	C3C-C4C-NC	2.35	113.44	110.43
18	A	4002	BCR	C8-C7-C6	-2.35	120.71	127.00
14	G	1102	CLA	CMD-C2D-C3D	-2.35	122.30	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1234	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
14	a	1102	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	b	1233	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	H	1233	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	B	1213	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	G	1111	CLA	CMB-C2B-C3B	2.35	132.08	126.55
14	A	1111	CLA	C4D-C3D-CAD	2.35	110.66	108.11
14	G	1132	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
14	A	1136	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
14	G	1106	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
14	a	1137	CLA	CMC-C2C-C1C	2.35	128.70	125.03
14	a	1102	CLA	C4D-C3D-CAD	2.35	110.66	108.11
14	A	1102	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
14	G	1137	CLA	C3C-C4C-NC	2.35	113.44	110.43
14	b	1206	CLA	CAA-C2A-C3A	-2.35	106.66	113.00
14	A	1137	CLA	C3C-C4C-NC	2.35	113.44	110.43
14	B	1232	CLA	C3C-C4C-NC	2.35	113.44	110.43
14	B	1235	CLA	C3C-C4C-NC	2.35	113.44	110.43
18	a	4003	BCR	C38-C26-C27	2.35	118.60	113.60
14	G	1112	CLA	C4D-C3D-CAD	2.35	110.65	108.11
14	B	1227	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
14	H	1206	CLA	CMB-C2B-C3B	2.34	132.06	126.55
14	G	1119	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	a	1105	CLA	C4D-C3D-CAD	2.34	110.65	108.11
14	a	1126	CLA	CMC-C2C-C1C	2.34	128.70	125.03
14	b	1232	CLA	C3C-C4C-NC	2.34	113.43	110.43
14	b	1227	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
14	G	1134	CLA	C4D-C3D-CAD	2.34	110.65	108.11
14	B	1222	CLA	C4D-C3D-CAD	2.34	110.65	108.11
15	A	1121	F6C	CMC-C2C-C1C	2.34	128.99	125.42
14	H	1233	CLA	C3C-C4C-NC	2.34	113.43	110.43
14	G	1013	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	B	1233	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
14	A	1114	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
14	a	1134	CLA	C4D-C3D-CAD	2.34	110.65	108.11
14	a	1106	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
14	A	1106	CLA	CMB-C2B-C3B	2.34	132.06	126.55
18	b	4014	BCR	C33-C5-C4	2.34	118.59	113.60
14	H	1202	CLA	C1-C2-C3	-2.34	122.36	126.20
18	A	4003	BCR	C38-C26-C27	2.34	118.58	113.60
14	b	1023	CLA	CMB-C2B-C1B	2.34	128.98	125.42
14	H	1228	CLA	CHC-C1C-C2C	-2.34	120.30	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	4019	BCR	C40-C30-C25	2.34	113.91	110.24
14	H	1214	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
14	A	1130	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
18	H	4014	BCR	C33-C5-C4	2.34	118.58	113.60
14	b	1211	CLA	C4D-C3D-CAD	2.34	110.65	108.11
18	G	4003	BCR	C38-C26-C27	2.34	118.58	113.60
15	G	1121	F6C	CMC-C2C-C1C	2.34	128.98	125.42
14	x	1701	CLA	C3D-C4D-ND	2.34	113.79	109.99
18	A	4001	BCR	C33-C5-C6	-2.34	121.93	124.48
18	L	4022	BCR	C37-C22-C21	-2.34	119.03	122.82
14	H	1023	CLA	CMB-C2B-C1B	2.34	128.98	125.42
14	b	1213	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
14	B	1210	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
14	a	1131	CLA	CMB-C2B-C1B	2.34	128.98	125.42
14	H	1206	CLA	CAA-C2A-C3A	-2.34	106.69	113.00
14	b	1228	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
18	U	4022	BCR	C37-C22-C21	-2.34	119.03	122.82
14	B	1225	CLA	C4D-C3D-CAD	2.33	110.64	108.11
14	B	1233	CLA	C3C-C4C-NC	2.33	113.42	110.43
14	B	1202	CLA	C1-C2-C3	-2.33	122.37	126.20
14	B	1228	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
14	L	1502	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
14	A	1117	CLA	CMB-C2B-C3B	2.33	132.04	126.55
14	B	1023	CLA	CMB-C2B-C1B	2.33	128.97	125.42
14	G	1106	CLA	CMB-C2B-C3B	2.33	132.03	126.55
14	B	1211	CLA	CMB-C2B-C3B	2.33	132.03	126.55
14	a	1112	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
14	a	1101	CLA	C4D-C3D-CAD	2.33	110.64	108.11
18	H	4014	BCR	C15-C14-C13	-2.33	124.01	127.28
14	b	1203	CLA	C4-C3-C5	2.33	119.27	115.23
14	G	1126	CLA	CMC-C2C-C1C	2.33	128.68	125.03
14	A	1101	CLA	C4D-C3D-CAD	2.33	110.64	108.11
14	A	1106	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
15	H	1238	F6C	O2D-CGD-O1D	-2.33	119.32	123.85
18	b	4005	BCR	C27-C26-C25	-2.33	119.56	122.70
14	B	1228	CLA	C4-C3-C5	2.33	119.27	115.23
14	H	1226	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
14	b	1226	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
15	a	1121	F6C	CMC-C2C-C1C	2.33	128.96	125.42
14	b	1239	CLA	C6-C5-C3	-2.33	107.80	113.47
14	b	1206	CLA	CMB-C2B-C3B	2.33	132.02	126.55
14	b	1210	CLA	CMD-C2D-C3D	-2.33	122.35	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1214	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
14	b	1222	CLA	O1D-CGD-CBD	-2.33	119.93	124.52
14	A	1125	CLA	C4B-CHC-C1C	2.33	131.72	126.25
18	B	4014	BCR	C33-C5-C4	2.33	118.56	113.60
14	b	1202	CLA	C1-C2-C3	-2.33	122.39	126.20
14	B	1206	CLA	CMB-C2B-C3B	2.33	132.02	126.55
14	A	1130	CLA	C3D-C4D-ND	2.33	113.77	109.99
18	H	4005	BCR	C27-C26-C25	-2.33	119.56	122.70
14	G	1114	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
14	b	1216	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
14	A	1105	CLA	C4D-C3D-CAD	2.32	110.63	108.11
14	B	1239	CLA	CAC-C3C-C4C	-2.32	121.77	124.79
14	B	1204	CLA	CMC-C2C-C1C	2.32	128.66	125.03
14	B	1214	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
18	L	4019	BCR	C30-C25-C26	-2.32	119.46	122.64
14	b	1228	CLA	C4-C3-C5	2.32	119.26	115.23
14	G	1114	CLA	C4D-C3D-CAD	2.32	110.63	108.11
14	a	1114	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
14	A	1114	CLA	C4D-C3D-CAD	2.32	110.63	108.11
14	A	1112	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
15	b	1230	F6C	C4C-C3C-C2C	-2.32	103.28	106.87
14	H	1216	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
14	H	1204	CLA	CMC-C2C-C1C	2.32	128.66	125.03
18	U	4019	BCR	C30-C25-C26	-2.32	119.47	122.64
18	l	4019	BCR	C30-C25-C26	-2.32	119.47	122.64
14	G	1105	CLA	C4D-C3D-CAD	2.32	110.63	108.11
18	U	4019	BCR	C40-C30-C25	2.32	113.88	110.24
14	H	1228	CLA	C4-C3-C5	2.32	119.25	115.23
14	B	1228	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
14	a	1106	CLA	CMB-C2B-C3B	2.32	132.00	126.55
14	b	1228	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
14	H	1210	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
14	H	1239	CLA	CAC-C3C-C4C	-2.32	121.77	124.79
14	A	1108	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
14	G	1108	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
14	B	1206	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
18	l	4022	BCR	C38-C26-C25	-2.31	121.96	124.48
14	a	1125	CLA	C4B-CHC-C1C	2.31	131.69	126.25
14	B	1210	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	b	1229	CLA	CMD-C2D-C3D	-2.31	122.38	127.69
14	A	1139	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
14	a	1102	CLA	C4-C3-C5	2.31	119.24	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1118	CLA	OBD-CAD-C3D	-2.31	123.01	128.42
14	a	1138	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
14	G	1131	CLA	CMB-C2B-C1B	2.31	128.94	125.42
14	G	1112	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
18	B	4005	BCR	C27-C26-C25	-2.31	119.58	122.70
14	B	1229	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
14	G	1101	CLA	C4D-C3D-CAD	2.31	110.61	108.11
14	G	1102	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	A	1102	CLA	C3C-C4C-NC	2.31	113.39	110.43
14	A	1118	CLA	OBD-CAD-C3D	-2.31	123.02	128.42
14	a	1117	CLA	CMB-C2B-C3B	2.31	131.98	126.55
14	G	1117	CLA	CMB-C2B-C3B	2.31	131.98	126.55
14	B	1226	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
14	G	1137	CLA	C5-C3-C4	2.31	119.90	114.59
14	G	1122	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
14	B	1228	CLA	C4D-C3D-CAD	2.31	110.61	108.11
14	H	1228	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
18	a	4011	BCR	C38-C26-C27	2.31	118.52	113.60
14	H	1239	CLA	C6-C5-C3	-2.31	107.85	113.47
14	A	1122	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
14	B	1239	CLA	C6-C5-C3	-2.31	107.85	113.47
14	b	1211	CLA	CMB-C2B-C3B	2.31	131.98	126.55
14	H	1222	CLA	C4D-C3D-CAD	2.31	110.61	108.11
14	G	1139	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
14	G	1101	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
18	b	4014	BCR	C15-C14-C13	-2.31	124.04	127.28
14	b	1235	CLA	C3C-C4C-NC	2.31	113.38	110.43
14	H	1211	CLA	CMB-C2B-C3B	2.31	131.97	126.55
18	G	4011	BCR	C38-C26-C27	2.30	118.51	113.60
14	A	1102	CLA	C4-C3-C5	2.30	119.23	115.23
14	l	1502	CLA	O1D-CGD-CBD	-2.30	119.97	124.52
14	a	1102	CLA	C3C-C4C-NC	2.30	113.38	110.43
18	A	4003	BCR	C33-C5-C4	2.30	118.51	113.60
14	b	1239	CLA	CAC-C3C-C4C	-2.30	121.79	124.79
14	B	1216	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
14	L	1503	CLA	C4D-C3D-CAD	2.30	110.61	108.11
14	H	1222	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
14	B	1222	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
16	G	2001	PQN	C12-C11-C3	-2.30	106.41	112.08
18	l	4019	BCR	C40-C30-C25	2.30	113.85	110.24
14	H	1201	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
14	G	1128	CLA	O1D-CGD-CBD	-2.30	119.98	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	4001	BCR	C19-C18-C17	2.30	122.63	119.01
14	a	1122	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
14	A	1126	CLA	CMC-C2C-C1C	2.30	128.63	125.03
14	A	1112	CLA	C4D-C3D-CAD	2.30	110.60	108.11
14	A	1112	CLA	CAA-CBA-CGA	-2.30	106.68	113.21
14	H	1235	CLA	C3C-C4C-NC	2.30	113.38	110.43
14	A	1131	CLA	C4-C3-C5	2.30	119.22	115.23
14	a	1137	CLA	C5-C3-C4	2.30	119.88	114.59
14	A	1128	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
14	G	1135	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
18	b	4014	BCR	C39-C30-C25	-2.30	106.64	110.24
14	b	1219	CLA	C3C-C4C-NC	2.30	113.37	110.43
14	G	1128	CLA	CHC-C1C-C2C	-2.30	120.42	126.95
18	G	4003	BCR	C33-C5-C4	2.30	118.49	113.60
14	A	1101	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
14	b	1210	CLA	C3C-C4C-NC	2.30	113.37	110.43
14	H	1229	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
14	B	1239	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
14	G	1123	CLA	CAC-C3C-C4C	2.30	127.78	124.79
14	A	1135	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
14	G	1125	CLA	C4B-CHC-C1C	2.29	131.64	126.25
14	b	1233	CLA	C3C-C4C-NC	2.29	113.37	110.43
18	a	4003	BCR	C33-C5-C4	2.29	118.49	113.60
14	G	1130	CLA	C4D-C3D-CAD	2.29	110.60	108.11
14	a	1108	CLA	C4D-C3D-CAD	2.29	110.60	108.11
14	A	1138	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
14	a	1117	CLA	C3D-C4D-ND	2.29	113.71	109.99
14	G	1117	CLA	C4D-C3D-CAD	2.29	110.60	108.11
14	H	1217	CLA	C4D-C3D-CAD	2.29	110.60	108.11
18	A	4011	BCR	C38-C26-C27	2.29	118.48	113.60
15	b	1238	F6C	O2D-CGD-O1D	-2.29	119.39	123.85
14	H	1225	CLA	C4D-C3D-CAD	2.29	110.59	108.11
14	B	1219	CLA	C4D-C3D-CAD	2.29	110.59	108.11
14	A	1123	CLA	CAC-C3C-C4C	2.29	127.77	124.79
16	A	2001	PQN	C12-C11-C3	-2.29	106.44	112.08
18	B	4014	BCR	C39-C30-C25	-2.29	106.65	110.24
14	a	1131	CLA	C4-C3-C5	2.29	119.20	115.23
18	H	4014	BCR	C39-C30-C25	-2.29	106.65	110.24
14	a	1101	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
15	H	1230	F6C	C4C-C3C-C2C	-2.29	103.32	106.87
14	G	1112	CLA	CAA-CBA-CGA	-2.29	106.71	113.21
14	G	1118	CLA	OBD-CAD-C3D	-2.29	123.06	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1122	CLA	CMA-C3A-C4A	2.29	117.93	111.77
18	B	4005	BCR	C33-C5-C4	2.29	118.48	113.60
14	A	1108	CLA	C4D-C3D-CAD	2.29	110.59	108.11
14	A	1107	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
14	a	1108	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
14	G	1122	CLA	CMA-C3A-C4A	2.29	117.92	111.77
14	H	1202	CLA	C4D-C3D-CAD	2.29	110.59	108.11
18	L	4022	BCR	C38-C26-C25	-2.29	121.99	124.48
14	B	1201	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
18	H	4005	BCR	C33-C5-C4	2.29	118.47	113.60
14	b	1229	CLA	O2A-C1-C2	2.29	116.91	108.11
14	A	1137	CLA	C5-C3-C4	2.29	119.85	114.59
18	G	4002	BCR	C27-C26-C25	-2.29	119.61	122.70
14	G	1117	CLA	C3D-C4D-ND	2.29	113.70	109.99
14	U	1502	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
14	B	1202	CLA	C4D-C3D-CAD	2.29	110.59	108.11
14	G	1117	CLA	CAC-C3C-C4C	2.29	127.76	124.79
14	a	1135	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
14	G	1131	CLA	C4-C3-C5	2.28	119.19	115.23
14	U	1503	CLA	C4D-C3D-CAD	2.28	110.59	108.11
14	a	1107	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
14	a	1139	CLA	O1D-CGD-CBD	-2.28	120.01	124.52
18	U	4022	BCR	C28-C27-C26	-2.28	109.98	114.06
14	B	1229	CLA	O2A-C1-C2	2.28	116.89	108.11
14	B	1219	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	G	1013	CLA	C6-C5-C3	-2.28	107.91	113.47
14	G	1138	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
14	a	1108	CLA	CMC-C2C-C1C	2.28	128.60	125.03
14	G	1102	CLA	C4-C3-C5	2.28	119.19	115.23
14	G	1135	CLA	CMB-C2B-C3B	2.28	131.92	126.55
14	H	1210	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	a	1013	CLA	C6-C5-C3	-2.28	107.91	113.47
14	a	1128	CLA	CHC-C1C-C2C	-2.28	120.47	126.95
18	B	4005	BCR	C30-C25-C26	-2.28	119.52	122.64
14	a	1123	CLA	CAC-C3C-C4C	2.28	127.76	124.79
14	H	1239	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
14	a	1124	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	b	1209	CLA	CAA-CBA-CGA	-2.28	106.41	112.49
14	a	1112	CLA	CAA-CBA-CGA	-2.28	106.74	113.21
16	a	2001	PQN	C12-C11-C3	-2.28	106.47	112.08
18	b	4005	BCR	C33-C5-C4	2.28	118.45	113.60
14	G	1140	CLA	CMB-C2B-C1B	2.28	128.89	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1202	CLA	C4D-C3D-CAD	2.28	110.58	108.11
14	B	1209	CLA	CAA-CBA-CGA	-2.28	106.41	112.49
14	A	1132	CLA	CMC-C2C-C1C	2.28	128.59	125.03
14	H	1229	CLA	O2A-C1-C2	2.28	116.88	108.11
14	a	1133	CLA	C3C-C4C-NC	2.28	113.35	110.43
15	B	1238	F6C	O2D-CGD-O1D	-2.28	119.41	123.85
14	a	1122	CLA	CMA-C3A-C4A	2.28	117.90	111.77
14	G	1132	CLA	CMC-C2C-C1C	2.28	128.59	125.03
14	b	1216	CLA	C1-O2A-CGA	2.28	122.17	116.65
14	b	1225	CLA	C4D-C3D-CAD	2.28	110.58	108.11
14	b	1201	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
14	A	1140	CLA	CMB-C2B-C1B	2.28	128.89	125.42
14	B	1221	CLA	CMC-C2C-C1C	2.28	128.59	125.03
14	G	1101	CLA	C3C-C4C-NC	2.28	113.35	110.43
14	a	1115	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
18	V	4021	BCR	C38-C26-C25	-2.28	122.00	124.48
14	B	1222	CLA	C4C-C3C-C2C	-2.28	103.58	106.89
14	H	1239	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
14	A	1135	CLA	CMB-C2B-C3B	2.28	131.90	126.55
18	G	4001	BCR	C19-C18-C17	2.28	122.59	119.01
14	b	1220	CLA	CHC-C1C-C2C	-2.28	120.48	126.95
14	G	1116	CLA	C4D-C3D-CAD	2.28	110.58	108.11
18	H	4005	BCR	C30-C25-C26	-2.27	119.53	122.64
14	A	1115	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
14	H	1021	CLA	CHD-C4C-C3C	-2.27	121.46	124.77
15	B	1230	F6C	C4C-C3C-C2C	-2.27	103.35	106.87
14	W	1701	CLA	CMA-C3A-C4A	2.27	117.89	111.77
18	U	4022	BCR	C38-C26-C25	-2.27	122.00	124.48
14	A	1124	CLA	CMA-C3A-C4A	2.27	117.88	111.77
14	A	1133	CLA	C3C-C4C-NC	2.27	113.34	110.43
14	a	1013	CLA	C4D-C3D-CAD	2.27	110.57	108.11
14	a	1117	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
14	B	1216	CLA	C1-O2A-CGA	2.27	122.15	116.65
18	A	4007	BCR	C35-C13-C12	2.27	121.56	118.09
14	b	1239	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
14	B	1212	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
14	A	1117	CLA	CAC-C3C-C4C	2.27	127.75	124.79
14	G	1124	CLA	CMA-C3A-C4A	2.27	117.88	111.77
18	a	4003	BCR	C15-C14-C13	-2.27	124.09	127.28
14	G	1115	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
14	H	1209	CLA	CAA-CBA-CGA	-2.27	106.43	112.49
14	U	1501	CLA	CMB-C2B-C3B	2.27	131.89	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1212	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
14	H	1228	CLA	C4D-C3D-CAD	2.27	110.57	108.11
14	a	1132	CLA	C3C-C4C-NC	2.27	113.34	110.43
14	b	1214	CLA	CAC-C3C-C4C	2.27	127.74	124.79
14	b	1239	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
18	G	4003	BCR	C15-C14-C13	-2.27	124.09	127.28
14	H	1212	CLA	CAA-C2A-C3A	-2.27	106.87	113.00
18	B	4013	BCR	C33-C5-C4	2.27	118.43	113.60
14	A	1117	CLA	C3D-C4D-ND	2.27	113.67	109.99
18	b	4006	BCR	C36-C18-C17	-2.27	119.14	122.82
14	A	1130	CLA	C4D-C3D-CAD	2.27	110.57	108.11
14	H	1220	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
18	L	4022	BCR	C28-C27-C26	-2.27	110.01	114.06
14	b	1222	CLA	C4C-C3C-C2C	-2.27	103.59	106.89
14	A	1013	CLA	C6-C5-C3	-2.27	107.94	113.47
14	H	1219	CLA	C3C-C4C-NC	2.27	113.33	110.43
14	a	1112	CLA	C4D-C3D-CAD	2.27	110.57	108.11
14	a	1128	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
14	A	1117	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
14	G	1107	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
14	A	1013	CLA	C4D-C3D-CAD	2.27	110.57	108.11
14	x	1701	CLA	CMA-C3A-C4A	2.27	117.86	111.77
14	B	1021	CLA	CHD-C4C-C3C	-2.27	121.47	124.77
14	H	1219	CLA	C4D-C3D-CAD	2.26	110.57	108.11
14	G	1117	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
14	G	1108	CLA	CMC-C2C-C1C	2.26	128.57	125.03
18	a	4002	BCR	C27-C26-C25	-2.26	119.64	122.70
14	H	1221	CLA	CMC-C2C-C1C	2.26	128.57	125.03
14	l	1501	CLA	CMB-C2B-C3B	2.26	131.87	126.55
15	b	1207	F6C	CHC-C1C-C2C	-2.26	120.86	127.43
14	G	1133	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	A	1128	CLA	O1D-CGD-CBD	-2.26	120.06	124.52
14	G	1013	CLA	C4D-C3D-CAD	2.26	110.56	108.11
14	A	1101	CLA	C3C-C4C-NC	2.26	113.33	110.43
14	G	1119	CLA	C4C-C3C-C2C	-2.26	103.60	106.89
18	G	4007	BCR	C35-C13-C12	2.26	121.54	118.09
14	H	1216	CLA	C1-O2A-CGA	2.26	122.12	116.65
14	b	1021	CLA	CHD-C4C-C3C	-2.26	121.48	124.77
14	a	1135	CLA	CMB-C2B-C3B	2.26	131.87	126.55
18	a	4001	BCR	C19-C18-C17	2.26	122.56	119.01
14	a	1110	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
14	a	1130	CLA	C4D-C3D-CAD	2.26	110.56	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1115	CLA	CAC-C3C-C4C	2.26	127.73	124.79
14	B	1239	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
14	a	1112	CLA	CMB-C2B-C3B	2.26	131.86	126.55
15	B	1207	F6C	CHC-C1C-C2C	-2.26	120.87	127.43
14	H	1222	CLA	C4C-C3C-C2C	-2.26	103.61	106.89
14	L	1501	CLA	CMB-C2B-C3B	2.26	131.86	126.55
14	a	1101	CLA	C3C-C4C-NC	2.26	113.32	110.43
14	A	1132	CLA	C3C-C4C-NC	2.26	113.32	110.43
14	b	1219	CLA	C4D-C3D-CAD	2.26	110.56	108.11
14	A	1117	CLA	C4D-C3D-CAD	2.26	110.56	108.11
14	B	1220	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
18	B	4016	BCR	C8-C7-C6	-2.26	120.97	127.00
14	A	1118	CLA	CAC-C3C-C4C	2.26	127.72	124.79
14	G	1118	CLA	CAC-C3C-C4C	2.26	127.72	124.79
18	R	4018	BCR	C1-C6-C5	-2.26	119.55	122.64
18	A	4002	BCR	C27-C26-C25	-2.25	119.66	122.70
14	a	1117	CLA	C4D-C3D-CAD	2.25	110.56	108.11
14	A	1104	CLA	CMC-C2C-C1C	2.25	128.56	125.03
14	G	1012	CLA	C11-C12-C13	-2.25	108.47	115.97
14	A	1012	CLA	C11-C12-C13	-2.25	108.47	115.97
18	M	4021	BCR	C38-C26-C25	-2.25	122.03	124.48
18	b	4016	BCR	C8-C7-C6	-2.25	120.98	127.00
14	l	1503	CLA	C4D-C3D-CAD	2.25	110.55	108.11
14	B	1217	CLA	C4D-C3D-CAD	2.25	110.55	108.11
14	A	1108	CLA	CMC-C2C-C1C	2.25	128.55	125.03
18	B	4004	BCR	C28-C27-C26	-2.25	110.04	114.06
18	b	4005	BCR	C30-C25-C26	-2.25	119.56	122.64
14	G	1115	CLA	CAC-C3C-C4C	2.25	127.72	124.79
14	A	1122	CLA	C1-O2A-CGA	2.25	122.10	116.65
14	a	1012	CLA	C11-C12-C13	-2.25	108.48	115.97
14	a	1132	CLA	CMC-C2C-C1C	2.25	128.55	125.03
18	b	4013	BCR	C33-C5-C4	2.25	118.40	113.60
14	G	1110	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
18	l	4022	BCR	C28-C27-C26	-2.25	110.04	114.06
14	G	1132	CLA	C3C-C4C-NC	2.25	113.31	110.43
14	a	1117	CLA	CAC-C3C-C4C	2.25	127.72	124.79
14	X	1701	CLA	CMA-C3A-C4A	2.25	117.82	111.77
14	A	1115	CLA	CAC-C3C-C4C	2.25	127.72	124.79
18	H	4013	BCR	C33-C5-C4	2.25	118.39	113.60
18	H	4006	BCR	C36-C18-C17	-2.25	119.17	122.82
14	a	1118	CLA	CAC-C3C-C4C	2.25	127.72	124.79
15	A	1121	F6C	CMD-C2D-C3D	-2.25	122.53	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1119	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
14	b	1216	CLA	C3C-C4C-NC	2.25	113.31	110.43
14	A	1110	CLA	CMA-C3A-C4A	2.25	117.81	111.77
18	b	4004	BCR	C28-C27-C26	-2.25	110.05	114.06
14	A	1119	CLA	C4C-C3C-C2C	-2.25	103.62	106.89
14	A	1112	CLA	CMB-C2B-C3B	2.25	131.84	126.55
14	b	1215	CLA	CHB-C1B-C2B	-2.25	120.91	127.43
14	G	1103	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
14	a	1103	CLA	CHC-C1C-C2C	-2.25	120.56	126.95
15	a	1121	F6C	CMD-C2D-C3D	-2.25	122.54	127.69
14	a	1104	CLA	CMC-C2C-C1C	2.24	128.54	125.03
18	a	4007	BCR	C35-C13-C12	2.24	121.52	118.09
18	H	4016	BCR	C8-C7-C6	-2.24	121.00	127.00
18	G	4002	BCR	C37-C22-C21	-2.24	119.18	122.82
14	G	1110	CLA	CMA-C3A-C4A	2.24	117.80	111.77
14	G	1136	CLA	CHB-C1B-C2B	-2.24	120.92	127.43
15	H	1230	F6C	CMA-C3A-C2A	-2.24	120.08	126.15
14	H	1216	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	A	1130	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	B	1216	CLA	C3C-C4C-NC	2.24	113.30	110.43
18	b	4013	BCR	C37-C22-C21	-2.24	119.18	122.82
14	a	1129	CLA	CMA-C3A-C4A	2.24	117.80	111.77
14	A	1110	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
14	a	1140	CLA	CMB-C2B-C1B	2.24	128.83	125.42
14	A	1103	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
14	b	1214	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
14	B	1209	CLA	CMA-C3A-C4A	2.24	117.80	111.77
14	G	1122	CLA	C1-O2A-CGA	2.24	122.07	116.65
14	B	1201	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	H	1222	CLA	CAC-C3C-C4C	2.24	127.70	124.79
18	A	4003	BCR	C15-C14-C13	-2.24	124.14	127.28
14	a	1122	CLA	C1-O2A-CGA	2.24	122.07	116.65
14	G	1108	CLA	C3C-C4C-NC	2.24	113.30	110.43
14	A	1129	CLA	CMA-C3A-C4A	2.24	117.79	111.77
18	B	4013	BCR	C37-C22-C21	-2.24	119.19	122.82
14	b	1228	CLA	C4D-C3D-CAD	2.24	110.54	108.11
14	A	1116	CLA	C4D-C3D-CAD	2.24	110.54	108.11
14	G	1129	CLA	CMA-C3A-C4A	2.24	117.79	111.77
14	B	1214	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
14	B	1239	CLA	C11-C10-C8	-2.24	108.53	115.97
14	A	1140	CLA	CMA-C3A-C4A	2.24	117.78	111.77
14	G	1126	CLA	CMD-C2D-C3D	-2.24	122.56	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	1121	F6C	O1D-CGD-CBD	-2.24	120.11	124.52
14	G	1130	CLA	C3C-C4C-NC	2.24	113.29	110.43
18	A	4002	BCR	C37-C22-C21	-2.24	119.19	122.82
14	B	1221	CLA	CMB-C2B-C3B	2.24	131.81	126.55
18	A	4011	BCR	C15-C14-C13	-2.23	124.14	127.28
14	G	1108	CLA	C4D-C3D-CAD	2.23	110.53	108.11
18	m	4021	BCR	C38-C26-C25	-2.23	122.05	124.48
14	a	1130	CLA	C3C-C4C-NC	2.23	113.29	110.43
15	H	1207	F6C	CHC-C1C-C2C	-2.23	120.94	127.43
18	U	4019	BCR	C7-C8-C9	-2.23	122.93	126.23
14	A	1136	CLA	CHB-C1B-C2B	-2.23	120.94	127.43
14	B	1214	CLA	CAC-C3C-C4C	2.23	127.69	124.79
14	b	1221	CLA	CMC-C2C-C1C	2.23	128.52	125.03
15	G	1121	F6C	CMD-C2D-C3D	-2.23	122.57	127.69
14	H	1214	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
13	A	1011	CL0	C4C-CHD-C1D	2.23	124.05	116.07
18	H	4004	BCR	C28-C27-C26	-2.23	110.08	114.06
14	b	1217	CLA	C4D-C3D-CAD	2.23	110.53	108.11
14	G	1109	CLA	CMC-C2C-C1C	2.23	128.52	125.03
14	a	1136	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
18	U	4019	BCR	C33-C5-C6	-2.23	122.05	124.48
18	L	4019	BCR	C33-C5-C6	-2.23	122.05	124.48
18	H	4013	BCR	C37-C22-C21	-2.23	119.20	122.82
14	H	1212	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
14	G	1112	CLA	CMB-C2B-C3B	2.23	131.79	126.55
14	b	1221	CLA	CMB-C2B-C3B	2.23	131.79	126.55
14	a	1109	CLA	CMC-C2C-C1C	2.23	128.52	125.03
18	L	4019	BCR	C7-C8-C9	-2.23	122.94	126.23
14	a	1112	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
18	G	4008	BCR	C36-C18-C17	-2.23	119.21	122.82
14	b	1209	CLA	CMA-C3A-C4A	2.23	117.76	111.77
13	G	1011	CL0	C4C-CHD-C1D	2.23	124.03	116.07
18	B	4006	BCR	C36-C18-C17	-2.23	119.21	122.82
14	a	1125	CLA	C1D-CHD-C4C	-2.23	121.29	126.02
14	a	1140	CLA	CMA-C3A-C4A	2.23	117.75	111.77
18	a	4011	BCR	C15-C14-C13	-2.23	124.16	127.28
14	b	1022	CLA	C4C-C3C-C2C	-2.22	103.65	106.89
14	H	1215	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
14	H	1203	CLA	C3D-C4D-ND	2.22	113.60	109.99
14	H	1201	CLA	C3C-C4C-NC	2.22	113.28	110.43
14	G	1125	CLA	C1D-CHD-C4C	-2.22	121.29	126.02
18	A	4008	BCR	C36-C18-C17	-2.22	119.21	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	A	1121	F6C	O1D-CGD-CBD	-2.22	120.13	124.52
14	H	1239	CLA	C11-C10-C8	-2.22	108.58	115.97
15	B	1230	F6C	CMA-C3A-C2A	-2.22	120.14	126.15
14	A	1110	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
14	A	1105	CLA	C3C-C4C-NC	2.22	113.28	110.43
13	a	1011	CL0	C4C-CHD-C1D	2.22	124.02	116.07
14	B	1215	CLA	CHB-C1B-C2B	-2.22	120.98	127.43
14	A	1126	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
16	G	2001	PQN	C21-C22-C23	-2.22	108.58	115.97
14	b	1210	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
18	a	4002	BCR	C37-C22-C21	-2.22	119.22	122.82
14	a	1114	CLA	CAC-C3C-C4C	2.22	127.68	124.79
14	b	1203	CLA	C3D-C4D-ND	2.22	113.60	109.99
14	H	1221	CLA	CMB-C2B-C3B	2.22	131.77	126.55
18	I	4018	BCR	C1-C6-C5	-2.22	119.60	122.64
14	a	1116	CLA	CHD-C4C-C3C	-2.22	121.54	124.77
14	a	1110	CLA	CMA-C3A-C4A	2.22	117.74	111.77
14	B	1222	CLA	CAC-C3C-C4C	2.22	127.68	124.79
14	G	1131	CLA	C4D-C3D-CAD	2.22	110.52	108.11
18	l	4019	BCR	C7-C8-C9	-2.22	122.95	126.23
14	b	1239	CLA	C11-C10-C8	-2.22	108.59	115.97
14	A	1108	CLA	C3C-C4C-NC	2.22	113.27	110.43
14	A	1136	CLA	C3C-C4C-NC	2.22	113.27	110.43
14	G	1114	CLA	CAC-C3C-C4C	2.22	127.68	124.79
14	U	1501	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	a	1105	CLA	C3C-C4C-NC	2.22	113.27	110.43
14	b	1227	CLA	C3C-C4C-NC	2.22	113.27	110.43
14	A	1112	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
14	G	1140	CLA	CMA-C3A-C4A	2.22	117.73	111.77
14	U	1503	CLA	CMA-C3A-C4A	2.22	117.73	111.77
14	b	1206	CLA	CMC-C2C-C3C	2.22	132.15	126.15
16	a	2001	PQN	C21-C22-C23	-2.22	108.60	115.97
14	B	1210	CLA	C4C-C3C-C2C	-2.22	103.67	106.89
14	G	1104	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
14	a	1126	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
16	A	2001	PQN	C21-C22-C23	-2.22	108.60	115.97
14	a	1116	CLA	C4D-C3D-CAD	2.22	110.51	108.11
18	i	4020	BCR	C37-C22-C21	-2.22	119.23	122.82
18	I	4020	BCR	C37-C22-C21	-2.22	119.23	122.82
14	l	1503	CLA	CMA-C3A-C4A	2.22	117.73	111.77
14	A	1124	CLA	CHB-C1B-C2B	-2.22	121.00	127.43
14	H	1209	CLA	CMA-C3A-C4A	2.21	117.72	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	K	1401	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
14	A	1125	CLA	C1D-CHD-C4C	-2.21	121.31	126.02
14	L	1501	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
14	b	1208	CLA	CMB-C2B-C3B	2.21	131.75	126.55
14	A	1127	CLA	CMB-C2B-C3B	2.21	131.75	126.55
14	H	1221	CLA	C1-O2A-CGA	2.21	122.00	116.65
14	A	1116	CLA	C1-O2A-CGA	2.21	122.00	116.65
14	A	1109	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	L	1503	CLA	CMA-C3A-C4A	2.21	117.72	111.77
15	B	1238	F6C	O1D-CGD-CBD	-2.21	120.16	124.52
14	G	1112	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
14	A	1116	CLA	CHD-C4C-C3C	-2.21	121.55	124.77
14	T	1401	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
14	B	1208	CLA	CMB-C2B-C3B	2.21	131.75	126.55
15	b	1230	F6C	CMA-C3A-C2A	-2.21	120.17	126.15
14	G	1104	CLA	CMC-C2C-C1C	2.21	128.49	125.03
14	a	1122	CLA	C4D-C3D-CAD	2.21	110.50	108.11
18	a	4001	BCR	C34-C9-C8	2.21	121.46	118.09
14	a	1107	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
14	a	1124	CLA	CHB-C1B-C2B	-2.21	121.02	127.43
14	H	1214	CLA	CAC-C3C-C4C	2.21	127.66	124.79
14	a	1127	CLA	CMB-C2B-C3B	2.21	131.74	126.55
14	B	1023	CLA	CMC-C2C-C3C	2.21	132.12	126.15
14	B	1212	CLA	CMA-C3A-C4A	2.21	117.70	111.77
14	a	1132	CLA	CBB-CAB-C3B	-2.21	116.50	127.53
14	k	1401	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
14	H	1219	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
14	B	1206	CLA	CMC-C2C-C3C	2.21	132.12	126.15
14	H	1224	CLA	CHD-C4C-C3C	-2.21	121.56	124.77
14	A	1110	CLA	CMB-C2B-C1B	2.21	128.78	125.42
14	G	1122	CLA	C4D-C3D-CAD	2.21	110.50	108.11
14	a	1110	CLA	CAA-C2A-C3A	-2.20	107.04	113.00
14	G	1105	CLA	C3C-C4C-NC	2.20	113.25	110.43
15	H	1238	F6C	O1D-CGD-CBD	-2.20	120.17	124.52
14	b	1212	CLA	CMA-C3A-C4A	2.20	117.69	111.77
14	b	1222	CLA	CAC-C3C-C4C	2.20	127.66	124.79
14	G	1111	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
14	b	1221	CLA	C1-O2A-CGA	2.20	121.98	116.65
14	H	1239	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
18	U	4019	BCR	C2-C1-C6	2.20	113.64	110.44
15	a	1121	F6C	O1D-CGD-CBD	-2.20	120.17	124.52
14	G	1127	CLA	CMB-C2B-C3B	2.20	131.73	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1110	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
14	H	1220	CLA	C4D-C3D-CAD	2.20	110.50	108.11
14	G	1123	CLA	CMB-C2B-C3B	2.20	131.73	126.55
14	a	1116	CLA	C1-O2A-CGA	2.20	121.98	116.65
14	l	1501	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
18	R	4020	BCR	C37-C22-C21	-2.20	119.25	122.82
14	G	1119	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
15	H	1207	F6C	CHB-C1B-C2B	-2.20	120.68	125.07
15	b	1207	F6C	CHB-C1B-C2B	-2.20	120.68	125.07
14	b	1221	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
14	G	1110	CLA	CMB-C2B-C1B	2.20	128.77	125.42
14	A	1107	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
14	A	1122	CLA	C4D-C3D-CAD	2.20	110.50	108.11
14	H	1023	CLA	CMC-C2C-C3C	2.20	132.10	126.15
14	H	1221	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
14	G	1116	CLA	CHD-C4C-C3C	-2.20	121.57	124.77
14	b	1229	CLA	C1-C2-C3	-2.20	122.59	126.20
15	H	1237	F6C	CAA-CBA-CGA	-2.20	106.92	113.44
14	G	1132	CLA	CBB-CAB-C3B	-2.20	116.54	127.53
14	B	1219	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
18	l	4019	BCR	C33-C5-C6	-2.20	122.08	124.48
14	b	1208	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
14	b	1208	CLA	C4D-C3D-CAD	2.20	110.49	108.11
18	a	4008	BCR	C36-C18-C17	-2.20	119.26	122.82
18	G	4001	BCR	C34-C9-C8	2.20	121.44	118.09
15	B	1207	F6C	CHB-C1B-C2B	-2.20	120.69	125.07
14	a	1110	CLA	CMB-C2B-C1B	2.20	128.76	125.42
18	A	4003	BCR	C36-C18-C17	-2.20	119.26	122.82
14	B	1239	CLA	CHC-C1C-C2C	-2.20	120.71	126.95
14	a	1111	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
14	G	1124	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
14	H	1206	CLA	CMC-C2C-C3C	2.20	132.09	126.15
15	b	1238	F6C	O1D-CGD-CBD	-2.20	120.19	124.52
14	B	1203	CLA	C3D-C4D-ND	2.20	113.56	109.99
14	b	1219	CLA	CMD-C2D-C3D	-2.20	122.66	127.69
14	b	1023	CLA	CMC-C2C-C3C	2.19	132.09	126.15
14	U	1502	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
14	b	1239	CLA	CHC-C1C-C2C	-2.19	120.71	126.95
14	B	1234	CLA	CAC-C3C-C4C	2.19	127.64	124.79
14	H	1022	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
14	b	1224	CLA	CHD-C4C-C3C	-2.19	121.58	124.77
14	H	1212	CLA	CMA-C3A-C4A	2.19	117.67	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1112	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
18	b	4009	BCR	C33-C5-C4	2.19	118.27	113.60
14	A	1114	CLA	CAC-C3C-C4C	2.19	127.64	124.79
14	A	1132	CLA	CBB-CAB-C3B	-2.19	116.57	127.53
18	a	4011	BCR	C8-C9-C10	2.19	122.46	119.01
15	B	1237	F6C	CAA-CBA-CGA	-2.19	106.94	113.44
18	A	4011	BCR	C8-C9-C10	2.19	122.46	119.01
13	a	1011	CL0	O1D-CGD-CBD	-2.19	121.40	124.72
14	a	1112	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
14	B	1221	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
18	G	4011	BCR	C15-C14-C13	-2.19	124.21	127.28
15	b	1237	F6C	CAA-CBA-CGA	-2.19	106.94	113.44
18	i	4018	BCR	C1-C6-C5	-2.19	119.64	122.64
14	H	1206	CLA	CAC-C3C-C4C	2.19	127.64	124.79
14	B	1022	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
18	L	4022	BCR	C31-C1-C6	-2.19	106.81	110.24
14	B	1221	CLA	C1-O2A-CGA	2.19	121.95	116.65
14	a	1135	CLA	CMC-C2C-C1C	2.19	128.46	125.03
14	A	1123	CLA	CMB-C2B-C3B	2.19	131.70	126.55
18	B	4016	BCR	C3-C4-C5	-2.19	110.15	114.06
14	B	1023	CLA	C3C-C4C-NC	2.19	113.23	110.43
14	a	1123	CLA	CMB-C2B-C3B	2.19	131.70	126.55
14	G	1107	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
13	a	1011	CL0	C1-O2A-CGA	2.19	121.95	116.65
14	G	1130	CLA	CHB-C1B-C2B	-2.19	121.07	127.43
14	b	1226	CLA	CHB-C1B-C2B	-2.19	121.07	127.43
14	a	1130	CLA	CHB-C1B-C2B	-2.19	121.08	127.43
14	B	1229	CLA	C1-C2-C3	-2.19	122.61	126.20
14	b	1212	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
18	G	4011	BCR	C37-C22-C21	-2.19	119.27	122.82
14	a	1119	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
14	A	1119	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
14	A	1135	CLA	CMC-C2C-C1C	2.19	128.45	125.03
14	A	1136	CLA	CMC-C2C-C1C	2.19	128.45	125.03
14	H	1208	CLA	CMB-C2B-C3B	2.19	131.69	126.55
14	A	1104	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
14	L	1502	CLA	CMD-C2D-C3D	-2.19	122.68	127.69
14	B	1224	CLA	CHD-C4C-C3C	-2.18	121.59	124.77
18	l	4022	BCR	C31-C1-C6	-2.18	106.82	110.24
14	G	1116	CLA	C1-O2A-CGA	2.18	121.94	116.65
14	G	1108	CLA	CMD-C2D-C3D	-2.18	122.68	127.69
14	a	1125	CLA	CHD-C4C-C3C	-2.18	121.59	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1201	CLA	C3C-C4C-NC	2.18	113.23	110.43
14	A	1130	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
14	b	1206	CLA	CAC-C3C-C4C	2.18	127.63	124.79
14	B	1212	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
15	B	1237	F6C	CHC-C1C-C2C	-2.18	121.09	127.43
14	a	1107	CLA	CAC-C3C-C4C	2.18	127.63	124.79
14	G	1108	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
18	H	4016	BCR	C3-C4-C5	-2.18	110.16	114.06
14	A	1112	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
14	H	1208	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
14	H	1210	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
14	a	1139	CLA	CAC-C3C-C4C	2.18	127.63	124.79
14	A	1111	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
14	H	1022	CLA	CHA-C1A-NA	-2.18	121.45	126.39
13	G	1011	CL0	C1-O2A-CGA	2.18	121.93	116.65
15	b	1230	F6C	CHC-C1C-C2C	-2.18	121.10	127.43
14	A	1139	CLA	CAC-C3C-C4C	2.18	127.63	124.79
14	A	1109	CLA	C3C-C4C-NC	2.18	113.22	110.43
18	B	4014	BCR	C37-C22-C21	-2.18	119.28	122.82
14	a	1138	CLA	CHB-C4A-NA	2.18	127.55	124.40
14	a	1012	CLA	CAA-CBA-CGA	-2.18	107.02	113.21
18	l	4019	BCR	C2-C1-C6	2.18	113.60	110.44
18	L	4019	BCR	C2-C1-C6	2.18	113.60	110.44
13	G	1011	CL0	O1D-CGD-CBD	-2.18	121.42	124.72
14	G	1112	CLA	C3C-C4C-NC	2.18	113.22	110.43
14	a	1138	CLA	CHB-C1B-C2B	-2.18	121.10	127.43
14	H	1223	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
18	A	4001	BCR	C34-C9-C8	2.18	121.42	118.09
14	G	1135	CLA	CMC-C2C-C1C	2.18	128.44	125.03
14	a	1136	CLA	CMC-C2C-C1C	2.18	128.44	125.03
14	a	1104	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
14	G	1113	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
15	A	1121	F6C	CHC-C1C-C2C	-2.18	121.11	127.43
14	A	1113	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
18	a	4003	BCR	C36-C18-C17	-2.18	119.29	122.82
13	A	1011	CL0	O1D-CGD-CBD	-2.18	121.42	124.72
18	I	4020	BCR	C23-C24-C25	-2.18	121.19	127.00
14	a	1108	CLA	C3C-C4C-NC	2.18	113.22	110.43
14	H	1226	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
14	G	1139	CLA	CAC-C3C-C4C	2.18	127.62	124.79
15	G	1121	F6C	CHC-C1C-C2C	-2.18	121.11	127.43
18	G	4003	BCR	C36-C18-C17	-2.18	119.29	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1012	CLA	CAA-CBA-CGA	-2.18	107.03	113.21
14	A	1125	CLA	CHD-C4C-C3C	-2.17	121.60	124.77
18	R	4020	BCR	C23-C24-C25	-2.17	121.19	127.00
18	a	4003	BCR	C34-C9-C10	-2.17	119.29	122.82
15	a	1121	F6C	CHC-C1C-C2C	-2.17	121.11	127.43
14	a	1140	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
14	H	1023	CLA	C3C-C4C-NC	2.17	113.22	110.43
14	G	1107	CLA	CAC-C3C-C4C	2.17	127.62	124.79
14	a	1108	CLA	CMD-C2D-C3D	-2.17	122.70	127.69
15	H	1230	F6C	CHC-C1C-C2C	-2.17	121.12	127.43
14	G	1125	CLA	CHD-C4C-C3C	-2.17	121.61	124.77
14	H	1023	CLA	C6-C5-C3	-2.17	108.18	113.47
14	B	1023	CLA	C6-C5-C3	-2.17	108.18	113.47
18	G	4003	BCR	C34-C9-C10	-2.17	119.30	122.82
14	G	1140	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
14	B	1226	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
14	B	1204	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
14	A	1108	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
14	l	1502	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
14	B	1227	CLA	C3C-C4C-NC	2.17	113.21	110.43
18	G	4011	BCR	C8-C9-C10	2.17	122.42	119.01
15	b	1237	F6C	CHC-C1C-C2C	-2.17	121.13	127.43
14	B	1236	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
18	B	4009	BCR	C33-C5-C4	2.17	118.22	113.60
14	b	1229	CLA	C3C-C4C-NC	2.17	113.21	110.43
14	A	1140	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
14	G	1127	CLA	C4D-C3D-CAD	2.17	110.46	108.11
14	G	1138	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
14	a	1108	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
14	a	1133	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
14	B	1208	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
14	B	1223	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
14	B	1022	CLA	CHA-C1A-NA	-2.17	121.48	126.39
14	a	1103	CLA	C4D-C3D-CAD	2.17	110.46	108.11
14	A	1138	CLA	CHB-C1B-C2B	-2.17	121.14	127.43
14	H	1229	CLA	C1-C2-C3	-2.17	122.65	126.20
14	G	1126	CLA	CMB-C2B-C1B	2.17	128.72	125.42
14	b	1220	CLA	C4D-C3D-CAD	2.17	110.46	108.11
18	A	4007	BCR	C38-C26-C27	2.17	118.22	113.60
18	b	4006	BCR	C23-C24-C25	-2.17	121.21	127.00
14	A	1118	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
15	B	1230	F6C	CHC-C1C-C2C	-2.17	121.14	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1227	CLA	C3C-C4C-NC	2.17	113.20	110.43
14	A	1107	CLA	CAC-C3C-C4C	2.17	127.61	124.79
18	b	4016	BCR	C3-C4-C5	-2.17	110.19	114.06
18	i	4020	BCR	C23-C24-C25	-2.17	121.21	127.00
14	G	1136	CLA	CMC-C2C-C1C	2.17	128.42	125.03
18	b	4014	BCR	C37-C22-C21	-2.17	119.31	122.82
14	B	1216	CLA	C4D-C3D-CAD	2.16	110.46	108.11
14	b	1204	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
14	a	1113	CLA	CHB-C1B-C2B	-2.16	121.14	127.43
14	G	1138	CLA	CHB-C4A-NA	2.16	127.52	124.40
14	A	1108	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
14	A	1133	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
18	b	4016	BCR	C35-C13-C14	-2.16	119.31	122.82
18	B	4006	BCR	C23-C24-C25	-2.16	121.22	127.00
14	G	1136	CLA	C3C-C4C-NC	2.16	113.20	110.43
14	A	1138	CLA	CHB-C4A-NA	2.16	127.52	124.40
14	G	1128	CLA	C3D-C4D-ND	2.16	113.50	109.99
13	A	1011	CL0	C1-O2A-CGA	2.16	121.88	116.65
14	a	1133	CLA	C1-O2A-CGA	2.16	121.88	116.65
14	B	1216	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
14	a	1109	CLA	C3C-C4C-NC	2.16	113.20	110.43
14	b	1239	CLA	C4C-C3C-C2C	-2.16	103.75	106.89
18	A	4003	BCR	C37-C22-C21	-2.16	119.31	122.82
14	H	1236	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
14	G	1012	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
14	B	1223	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
15	H	1237	F6C	CHC-C1C-C2C	-2.16	121.16	127.43
18	H	4009	BCR	C33-C5-C4	2.16	118.20	113.60
18	A	4003	BCR	C34-C9-C10	-2.16	119.32	122.82
18	B	4016	BCR	C35-C13-C14	-2.16	119.32	122.82
14	G	1118	CLA	CMD-C2D-C3D	-2.16	122.74	127.69
14	A	1133	CLA	C1-O2A-CGA	2.16	121.88	116.65
14	a	1128	CLA	C3D-C4D-ND	2.16	113.49	109.99
14	G	1126	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
18	a	4007	BCR	C38-C26-C27	2.16	118.19	113.60
14	b	1236	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
18	H	4014	BCR	C37-C22-C21	-2.16	119.32	122.82
14	G	1133	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
14	G	1133	CLA	C1-O2A-CGA	2.16	121.87	116.65
14	A	1012	CLA	C1-O2A-CGA	2.16	121.87	116.65
14	b	1216	CLA	CMD-C2D-C3D	-2.16	122.75	127.69
14	b	1229	CLA	CAA-CBA-CGA	-2.16	107.09	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1126	CLA	CHB-C1B-C2B	-2.16	121.17	127.43
18	a	4001	BCR	C29-C30-C25	2.16	113.57	110.44
14	H	1216	CLA	CHB-C1B-C2B	-2.16	121.17	127.43
14	G	1012	CLA	C1-O2A-CGA	2.15	121.87	116.65
14	G	1135	CLA	CHC-C1C-C2C	-2.15	120.82	126.95
18	G	4003	BCR	C37-C22-C21	-2.15	119.33	122.82
14	H	1234	CLA	CAC-C3C-C4C	2.15	127.59	124.79
14	H	1206	CLA	C3C-C4C-NC	2.15	113.19	110.43
14	b	1223	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
14	b	1022	CLA	CHA-C1A-NA	-2.15	121.52	126.39
14	b	1023	CLA	C3C-C4C-NC	2.15	113.19	110.43
14	b	1216	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
14	H	1215	CLA	CMA-C3A-C4A	2.15	117.56	111.77
14	H	1216	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	B	1208	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	H	1235	CLA	C4-C3-C2	-2.15	118.10	123.63
14	A	1126	CLA	CAC-C3C-C4C	2.15	127.59	124.79
14	a	1118	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
14	G	1109	CLA	C3C-C4C-NC	2.15	113.19	110.43
14	X	1701	CLA	CMB-C2B-C3B	2.15	131.61	126.55
18	U	4022	BCR	C31-C1-C6	-2.15	106.87	110.24
14	B	1215	CLA	CMA-C3A-C4A	2.15	117.55	111.77
14	a	1135	CLA	CHC-C1C-C2C	-2.15	120.84	126.95
14	b	1223	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
14	A	1126	CLA	CMB-C2B-C1B	2.15	128.69	125.42
18	b	4013	BCR	C35-C13-C12	2.15	121.37	118.09
14	H	1208	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	b	1236	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	b	1234	CLA	CMC-C2C-C1C	2.15	128.39	125.03
14	A	1131	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	B	1219	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
15	H	1237	F6C	CMC-C2C-C3C	2.15	130.18	125.62
14	L	1502	CLA	CAC-C3C-C4C	2.15	127.58	124.79
18	A	4001	BCR	C29-C30-C25	2.15	113.56	110.44
18	L	4019	BCR	C32-C1-C6	-2.15	106.88	110.24
14	a	1136	CLA	C3C-C4C-NC	2.15	113.18	110.43
14	a	1131	CLA	C4D-C3D-CAD	2.15	110.44	108.11
14	x	1701	CLA	CMB-C2B-C3B	2.15	131.60	126.55
14	A	1122	CLA	CMB-C2B-C1B	2.14	128.69	125.42
14	G	1102	CLA	CHB-C4A-NA	2.14	127.49	124.40
14	B	1229	CLA	C3C-C4C-NC	2.14	113.18	110.43
14	b	1216	CLA	C4D-C3D-CAD	2.14	110.43	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1226	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
14	b	1023	CLA	C6-C5-C3	-2.14	108.25	113.47
18	I	4018	BCR	C30-C25-C26	-2.14	119.71	122.64
18	a	4011	BCR	C37-C22-C21	-2.14	119.34	122.82
14	b	1224	CLA	CMA-C3A-C4A	2.14	117.53	111.77
14	H	1022	CLA	C6-C7-C8	-2.14	108.84	115.97
14	a	1012	CLA	C1-O2A-CGA	2.14	121.84	116.65
14	a	1126	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
14	G	1122	CLA	CMB-C2B-C1B	2.14	128.68	125.42
14	G	1127	CLA	CAC-C3C-C4C	2.14	127.58	124.79
14	W	1701	CLA	CMB-C2B-C3B	2.14	131.59	126.55
14	a	1139	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
18	G	4007	BCR	C38-C26-C27	2.14	118.16	113.60
18	A	4008	BCR	C27-C26-C25	-2.14	119.81	122.70
18	H	4006	BCR	C23-C24-C25	-2.14	121.28	127.00
18	a	4003	BCR	C37-C22-C21	-2.14	119.35	122.82
18	A	4011	BCR	C37-C22-C21	-2.14	119.35	122.82
14	b	1215	CLA	CMA-C3A-C4A	2.14	117.52	111.77
14	B	1216	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
14	G	1124	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	H	1228	CLA	C3C-C4C-NC	2.14	113.17	110.43
14	B	1224	CLA	CMA-C3A-C4A	2.14	117.52	111.77
14	H	1239	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
14	G	1124	CLA	CMB-C2B-C3B	2.14	131.58	126.55
14	a	1122	CLA	CMB-C2B-C1B	2.14	128.68	125.42
18	G	4002	BCR	C33-C5-C4	2.14	118.16	113.60
14	B	1226	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
21	G	6002	LMT	O1'-C1'-C2'	2.14	111.52	108.27
18	b	4014	BCR	C29-C28-C27	-2.14	106.58	111.28
18	U	4019	BCR	C32-C1-C6	-2.14	106.89	110.24
14	B	1022	CLA	C6-C7-C8	-2.14	108.86	115.97
14	H	1202	CLA	CHB-C4A-NA	2.14	127.48	124.40
14	a	1120	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
14	G	1126	CLA	CAC-C3C-C4C	2.14	127.57	124.79
14	b	1219	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
14	H	1216	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
18	a	4002	BCR	C33-C5-C4	2.14	118.15	113.60
14	G	1117	CLA	C4-C3-C5	2.14	118.94	115.23
14	B	1239	CLA	C4C-C3C-C2C	-2.14	103.78	106.89
14	H	1204	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
15	b	1237	F6C	CMC-C2C-C3C	2.13	130.15	125.62
14	A	1135	CLA	CHC-C1C-C2C	-2.13	120.88	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1224	CLA	CMA-C3A-C4A	2.13	117.51	111.77
14	B	1211	CLA	C3C-C4C-NC	2.13	113.16	110.43
14	A	1139	CLA	O2D-CGD-O1D	-2.13	119.69	123.85
14	A	1116	CLA	CBA-CAA-C2A	2.13	120.14	113.79
14	a	1126	CLA	CAC-C3C-C4C	2.13	127.57	124.79
14	H	1235	CLA	C1-C2-C3	-2.13	122.70	126.20
14	b	1235	CLA	C4-C3-C2	-2.13	118.15	123.63
18	R	4018	BCR	C30-C25-C26	-2.13	119.72	122.64
14	H	1223	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
14	B	1220	CLA	C4D-C3D-CAD	2.13	110.42	108.11
14	H	1229	CLA	C3C-C4C-NC	2.13	113.16	110.43
14	H	1222	CLA	C4-C3-C2	-2.13	118.15	123.63
14	G	1120	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
14	B	1206	CLA	CAC-C3C-C4C	2.13	127.56	124.79
14	A	1103	CLA	C4D-C3D-CAD	2.13	110.42	108.11
14	H	1229	CLA	CAA-CBA-CGA	-2.13	107.16	113.21
18	H	4014	BCR	C29-C28-C27	-2.13	106.59	111.28
18	U	4019	BCR	C29-C30-C25	-2.13	107.34	110.44
18	a	4011	BCR	C1-C6-C7	2.13	121.43	115.65
21	A	6002	LMT	O1'-C1'-C2'	2.13	111.51	108.27
14	b	1234	CLA	CAC-C3C-C4C	2.13	127.56	124.79
14	B	1222	CLA	C4-C3-C2	-2.13	118.16	123.63
14	a	1102	CLA	CHB-C4A-NA	2.13	127.47	124.40
18	B	4014	BCR	C29-C28-C27	-2.13	106.59	111.28
18	G	4011	BCR	C1-C6-C7	2.13	121.43	115.65
14	b	1226	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
14	B	1235	CLA	C4-C3-C2	-2.13	118.16	123.63
18	l	4019	BCR	C32-C1-C6	-2.13	106.91	110.24
14	H	1234	CLA	CMC-C2C-C1C	2.13	128.36	125.03
14	A	1120	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
18	b	4006	BCR	C33-C5-C4	2.13	118.13	113.60
18	A	4002	BCR	C33-C5-C4	2.13	118.13	113.60
14	b	1228	CLA	C3C-C4C-NC	2.13	113.16	110.43
18	A	4011	BCR	C1-C6-C7	2.13	121.42	115.65
14	G	1104	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
14	a	1118	CLA	CMA-C3A-C4A	2.13	117.49	111.77
14	b	1235	CLA	C1-C2-C3	-2.13	122.71	126.20
18	H	4016	BCR	C35-C13-C14	-2.13	119.37	122.82
14	A	1124	CLA	CMB-C2B-C3B	2.13	131.55	126.55
16	b	2002	PQN	C12-C11-C3	-2.13	106.84	112.08
14	b	1203	CLA	C4D-C3D-CAD	2.13	110.42	108.11
18	H	4009	BCR	C23-C24-C25	-2.13	121.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1211	CLA	C3C-C4C-NC	2.13	113.15	110.43
14	B	1209	CLA	C3C-C4C-NC	2.13	113.15	110.43
14	H	1239	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
14	A	1012	CLA	CHA-C1A-NA	-2.13	121.58	126.39
18	b	4009	BCR	C23-C24-C25	-2.13	121.32	127.00
14	H	1236	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
14	l	1502	CLA	CAC-C3C-C4C	2.13	127.56	124.79
14	G	1103	CLA	C4D-C3D-CAD	2.13	110.42	108.11
14	b	1206	CLA	C3C-C4C-NC	2.13	113.15	110.43
18	b	4017	BCR	C33-C5-C4	2.13	118.13	113.60
18	B	4013	BCR	C35-C13-C12	2.13	121.33	118.09
14	a	1126	CLA	CMB-C2B-C1B	2.13	128.66	125.42
14	a	1127	CLA	C4D-C3D-CAD	2.13	110.41	108.11
18	H	4013	BCR	C35-C13-C12	2.12	121.33	118.09
14	G	1103	CLA	C3C-C4C-NC	2.12	113.15	110.43
14	a	1112	CLA	C3C-C4C-NC	2.12	113.15	110.43
14	B	1235	CLA	C1-C2-C3	-2.12	122.72	126.20
18	G	4001	BCR	C29-C30-C25	2.12	113.53	110.44
14	H	1227	CLA	CHC-C1C-C2C	-2.12	120.91	126.95
14	G	1108	CLA	CMA-C3A-C4A	2.12	117.48	111.77
18	B	4017	BCR	C33-C5-C4	2.12	118.12	113.60
15	H	1238	F6C	C6-C5-C3	-2.12	108.30	113.47
14	H	1204	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
14	B	1228	CLA	C3C-C4C-NC	2.12	113.15	110.43
14	b	1217	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
14	H	1234	CLA	CBA-CAA-C2A	-2.12	107.48	113.79
14	b	1204	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
14	b	1022	CLA	CHD-C4C-C3C	-2.12	121.68	124.77
14	b	1234	CLA	CBA-CAA-C2A	-2.12	107.48	113.79
18	l	4019	BCR	C29-C30-C25	-2.12	107.36	110.44
15	b	1238	F6C	C6-C5-C3	-2.12	108.30	113.47
14	b	1022	CLA	C6-C7-C8	-2.12	108.91	115.97
14	b	1236	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
16	B	2002	PQN	C12-C11-C3	-2.12	106.86	112.08
14	B	1224	CLA	C4D-C3D-CAD	2.12	110.41	108.11
18	L	4019	BCR	C29-C30-C25	-2.12	107.36	110.44
18	i	4018	BCR	C27-C26-C25	-2.12	119.84	122.70
15	B	1237	F6C	CMC-C2C-C3C	2.12	130.12	125.62
14	A	1104	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
14	G	1129	CLA	C5-C3-C4	2.12	119.47	114.59
14	G	1012	CLA	CHA-C1A-NA	-2.12	121.59	126.39
14	B	1235	CLA	C6-C5-C3	-2.12	108.30	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1116	CLA	CBA-CAA-C2A	2.12	120.10	113.79
14	A	1118	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	A	1128	CLA	C3D-C4D-ND	2.12	113.43	109.99
18	G	4008	BCR	C27-C26-C25	-2.12	119.84	122.70
14	H	1219	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
14	B	1236	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
14	a	1116	CLA	CBA-CAA-C2A	2.12	120.10	113.79
14	G	1118	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	b	1202	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	B	1202	CLA	CHB-C4A-NA	2.12	127.46	124.40
14	B	1022	CLA	CHD-C4C-C3C	-2.12	121.69	124.77
14	b	1235	CLA	C6-C5-C3	-2.12	108.31	113.47
18	H	4017	BCR	C33-C5-C4	2.12	118.11	113.60
14	B	1206	CLA	C3C-C4C-NC	2.12	113.14	110.43
14	a	1108	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	b	1219	CLA	CMA-C3A-C4A	2.12	117.47	111.77
14	b	1222	CLA	C4-C3-C2	-2.12	118.19	123.63
14	a	1111	CLA	CAA-CBA-CGA	-2.12	107.20	113.21
14	G	1139	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
15	B	1238	F6C	C6-C5-C3	-2.12	108.31	113.47
14	a	1117	CLA	C4-C3-C5	2.12	118.90	115.23
14	b	1209	CLA	C3C-C4C-NC	2.12	113.14	110.43
14	H	1203	CLA	C4D-C3D-CAD	2.12	110.40	108.11
14	a	1124	CLA	CMB-C2B-C3B	2.12	131.53	126.55
14	a	1104	CLA	O1D-CGD-CBD	-2.12	120.35	124.52
14	W	1701	CLA	C4C-C3C-C2C	-2.12	103.81	106.89
14	B	1227	CLA	CHC-C1C-C2C	-2.11	120.94	126.95
14	a	1124	CLA	C3C-C4C-NC	2.11	113.14	110.43
14	b	1228	CLA	CMA-C3A-C4A	2.11	117.46	111.77
18	B	4009	BCR	C23-C24-C25	-2.11	121.35	127.00
18	B	4006	BCR	C33-C5-C4	2.11	118.10	113.60
14	H	1231	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
14	b	1211	CLA	C3C-C4C-NC	2.11	113.14	110.43
14	B	1234	CLA	CBA-CAA-C2A	-2.11	107.51	113.79
14	x	1701	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
14	B	1023	CLA	CHD-C4C-NC	-2.11	120.96	124.23
14	B	1229	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
14	A	1127	CLA	C4D-C3D-CAD	2.11	110.40	108.11
14	B	1210	CLA	C4D-C3D-CAD	2.11	110.40	108.11
18	A	4001	BCR	C23-C24-C25	-2.11	121.36	127.00
14	b	1023	CLA	CHD-C4C-NC	-2.11	120.96	124.23
14	H	1228	CLA	CMA-C3A-C4A	2.11	117.45	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1209	CLA	C3C-C4C-NC	2.11	113.14	110.43
14	b	1226	CLA	C3C-C4C-NC	2.11	113.14	110.43
14	a	1127	CLA	CAC-C3C-C4C	2.11	127.54	124.79
14	A	1127	CLA	CAC-C3C-C4C	2.11	127.54	124.79
14	H	1022	CLA	CHD-C4C-C3C	-2.11	121.69	124.77
14	B	1226	CLA	CMC-C2C-C3C	2.11	131.86	126.15
14	H	1219	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	B	1219	CLA	CMA-C3A-C4A	2.11	117.45	111.77
14	b	1227	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
14	H	1217	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
14	b	1239	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
14	B	1236	CLA	C4D-C3D-CAD	2.11	110.40	108.11
21	a	6002	LMT	O1'-C1'-C2'	2.11	111.48	108.27
14	a	1125	CLA	CHD-C1D-ND	-2.11	121.83	124.80
18	H	4006	BCR	C33-C5-C4	2.11	118.09	113.60
18	a	4008	BCR	C27-C26-C25	-2.11	119.85	122.70
14	B	1228	CLA	CMA-C3A-C4A	2.11	117.44	111.77
14	U	1503	CLA	C1-O2A-CGA	2.11	121.75	116.65
14	B	1225	CLA	C1-O2A-CGA	2.11	121.75	116.65
14	H	1226	CLA	CMC-C2C-C3C	2.11	131.85	126.15
18	b	4017	BCR	C35-C13-C12	2.11	121.31	118.09
15	b	1238	F6C	CHB-C1B-C2B	-2.11	120.86	125.07
14	H	1232	CLA	CMB-C2B-C3B	2.11	131.51	126.55
16	H	2002	PQN	C12-C11-C3	-2.11	106.89	112.08
14	B	1234	CLA	CMC-C2C-C1C	2.11	128.33	125.03
14	H	1236	CLA	C4D-C3D-CAD	2.11	110.39	108.11
18	i	4018	BCR	C30-C25-C26	-2.11	119.76	122.64
18	H	4017	BCR	C35-C13-C12	2.11	121.31	118.09
18	G	4001	BCR	C23-C24-C25	-2.11	121.37	127.00
18	b	4004	BCR	C31-C1-C6	-2.11	106.94	110.24
14	A	1108	CLA	CMA-C3A-C4A	2.11	117.43	111.77
14	A	1125	CLA	CHD-C1D-ND	-2.11	121.84	124.80
18	b	4004	BCR	C33-C5-C4	2.10	118.08	113.60
14	A	1104	CLA	CHB-C4A-NA	2.10	127.44	124.40
14	A	1124	CLA	C3C-C4C-NC	2.10	113.13	110.43
14	B	1217	CLA	CMD-C2D-C3D	-2.10	122.86	127.69
18	a	4001	BCR	C23-C24-C25	-2.10	121.38	127.00
18	H	4004	BCR	C33-C5-C4	2.10	118.08	113.60
15	H	1238	F6C	CHB-C1B-C2B	-2.10	120.87	125.07
14	H	1235	CLA	C6-C5-C3	-2.10	108.35	113.47
14	a	1124	CLA	C4-C3-C5	2.10	118.88	115.23
15	B	1238	F6C	CHB-C1B-C2B	-2.10	120.88	125.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1111	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
14	G	1125	CLA	CHD-C1D-ND	-2.10	121.84	124.80
14	a	1133	CLA	CAC-C3C-C4C	2.10	127.52	124.79
14	B	1232	CLA	CMB-C2B-C3B	2.10	131.49	126.55
14	H	1023	CLA	CHD-C4C-NC	-2.10	120.97	124.23
14	G	1125	CLA	C3D-C4D-ND	2.10	113.40	109.99
18	H	4004	BCR	C31-C1-C6	-2.10	106.95	110.24
14	B	1204	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
14	B	1203	CLA	C4D-C3D-CAD	2.10	110.39	108.11
14	b	1232	CLA	CMB-C2B-C3B	2.10	131.49	126.55
14	A	1108	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
14	a	1012	CLA	CHA-C1A-NA	-2.10	121.64	126.39
14	G	1124	CLA	C4-C3-C5	2.10	118.87	115.23
14	b	1226	CLA	CMC-C2C-C3C	2.10	131.83	126.15
14	G	1111	CLA	CAA-CBA-CGA	-2.10	107.25	113.21
14	L	1503	CLA	C1-O2A-CGA	2.10	121.73	116.65
14	l	1501	CLA	C1-O2A-CGA	2.10	121.73	116.65
14	a	1108	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
14	G	1108	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
14	l	1503	CLA	C1-O2A-CGA	2.10	121.72	116.65
14	B	1239	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
14	H	1226	CLA	C3C-C4C-NC	2.10	113.11	110.43
14	b	1226	CLA	C4B-C3B-C2B	-2.10	104.70	107.30
14	H	1225	CLA	C1-O2A-CGA	2.10	121.72	116.65
14	G	1133	CLA	CAC-C3C-C4C	2.10	127.52	124.79
14	G	1122	CLA	C3C-C4C-NC	2.10	113.11	110.43
14	a	1104	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	A	1102	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	b	1224	CLA	C4D-C3D-CAD	2.09	110.38	108.11
14	a	1129	CLA	C5-C3-C4	2.09	119.41	114.59
14	A	1102	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
14	B	1208	CLA	CAC-C3C-C4C	2.09	127.51	124.79
18	I	4020	BCR	C40-C30-C25	-2.09	106.96	110.24
14	b	1023	CLA	CBB-CAB-C3B	-2.09	117.07	127.53
14	G	1137	CLA	CAC-C3C-C4C	2.09	127.51	124.79
14	A	1133	CLA	CAC-C3C-C4C	2.09	127.51	124.79
13	G	1011	CL0	C4C-C3C-C2C	-2.09	105.10	113.37
14	G	1122	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
14	A	1104	CLA	C7-C6-C5	-2.09	107.68	113.26
18	i	4020	BCR	C40-C30-C25	-2.09	106.96	110.24
18	B	4004	BCR	C33-C5-C4	2.09	118.06	113.60
14	a	1116	CLA	CHB-C1B-C2B	-2.09	121.35	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1112	CLA	C3C-C4C-NC	2.09	113.11	110.43
14	b	1231	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
14	a	1111	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
14	a	1136	CLA	C4D-C3D-CAD	2.09	110.38	108.11
14	A	1113	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
14	H	1208	CLA	CAC-C3C-C4C	2.09	127.51	124.79
14	G	1124	CLA	CMC-C2C-C1C	2.09	128.30	125.03
14	A	1129	CLA	C5-C3-C4	2.09	119.40	114.59
14	a	1102	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
14	A	1116	CLA	CMA-C3A-C4A	2.09	117.39	111.77
14	U	1501	CLA	C1-O2A-CGA	2.09	121.71	116.65
14	A	1122	CLA	C3C-C4C-NC	2.09	113.11	110.43
15	B	1237	F6C	CHB-C4A-NA	2.09	127.74	124.80
14	G	1122	CLA	CMC-C2C-C1C	2.09	128.30	125.03
14	a	1128	CLA	CMC-C2C-C3C	2.09	131.80	126.15
16	a	2001	PQN	C16-C17-C18	-2.09	109.02	115.97
14	U	1502	CLA	CAC-C3C-C4C	2.09	127.51	124.79
14	A	1116	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
14	B	1226	CLA	C4B-C3B-C2B	-2.09	104.71	107.30
18	H	4014	BCR	C34-C9-C8	2.09	121.28	118.09
14	b	1218	CLA	CHD-C1D-ND	-2.09	121.86	124.80
14	A	1136	CLA	C4D-C3D-CAD	2.09	110.37	108.11
14	H	1227	CLA	CMC-C2C-C1C	2.09	128.29	125.03
14	L	1501	CLA	C16-C15-C13	-2.09	109.03	115.97
14	B	1023	CLA	CBB-CAB-C3B	-2.09	117.10	127.53
14	A	1111	CLA	C4C-C3C-C2C	-2.09	103.86	106.89
14	a	1113	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
14	b	1225	CLA	C1-O2A-CGA	2.09	121.70	116.65
14	G	1102	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
14	b	1208	CLA	C6-C5-C3	-2.09	108.39	113.47
14	b	1206	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
14	H	1023	CLA	CBB-CAB-C3B	-2.09	117.11	127.53
14	L	1503	CLA	C4C-C3C-C2C	-2.09	103.86	106.89
14	H	1232	CLA	CAC-C3C-C4C	2.09	127.50	124.79
14	A	1137	CLA	CHC-C1C-C2C	-2.09	121.02	126.95
14	a	1103	CLA	C3C-C4C-NC	2.09	113.10	110.43
13	A	1011	CL0	C4C-C3C-C2C	-2.08	105.14	113.37
14	A	1126	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
14	H	1214	CLA	CBB-CAB-C3B	-2.08	117.11	127.53
14	a	1126	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
14	l	1503	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
15	H	1207	F6C	C3D-C4D-ND	2.08	113.36	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1239	CLA	CMA-C3A-C4A	2.08	117.37	111.77
18	R	4020	BCR	C40-C30-C25	-2.08	106.98	110.24
14	B	1226	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
14	a	1116	CLA	CMA-C3A-C4A	2.08	117.37	111.77
14	a	1134	CLA	CAC-C3C-C4C	2.08	127.50	124.79
14	H	1226	CLA	C4B-C3B-C2B	-2.08	104.71	107.30
15	B	1207	F6C	C3D-C4D-ND	2.08	113.36	109.93
18	B	4009	BCR	C1-C6-C5	-2.08	119.79	122.64
14	G	1104	CLA	C7-C6-C5	-2.08	107.71	113.26
14	a	1013	CLA	CBC-CAC-C3C	-2.08	106.78	112.42
14	B	1206	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
14	A	1128	CLA	CMC-C2C-C3C	2.08	131.78	126.15
14	a	1137	CLA	CAC-C3C-C4C	2.08	127.50	124.79
14	H	1222	CLA	CMC-C2C-C1C	2.08	128.28	125.03
18	B	4017	BCR	C35-C13-C12	2.08	121.27	118.09
14	A	1124	CLA	C4-C3-C5	2.08	118.84	115.23
18	H	4009	BCR	C1-C6-C5	-2.08	119.79	122.64
14	G	1116	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
21	a	6002	LMT	O5B-C5B-C6B	2.08	111.59	106.44
14	b	1208	CLA	CAC-C3C-C4C	2.08	127.50	124.79
14	a	1109	CLA	C6-C7-C8	-2.08	109.06	115.97
14	A	1132	CLA	C4-C3-C5	2.08	118.84	115.23
14	B	1222	CLA	CMC-C2C-C1C	2.08	128.28	125.03
14	B	1231	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
21	A	6002	LMT	O5B-C5B-C6B	2.08	111.59	106.44
14	G	1116	CLA	CMA-C3A-C4A	2.08	117.36	111.77
14	X	1701	CLA	C4C-C3C-C2C	-2.08	103.87	106.89
16	G	2001	PQN	C16-C17-C18	-2.08	109.06	115.97
14	G	1117	CLA	CAA-C2A-C3A	-2.08	107.39	113.00
14	G	1133	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
14	G	1113	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
18	R	4018	BCR	C27-C26-C25	-2.08	119.90	122.70
14	G	1128	CLA	CMC-C2C-C3C	2.08	131.76	126.15
14	a	1118	CLA	CHC-C1C-C2C	-2.08	121.05	126.95
14	b	1210	CLA	C4D-C3D-CAD	2.08	110.36	108.11
13	a	1011	CL0	C2C-C1C-NC	2.08	116.33	110.46
14	b	1239	CLA	CMA-C3A-C4A	2.08	117.35	111.77
14	b	1214	CLA	C3C-C4C-NC	2.08	113.09	110.43
13	a	1011	CL0	C4C-C3C-C2C	-2.08	105.17	113.37
14	A	1137	CLA	CAC-C3C-C4C	2.08	127.49	124.79
14	a	1104	CLA	C7-C6-C5	-2.08	107.73	113.26
14	H	1231	CLA	CMD-C2D-C3D	-2.08	122.93	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1105	CLA	CMB-C2B-C3B	2.08	131.43	126.55
14	b	1214	CLA	CBB-CAB-C3B	-2.07	117.16	127.53
14	U	1503	CLA	C4C-C3C-C2C	-2.07	103.87	106.89
14	L	1501	CLA	C1-O2A-CGA	2.07	121.67	116.65
16	A	2001	PQN	C16-C17-C18	-2.07	109.07	115.97
18	B	4017	BCR	C2-C1-C6	2.07	113.45	110.44
14	G	1137	CLA	CHC-C1C-C2C	-2.07	121.05	126.95
14	G	1117	CLA	CMC-C2C-C3C	2.07	131.76	126.15
14	a	1105	CLA	CMB-C2B-C3B	2.07	131.43	126.55
14	a	1124	CLA	CMC-C2C-C1C	2.07	128.27	125.03
14	U	1501	CLA	C16-C15-C13	-2.07	109.08	115.97
14	G	1105	CLA	CMB-C2B-C3B	2.07	131.43	126.55
14	A	1118	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
14	b	1226	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
14	A	1117	CLA	C4-C3-C5	2.07	118.82	115.23
14	a	1125	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
14	A	1117	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
14	A	1125	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
14	a	1133	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
14	B	1214	CLA	CBB-CAB-C3B	-2.07	117.18	127.53
14	G	1109	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
15	b	1207	F6C	C3D-C4D-ND	2.07	113.34	109.93
14	a	1117	CLA	CMC-C2C-C3C	2.07	131.75	126.15
14	G	1118	CLA	CHC-C1C-C2C	-2.07	121.06	126.95
14	B	1208	CLA	C6-C5-C3	-2.07	108.43	113.47
14	b	1232	CLA	CHA-C1A-NA	-2.07	121.70	126.39
14	G	1013	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
14	B	1210	CLA	CMA-C3A-C4A	2.07	117.34	111.77
14	B	1228	CLA	CMB-C2B-C3B	2.07	131.42	126.55
14	A	1123	CLA	C4-C3-C2	-2.07	118.31	123.63
14	W	1701	CLA	C1-O2A-CGA	2.07	121.66	116.65
14	G	1132	CLA	C4-C3-C5	2.07	118.82	115.23
18	b	4006	BCR	C38-C26-C27	2.07	118.01	113.60
14	b	1205	CLA	CMB-C2B-C3B	2.07	131.42	126.55
14	H	1206	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
18	b	4017	BCR	C2-C1-C6	2.07	113.44	110.44
18	B	4014	BCR	C34-C9-C8	2.07	121.25	118.09
14	B	1239	CLA	CMA-C3A-C4A	2.07	117.33	111.77
18	l	4022	BCR	C36-C18-C17	-2.07	119.47	122.82
18	H	4013	BCR	C38-C26-C27	2.07	118.00	113.60
18	a	4007	BCR	C33-C5-C4	2.07	118.00	113.60
14	a	1132	CLA	C4-C3-C5	2.07	118.81	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	1109	CLA	OBD-CAD-C3D	-2.07	123.59	128.42
14	b	1227	CLA	CMC-C2C-C1C	2.07	128.26	125.03
14	H	1226	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
14	G	1104	CLA	CHB-C4A-NA	2.07	127.38	124.40
14	b	1222	CLA	CMC-C2C-C1C	2.07	128.26	125.03
14	G	1130	CLA	CHA-C1A-NA	-2.06	121.72	126.39
14	b	1228	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
14	H	1224	CLA	C4D-C3D-CAD	2.06	110.35	108.11
14	a	1125	CLA	C3D-C4D-ND	2.06	113.34	109.99
14	U	1501	CLA	C4-C3-C5	2.06	118.81	115.23
14	G	1126	CLA	C4C-C3C-C2C	-2.06	103.89	106.89
21	G	6002	LMT	O5B-C5B-C6B	2.06	111.56	106.44
14	B	1214	CLA	C3C-C4C-NC	2.06	113.07	110.43
14	A	1013	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
14	l	1501	CLA	C16-C15-C13	-2.06	109.11	115.97
14	H	1210	CLA	CMA-C3A-C4A	2.06	117.32	111.77
14	H	1228	CLA	CMC-C2C-C3C	2.06	131.73	126.15
14	A	1124	CLA	CMC-C2C-C1C	2.06	128.26	125.03
14	A	1117	CLA	CMC-C2C-C3C	2.06	131.73	126.15
14	b	1204	CLA	OBD-CAD-C3D	-2.06	123.59	128.42
14	l	1501	CLA	C4-C3-C5	2.06	118.81	115.23
14	G	1134	CLA	CAC-C3C-C4C	2.06	127.47	124.79
18	I	4018	BCR	C28-C27-C26	-2.06	110.38	114.06
14	G	1140	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
14	a	1117	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
14	B	1204	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
14	a	1122	CLA	CHC-C1C-C2C	-2.06	121.09	126.95
14	a	1122	CLA	C3C-C4C-NC	2.06	113.07	110.43
14	b	1210	CLA	CMA-C3A-C4A	2.06	117.31	111.77
18	R	4020	BCR	C28-C29-C30	-2.06	107.14	114.43
18	b	4009	BCR	C1-C6-C5	-2.06	119.82	122.64
14	x	1701	CLA	C1-O2A-CGA	2.06	121.64	116.65
14	A	1109	CLA	C6-C7-C8	-2.06	109.12	115.97
18	U	4022	BCR	C36-C18-C17	-2.06	119.48	122.82
13	A	1011	CL0	C2C-C1C-NC	2.06	116.29	110.46
18	b	4014	BCR	C34-C9-C8	2.06	121.23	118.09
14	a	1130	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	a	1140	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
14	G	1125	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
14	A	1133	CLA	CHC-C1C-C2C	-2.06	121.10	126.95
13	G	1011	CL0	C2C-C1C-NC	2.06	116.28	110.46
14	A	1128	CLA	CHB-C1B-C2B	-2.06	121.45	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1232	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	B	1232	CLA	CHA-C1A-NA	-2.06	121.73	126.39
14	G	1136	CLA	C4D-C3D-CAD	2.06	110.34	108.11
14	H	1205	CLA	CMB-C2B-C3B	2.06	131.39	126.55
14	A	1113	CLA	C4C-C3C-C2C	-2.06	103.90	106.89
14	B	1228	CLA	C4C-C3C-C2C	-2.06	103.90	106.89
14	A	1140	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
18	I	4018	BCR	C27-C26-C25	-2.06	119.92	122.70
18	B	4004	BCR	C31-C1-C6	-2.06	107.02	110.24
18	B	4006	BCR	C38-C26-C27	2.06	117.98	113.60
14	B	1231	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
14	H	1208	CLA	C6-C5-C3	-2.06	108.46	113.47
14	A	1122	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
15	b	1237	F6C	CHB-C4A-NA	2.05	127.69	124.80
14	b	1203	CLA	CHA-C4D-ND	2.05	136.79	132.55
14	A	1130	CLA	CHA-C4D-ND	2.05	136.79	132.55
14	B	1232	CLA	CAC-C3C-C4C	2.05	127.46	124.79
18	H	4017	BCR	C2-C1-C6	2.05	113.42	110.44
18	I	4020	BCR	C28-C29-C30	-2.05	107.16	114.43
14	B	1218	CLA	CHD-C1D-ND	-2.05	121.91	124.80
14	a	1128	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
14	a	1130	CLA	CHA-C4D-ND	2.05	136.78	132.55
14	a	1137	CLA	CHC-C1C-C2C	-2.05	121.11	126.95
14	A	1103	CLA	C3C-C4C-NC	2.05	113.06	110.43
14	G	1137	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
14	b	1231	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
18	i	4018	BCR	C28-C27-C26	-2.05	110.40	114.06
14	b	1221	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	B	1218	CLA	CHD-C4C-C3C	-2.05	121.78	124.77
18	i	4020	BCR	C28-C29-C30	-2.05	107.17	114.43
18	G	4007	BCR	C33-C5-C4	2.05	117.97	113.60
14	G	1123	CLA	C4-C3-C2	-2.05	118.36	123.63
14	X	1701	CLA	C1-O2A-CGA	2.05	121.61	116.65
18	H	4014	BCR	C3-C4-C5	-2.05	110.40	114.06
14	B	1226	CLA	C3C-C4C-NC	2.05	113.06	110.43
14	H	1218	CLA	CHD-C1D-ND	-2.05	121.92	124.80
14	H	1021	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	H	1223	CLA	CHA-C4D-ND	2.05	136.78	132.55
14	B	1203	CLA	CHA-C4D-ND	2.05	136.78	132.55
18	B	4013	BCR	C38-C26-C27	2.05	117.96	113.60
14	b	1202	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
14	B	1235	CLA	CHB-C1B-C2B	-2.05	121.48	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	H	1022	CLA	CHC-C1C-NC	-2.05	121.23	124.31
18	R	4018	BCR	C28-C27-C26	-2.05	110.40	114.06
14	b	1228	CLA	CMB-C2B-C3B	2.05	131.37	126.55
14	B	1202	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
14	G	1135	CLA	CHA-C4D-ND	2.05	136.77	132.55
14	a	1123	CLA	C4-C3-C2	-2.05	118.37	123.63
14	H	1216	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
14	B	1227	CLA	CMC-C2C-C1C	2.05	128.23	125.03
14	G	1012	CLA	C11-C10-C8	-2.05	109.16	115.97
14	G	1109	CLA	C6-C7-C8	-2.05	109.16	115.97
14	A	1134	CLA	CAC-C3C-C4C	2.05	127.45	124.79
15	B	1230	F6C	CMC-C2C-C3C	2.05	129.97	125.62
14	H	1235	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
14	b	1223	CLA	CHA-C4D-ND	2.05	136.77	132.55
14	H	1210	CLA	C4D-C3D-CAD	2.05	110.33	108.11
14	B	1205	CLA	CMB-C2B-C3B	2.05	131.36	126.55
14	A	1124	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
14	B	1228	CLA	CMC-C2C-C3C	2.05	131.68	126.15
15	b	1237	F6C	CAC-C3C-C4C	2.05	127.73	124.91
18	A	4007	BCR	C33-C5-C4	2.05	117.96	113.60
15	H	1237	F6C	CHB-C4A-NA	2.04	127.68	124.80
18	M	4021	BCR	C37-C22-C21	-2.04	119.50	122.82
14	H	1228	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
14	a	1137	CLA	CBC-CAC-C3C	-2.04	106.88	112.42
15	B	1237	F6C	CAC-C3C-C4C	2.04	127.72	124.91
14	b	1232	CLA	CAC-C3C-C4C	2.04	127.45	124.79
14	G	1128	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
14	G	1111	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
14	G	1113	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
14	H	1204	CLA	CBB-CAB-C3B	-2.04	117.32	127.53
18	b	4013	BCR	C38-C26-C27	2.04	117.95	113.60
13	a	1011	CL0	CMA-C3A-C2A	-2.04	106.24	114.13
14	G	1130	CLA	CHA-C4D-ND	2.04	136.76	132.55
14	b	1202	CLA	C4-C3-C2	-2.04	118.38	123.63
14	B	1218	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
14	H	1202	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
14	G	1118	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
14	H	1203	CLA	CHA-C4D-ND	2.04	136.76	132.55
14	G	1123	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	a	1118	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
14	b	1223	CLA	C3D-C4D-ND	2.04	113.30	109.99
18	b	4014	BCR	C3-C4-C5	-2.04	110.42	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1235	CLA	CHB-C1B-C2B	-2.04	121.51	127.43
14	B	1216	CLA	CHC-C1C-C2C	-2.04	121.15	126.95
14	b	1228	CLA	CMC-C2C-C3C	2.04	131.66	126.15
14	H	1228	CLA	CMB-C2B-C3B	2.04	131.35	126.55
14	B	1022	CLA	CHC-C1C-NC	-2.04	121.24	124.31
14	a	1116	CLA	CBB-CAB-C3B	-2.04	117.34	127.53
14	b	1223	CLA	CHA-C1A-NA	-2.04	121.77	126.39
14	B	1202	CLA	C4-C3-C2	-2.04	118.39	123.63
14	B	1204	CLA	CBB-CAB-C3B	-2.04	117.34	127.53
14	A	1137	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
14	A	1138	CLA	C3C-C4C-NC	2.04	113.04	110.43
14	U	1501	CLA	CMA-C3A-C4A	2.04	117.25	111.77
14	b	1204	CLA	CBB-CAB-C3B	-2.04	117.34	127.53
14	G	1112	CLA	CMA-C3A-C4A	2.04	117.25	111.77
13	A	1011	CL0	CMA-C3A-C2A	-2.04	106.26	114.13
15	H	1237	F6C	CAC-C3C-C4C	2.04	127.71	124.91
14	A	1122	CLA	CMC-C2C-C1C	2.04	128.22	125.03
14	b	1206	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
14	A	1125	CLA	C3D-C4D-ND	2.04	113.30	109.99
14	H	1214	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
14	b	1216	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
14	L	1501	CLA	C4-C3-C5	2.04	118.76	115.23
14	a	1109	CLA	OBD-CAD-C3D	-2.04	123.66	128.42
15	G	1121	F6C	CMC-C2C-C3C	2.03	129.94	125.62
18	B	4014	BCR	C3-C4-C5	-2.03	110.43	114.06
14	A	1012	CLA	C11-C10-C8	-2.03	109.20	115.97
15	a	1121	F6C	CMC-C2C-C3C	2.03	129.94	125.62
14	A	1126	CLA	CMB-C2B-C3B	2.03	131.33	126.55
14	G	1116	CLA	CBB-CAB-C3B	-2.03	117.37	127.53
14	H	1202	CLA	C4-C3-C2	-2.03	118.41	123.63
14	H	1204	CLA	OBD-CAD-C3D	-2.03	123.66	128.42
14	B	1221	CLA	C4D-C3D-CAD	2.03	110.31	108.11
14	a	1112	CLA	CMA-C3A-C4A	2.03	117.24	111.77
14	B	1223	CLA	C3D-C4D-ND	2.03	113.29	109.99
15	b	1230	F6C	CMC-C2C-C3C	2.03	129.94	125.62
14	B	1226	CLA	CMA-C3A-C4A	2.03	117.24	111.77
14	B	1211	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
14	U	1503	CLA	CAC-C3C-C4C	2.03	127.43	124.79
14	H	1239	CLA	C11-C12-C13	-2.03	109.21	115.97
14	A	1123	CLA	CHA-C1A-NA	-2.03	121.79	126.39
18	L	4022	BCR	C36-C18-C17	-2.03	119.52	122.82
14	H	1218	CLA	CHD-C4C-C3C	-2.03	121.81	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	b	1218	CLA	CHD-C4C-C3C	-2.03	121.81	124.77
14	B	1223	CLA	CHA-C4D-ND	2.03	136.74	132.55
14	a	1124	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
14	A	1116	CLA	CBB-CAB-C3B	-2.03	117.38	127.53
14	l	1501	CLA	CMA-C3A-C4A	2.03	117.23	111.77
14	b	1211	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
14	b	1239	CLA	C11-C12-C13	-2.03	109.21	115.97
14	A	1130	CLA	CHA-C1A-NA	-2.03	121.79	126.39
14	A	1135	CLA	CHA-C4D-ND	2.03	136.74	132.55
14	A	1113	CLA	CAC-C3C-C4C	2.03	127.43	124.79
14	a	1123	CLA	CHA-C1A-NA	-2.03	121.79	126.39
14	G	1106	CLA	C6-C5-C3	-2.03	108.52	113.47
20	R	5006	LMG	O7-C10-O9	-2.03	118.96	123.70
18	H	4005	BCR	C34-C9-C8	2.03	121.19	118.09
14	B	1239	CLA	C11-C12-C13	-2.03	109.22	115.97
14	B	1216	CLA	CMC-C2C-C1C	2.03	128.21	125.03
14	H	1214	CLA	C3C-C4C-NC	2.03	113.03	110.43
14	A	1112	CLA	CMA-C3A-C4A	2.03	117.22	111.77
13	G	1011	CL0	CMA-C3A-C2A	-2.03	106.30	114.13
18	H	4006	BCR	C38-C26-C27	2.03	117.92	113.60
14	b	1218	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
14	b	1022	CLA	CHC-C1C-NC	-2.03	121.26	124.31
14	a	1012	CLA	C11-C10-C8	-2.03	109.23	115.97
14	A	1106	CLA	C6-C5-C3	-2.03	108.53	113.47
20	i	5006	LMG	O7-C10-O9	-2.03	118.97	123.70
18	V	4021	BCR	C37-C22-C21	-2.03	119.53	122.82
14	B	1202	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
14	A	1114	CLA	CMC-C2C-C3C	2.02	131.62	126.15
15	A	1121	F6C	CMC-C2C-C3C	2.02	129.92	125.62
14	G	1112	CLA	C1-O2A-CGA	2.02	121.55	116.65
14	G	1114	CLA	CMC-C2C-C3C	2.02	131.62	126.15
15	H	1230	F6C	CMC-C2C-C3C	2.02	129.92	125.62
14	A	1115	CLA	CMA-C3A-C4A	2.02	117.21	111.77
14	b	1208	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
14	H	1223	CLA	C3D-C4D-ND	2.02	113.28	109.99
14	a	1103	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
14	a	1112	CLA	C1-O2A-CGA	2.02	121.55	116.65
14	A	1118	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
14	H	1233	CLA	CAC-C3C-C4C	2.02	127.42	124.79
14	H	1206	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
14	L	1501	CLA	CMA-C3A-C4A	2.02	117.21	111.77
14	b	1214	CLA	CHC-C1C-C2C	-2.02	121.20	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	a	1122	CLA	CMC-C2C-C1C	2.02	128.19	125.03
14	B	1206	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
14	G	1115	CLA	CMA-C3A-C4A	2.02	117.20	111.77
14	H	1218	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
14	b	1215	CLA	CHC-C1C-C2C	-2.02	121.21	126.95
14	A	1128	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
14	G	1124	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
20	I	5006	LMG	O7-C10-O9	-2.02	118.98	123.70
14	a	1135	CLA	CHA-C4D-ND	2.02	136.72	132.55
14	a	1113	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
16	H	2002	PQN	O4-C4-C5	-2.02	118.34	121.57
14	B	1205	CLA	C1-C2-C3	-2.02	122.89	126.20
14	b	1223	CLA	C6-C7-C8	-2.02	109.26	115.97
14	b	1202	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
14	b	1216	CLA	CMC-C2C-C1C	2.02	128.19	125.03
14	a	1114	CLA	CMC-C2C-C3C	2.02	131.60	126.15
14	B	1208	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
14	H	1211	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
14	a	1135	CLA	C1-O2A-CGA	2.02	121.53	116.65
14	H	1226	CLA	CMA-C3A-C4A	2.02	117.19	111.77
14	B	1214	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
14	H	1221	CLA	C4D-C3D-CAD	2.02	110.30	108.11
14	l	1503	CLA	CAC-C3C-C4C	2.02	127.41	124.79
18	b	4005	BCR	C34-C9-C8	2.02	121.17	118.09
14	A	1135	CLA	C1-O2A-CGA	2.02	121.53	116.65
14	G	1140	CLA	C4C-C3C-C2C	-2.02	103.96	106.89
14	A	1112	CLA	C1-O2A-CGA	2.02	121.53	116.65
14	b	1226	CLA	CMA-C3A-C4A	2.02	117.19	111.77
14	B	1215	CLA	CHC-C1C-C2C	-2.02	121.22	126.95
14	a	1106	CLA	C6-C5-C3	-2.01	108.56	113.47
14	a	1119	CLA	CMB-C2B-C3B	2.01	131.29	126.55
18	b	4014	BCR	C38-C26-C25	-2.01	122.29	124.48
14	a	1126	CLA	CMB-C2B-C3B	2.01	131.29	126.55
14	A	1131	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
14	B	1223	CLA	CHA-C1A-NA	-2.01	121.83	126.39
14	b	1202	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
14	H	1215	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
14	G	1138	CLA	C3C-C4C-NC	2.01	113.01	110.43
14	H	1235	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
18	b	4016	BCR	C34-C9-C10	-2.01	119.56	122.82
18	m	4021	BCR	C37-C22-C21	-2.01	119.56	122.82
14	H	1223	CLA	CHA-C1A-NA	-2.01	121.83	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	1135	CLA	C1-O2A-CGA	2.01	121.52	116.65
14	a	1109	CLA	CMB-C2B-C1B	2.01	128.48	125.42
14	A	1134	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
14	H	1202	CLA	C4C-C3C-C2C	-2.01	103.96	106.89
14	a	1115	CLA	CMA-C3A-C4A	2.01	117.18	111.77
14	b	1205	CLA	CMA-C3A-C4A	2.01	117.18	111.77
14	B	1233	CLA	CAC-C3C-C4C	2.01	127.41	124.79
14	B	1235	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
14	H	1223	CLA	C6-C7-C8	-2.01	109.28	115.97
14	G	1126	CLA	CMB-C2B-C3B	2.01	131.28	126.55
14	A	1119	CLA	CMB-C2B-C3B	2.01	131.28	126.55
14	b	1232	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
14	b	1235	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
14	L	1503	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
14	G	1134	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
14	a	1134	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
14	a	1136	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
14	A	1138	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
14	b	1210	CLA	CGD-CBD-CAD	-2.01	104.35	110.85
14	H	1210	CLA	CGD-CBD-CAD	-2.01	104.35	110.85
14	A	1103	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
14	a	1114	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
14	H	1202	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
14	B	1202	CLA	CAA-C2A-C3A	-2.01	107.58	113.00
14	B	1227	CLA	CHA-C4D-ND	2.01	136.69	132.55
14	G	1130	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
18	H	4016	BCR	C34-C9-C10	-2.01	119.57	122.82
14	G	1138	CLA	CMD-C2D-C3D	-2.01	123.09	127.69
14	H	1205	CLA	CMA-C3A-C4A	2.01	117.16	111.77
14	H	1216	CLA	CMC-C2C-C1C	2.00	128.17	125.03
14	A	1119	CLA	C4D-C3D-CAD	2.00	110.28	108.11
14	G	1131	CLA	CAA-CBA-CGA	-2.00	107.52	113.21
14	H	1205	CLA	C1-C2-C3	-2.00	122.91	126.20
14	b	1225	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
14	B	1223	CLA	C4C-C3C-C2C	-2.00	103.98	106.89
14	U	1503	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
18	H	4004	BCR	C30-C25-C26	-2.00	119.90	122.64
18	b	4004	BCR	C30-C25-C26	-2.00	119.90	122.64
14	a	1134	CLA	CHC-C1C-C2C	-2.00	121.26	126.95
14	G	1113	CLA	CAC-C3C-C4C	2.00	127.39	124.79
14	H	1203	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
14	H	1232	CLA	OBD-CAD-C3D	-2.00	123.74	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	1223	CLA	C6-C7-C8	-2.00	109.31	115.97
14	B	1225	CLA	CHB-C1B-C2B	-2.00	121.62	127.43
14	b	1203	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
14	A	1013	CLA	CHD-C4C-C3C	-2.00	121.86	124.77
18	B	4004	BCR	C30-C25-C26	-2.00	119.90	122.64

All (276) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	1011	CL0	NC
13	G	1011	CL0	NA
13	G	1011	CL0	ND
13	a	1011	CL0	NC
13	a	1011	CL0	NA
13	a	1011	CL0	ND
13	A	1011	CL0	NC
13	A	1011	CL0	NA
13	A	1011	CL0	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
14	G	1114	CLA	ND
14	G	1115	CLA	ND
14	G	1116	CLA	ND
14	G	1117	CLA	ND
14	G	1118	CLA	ND
14	G	1119	CLA	ND
14	G	1120	CLA	ND
14	G	1122	CLA	ND
14	G	1123	CLA	ND

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Mol	Chain	Res	Type	Atom
14	G	1124	CLA	ND
14	G	1125	CLA	ND
14	G	1126	CLA	ND
14	G	1127	CLA	ND
14	G	1128	CLA	ND
14	G	1129	CLA	ND
14	G	1130	CLA	ND
14	G	1131	CLA	ND
14	G	1132	CLA	ND
14	G	1133	CLA	ND
14	G	1134	CLA	ND
14	G	1135	CLA	ND
14	G	1136	CLA	ND
14	G	1137	CLA	ND
14	G	1138	CLA	ND
14	G	1139	CLA	ND
14	G	1140	CLA	ND
14	H	1021	CLA	ND
14	H	1022	CLA	ND
14	H	1023	CLA	ND
14	H	1201	CLA	ND
14	H	1202	CLA	ND
14	H	1203	CLA	ND
14	H	1204	CLA	ND
14	H	1205	CLA	ND
14	H	1206	CLA	ND
14	H	1208	CLA	ND
14	H	1209	CLA	ND
14	H	1210	CLA	ND
14	H	1211	CLA	ND
14	H	1212	CLA	ND
14	H	1213	CLA	ND
14	H	1214	CLA	ND
14	H	1215	CLA	ND
14	H	1216	CLA	ND
14	H	1217	CLA	ND
14	H	1218	CLA	ND
14	H	1219	CLA	ND
14	H	1220	CLA	ND
14	H	1221	CLA	ND
14	H	1222	CLA	ND
14	H	1223	CLA	ND

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Mol	Chain	Res	Type	Atom
14	H	1224	CLA	ND
14	H	1225	CLA	ND
14	H	1226	CLA	ND
14	H	1227	CLA	ND
14	H	1228	CLA	ND
14	H	1229	CLA	ND
14	H	1231	CLA	ND
14	H	1232	CLA	ND
14	H	1233	CLA	ND
14	H	1234	CLA	ND
14	H	1235	CLA	ND
14	H	1236	CLA	ND
14	H	1239	CLA	ND
14	T	1401	CLA	ND
14	U	1501	CLA	ND
14	U	1502	CLA	ND
14	U	1503	CLA	ND
14	W	1701	CLA	ND
14	a	1012	CLA	ND
14	a	1013	CLA	ND
14	a	1101	CLA	ND
14	a	1102	CLA	ND
14	a	1103	CLA	ND
14	a	1104	CLA	ND
14	a	1105	CLA	ND
14	a	1106	CLA	ND
14	a	1107	CLA	ND
14	a	1108	CLA	ND
14	a	1109	CLA	ND
14	a	1110	CLA	ND
14	a	1111	CLA	ND
14	a	1112	CLA	ND
14	a	1113	CLA	ND
14	a	1114	CLA	ND
14	a	1115	CLA	ND
14	a	1116	CLA	ND
14	a	1117	CLA	ND
14	a	1118	CLA	ND
14	a	1119	CLA	ND
14	a	1120	CLA	ND
14	a	1122	CLA	ND
14	a	1123	CLA	ND

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Mol	Chain	Res	Type	Atom
14	a	1124	CLA	ND
14	a	1125	CLA	ND
14	a	1126	CLA	ND
14	a	1127	CLA	ND
14	a	1128	CLA	ND
14	a	1129	CLA	ND
14	a	1130	CLA	ND
14	a	1131	CLA	ND
14	a	1132	CLA	ND
14	a	1133	CLA	ND
14	a	1134	CLA	ND
14	a	1135	CLA	ND
14	a	1136	CLA	ND
14	a	1137	CLA	ND
14	a	1138	CLA	ND
14	a	1139	CLA	ND
14	a	1140	CLA	ND
14	b	1021	CLA	ND
14	b	1022	CLA	ND
14	b	1023	CLA	ND
14	b	1201	CLA	ND
14	b	1202	CLA	ND
14	b	1203	CLA	ND
14	b	1204	CLA	ND
14	b	1205	CLA	ND
14	b	1206	CLA	ND
14	b	1208	CLA	ND
14	b	1209	CLA	ND
14	b	1210	CLA	ND
14	b	1211	CLA	ND
14	b	1212	CLA	ND
14	b	1213	CLA	ND
14	b	1214	CLA	ND
14	b	1215	CLA	ND
14	b	1216	CLA	ND
14	b	1217	CLA	ND
14	b	1218	CLA	ND
14	b	1219	CLA	ND
14	b	1220	CLA	ND
14	b	1221	CLA	ND
14	b	1222	CLA	ND
14	b	1223	CLA	ND

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Mol	Chain	Res	Type	Atom
14	b	1224	CLA	ND
14	b	1225	CLA	ND
14	b	1226	CLA	ND
14	b	1227	CLA	ND
14	b	1228	CLA	ND
14	b	1229	CLA	ND
14	b	1231	CLA	ND
14	b	1232	CLA	ND
14	b	1233	CLA	ND
14	b	1234	CLA	ND
14	b	1235	CLA	ND
14	b	1236	CLA	ND
14	b	1239	CLA	ND
14	k	1401	CLA	ND
14	l	1501	CLA	ND
14	l	1502	CLA	ND
14	l	1503	CLA	ND
14	x	1701	CLA	ND
14	A	1012	CLA	ND
14	A	1013	CLA	ND
14	A	1101	CLA	ND
14	A	1102	CLA	ND
14	A	1103	CLA	ND
14	A	1104	CLA	ND
14	A	1105	CLA	ND
14	A	1106	CLA	ND
14	A	1107	CLA	ND
14	A	1108	CLA	ND
14	A	1109	CLA	ND
14	A	1110	CLA	ND
14	A	1111	CLA	ND
14	A	1112	CLA	ND
14	A	1113	CLA	ND
14	A	1114	CLA	ND
14	A	1115	CLA	ND
14	A	1116	CLA	ND
14	A	1117	CLA	ND
14	A	1118	CLA	ND
14	A	1119	CLA	ND
14	A	1120	CLA	ND
14	A	1122	CLA	ND
14	A	1123	CLA	ND

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Mol	Chain	Res	Type	Atom
14	A	1124	CLA	ND
14	A	1125	CLA	ND
14	A	1126	CLA	ND
14	A	1127	CLA	ND
14	A	1128	CLA	ND
14	A	1129	CLA	ND
14	A	1130	CLA	ND
14	A	1131	CLA	ND
14	A	1132	CLA	ND
14	A	1133	CLA	ND
14	A	1134	CLA	ND
14	A	1135	CLA	ND
14	A	1136	CLA	ND
14	A	1137	CLA	ND
14	A	1138	CLA	ND
14	A	1139	CLA	ND
14	A	1140	CLA	ND
14	B	1021	CLA	ND
14	B	1022	CLA	ND
14	B	1023	CLA	ND
14	B	1201	CLA	ND
14	B	1202	CLA	ND
14	B	1203	CLA	ND
14	B	1204	CLA	ND
14	B	1205	CLA	ND
14	B	1206	CLA	ND
14	B	1208	CLA	ND
14	B	1209	CLA	ND
14	B	1210	CLA	ND
14	B	1211	CLA	ND
14	B	1212	CLA	ND
14	B	1213	CLA	ND
14	B	1214	CLA	ND
14	B	1215	CLA	ND
14	B	1216	CLA	ND
14	B	1217	CLA	ND
14	B	1218	CLA	ND
14	B	1219	CLA	ND
14	B	1220	CLA	ND
14	B	1221	CLA	ND
14	B	1222	CLA	ND
14	B	1223	CLA	ND

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Mol	Chain	Res	Type	Atom
14	B	1224	CLA	ND
14	B	1225	CLA	ND
14	B	1226	CLA	ND
14	B	1227	CLA	ND
14	B	1228	CLA	ND
14	B	1229	CLA	ND
14	B	1231	CLA	ND
14	B	1232	CLA	ND
14	B	1233	CLA	ND
14	B	1234	CLA	ND
14	B	1235	CLA	ND
14	B	1236	CLA	ND
14	B	1239	CLA	ND
14	K	1401	CLA	ND
14	L	1501	CLA	ND
14	L	1502	CLA	ND
14	L	1503	CLA	ND
14	X	1701	CLA	ND
15	G	1121	F6C	NA
15	H	1207	F6C	NA
15	H	1230	F6C	NA
15	H	1237	F6C	NA
15	H	1238	F6C	NA
15	a	1121	F6C	NA
15	b	1207	F6C	NA
15	b	1230	F6C	NA
15	b	1237	F6C	NA
15	b	1238	F6C	NA
15	A	1121	F6C	NA
15	B	1207	F6C	NA
15	B	1230	F6C	NA
15	B	1237	F6C	NA
15	B	1238	F6C	NA

All (4356) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	1013	CLA	C1A-C2A-CAA-CBA
14	G	1013	CLA	C3A-C2A-CAA-CBA
14	G	1013	CLA	C11-C10-C8-C9
14	G	1101	CLA	CHA-CBD-CGD-O1D
14	G	1101	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	G	1102	CLA	C1A-C2A-CAA-CBA
14	G	1102	CLA	CBA-CGA-O2A-C1
14	G	1102	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	CAD-CBD-CGD-O1D
14	G	1103	CLA	CAD-CBD-CGD-O2D
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	1107	CLA	CBD-CGD-O2D-CED
14	G	1108	CLA	CBD-CGD-O2D-CED
14	G	1109	CLA	C1A-C2A-CAA-CBA
14	G	1109	CLA	C3A-C2A-CAA-CBA
14	G	1111	CLA	CBA-CGA-O2A-C1
14	G	1111	CLA	O1A-CGA-O2A-C1
14	G	1112	CLA	C1A-C2A-CAA-CBA
14	G	1112	CLA	C2-C1-O2A-CGA
14	G	1114	CLA	C1A-C2A-CAA-CBA
14	G	1114	CLA	C3A-C2A-CAA-CBA
14	G	1114	CLA	CHA-CBD-CGD-O1D
14	G	1114	CLA	CHA-CBD-CGD-O2D
14	G	1115	CLA	C1A-C2A-CAA-CBA
14	G	1115	CLA	C3A-C2A-CAA-CBA
14	G	1115	CLA	CHA-CBD-CGD-O1D
14	G	1115	CLA	CHA-CBD-CGD-O2D
14	G	1116	CLA	C3A-C2A-CAA-CBA
14	G	1117	CLA	C1A-C2A-CAA-CBA
14	G	1117	CLA	C3A-C2A-CAA-CBA
14	G	1117	CLA	CBD-CGD-O2D-CED
14	G	1118	CLA	C2-C1-O2A-CGA
14	G	1119	CLA	CBD-CGD-O2D-CED
14	G	1120	CLA	C1A-C2A-CAA-CBA
14	G	1120	CLA	C3A-C2A-CAA-CBA
14	G	1120	CLA	CHA-CBD-CGD-O1D
14	G	1120	CLA	CHA-CBD-CGD-O2D
14	G	1122	CLA	C4-C3-C5-C6
14	G	1124	CLA	C1A-C2A-CAA-CBA
14	G	1125	CLA	C1A-C2A-CAA-CBA
14	G	1127	CLA	C1A-C2A-CAA-CBA
14	G	1128	CLA	CHA-CBD-CGD-O1D
14	G	1128	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	G	1130	CLA	C1A-C2A-CAA-CBA
14	G	1131	CLA	C2-C1-O2A-CGA
14	G	1131	CLA	C2B-C3B-CAB-CBB
14	G	1131	CLA	C4B-C3B-CAB-CBB
14	G	1132	CLA	CHA-CBD-CGD-O1D
14	G	1132	CLA	CHA-CBD-CGD-O2D
14	G	1132	CLA	CBD-CGD-O2D-CED
14	G	1133	CLA	O1A-CGA-O2A-C1
14	G	1135	CLA	C3A-C2A-CAA-CBA
14	G	1135	CLA	CHA-CBD-CGD-O2D
14	G	1137	CLA	C2-C1-O2A-CGA
14	G	1138	CLA	C1A-C2A-CAA-CBA
14	G	1140	CLA	C1A-C2A-CAA-CBA
14	G	1140	CLA	C3A-C2A-CAA-CBA
14	G	1140	CLA	C6-C7-C8-C9
14	H	1201	CLA	CHA-CBD-CGD-O1D
14	H	1201	CLA	CHA-CBD-CGD-O2D
14	H	1202	CLA	CHA-CBD-CGD-O1D
14	H	1202	CLA	CHA-CBD-CGD-O2D
14	H	1203	CLA	C1A-C2A-CAA-CBA
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	1209	CLA	C1A-C2A-CAA-CBA
14	H	1210	CLA	C1A-C2A-CAA-CBA
14	H	1210	CLA	C2-C1-O2A-CGA
14	H	1211	CLA	C2-C1-O2A-CGA
14	H	1213	CLA	CHA-CBD-CGD-O1D
14	H	1213	CLA	CHA-CBD-CGD-O2D
14	H	1213	CLA	C6-C7-C8-C9
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	1216	CLA	C1A-C2A-CAA-CBA
14	H	1216	CLA	C3A-C2A-CAA-CBA
14	H	1217	CLA	C1A-C2A-CAA-CBA
14	H	1217	CLA	C3A-C2A-CAA-CBA
14	H	1217	CLA	CBD-CGD-O2D-CED
14	H	1218	CLA	CHA-CBD-CGD-O1D
14	H	1218	CLA	CHA-CBD-CGD-O2D
14	H	1221	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	H	1222	CLA	CHA-CBD-CGD-O1D
14	H	1222	CLA	CHA-CBD-CGD-O2D
14	H	1225	CLA	C1A-C2A-CAA-CBA
14	H	1225	CLA	C3A-C2A-CAA-CBA
14	H	1226	CLA	C2-C1-O2A-CGA
14	H	1227	CLA	C3A-C2A-CAA-CBA
14	H	1228	CLA	C1A-C2A-CAA-CBA
14	H	1229	CLA	C2-C1-O2A-CGA
14	H	1234	CLA	C2B-C3B-CAB-CBB
14	H	1234	CLA	C4B-C3B-CAB-CBB
14	T	1401	CLA	C1A-C2A-CAA-CBA
14	T	1401	CLA	C3A-C2A-CAA-CBA
14	T	1401	CLA	CHA-CBD-CGD-O1D
14	T	1401	CLA	CHA-CBD-CGD-O2D
14	U	1502	CLA	C2B-C3B-CAB-CBB
14	U	1502	CLA	C4B-C3B-CAB-CBB
14	U	1503	CLA	C1A-C2A-CAA-CBA
14	U	1503	CLA	CBA-CGA-O2A-C1
14	U	1503	CLA	O1A-CGA-O2A-C1
14	U	1503	CLA	C4-C3-C5-C6
14	a	1013	CLA	C1A-C2A-CAA-CBA
14	a	1013	CLA	C3A-C2A-CAA-CBA
14	a	1013	CLA	C11-C10-C8-C9
14	a	1101	CLA	CHA-CBD-CGD-O1D
14	a	1101	CLA	CHA-CBD-CGD-O2D
14	a	1102	CLA	C1A-C2A-CAA-CBA
14	a	1102	CLA	CBA-CGA-O2A-C1
14	a	1102	CLA	O1A-CGA-O2A-C1
14	a	1103	CLA	CAD-CBD-CGD-O1D
14	a	1103	CLA	CAD-CBD-CGD-O2D
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	1107	CLA	CBD-CGD-O2D-CED
14	a	1108	CLA	CBD-CGD-O2D-CED
14	a	1109	CLA	C1A-C2A-CAA-CBA
14	a	1109	CLA	C3A-C2A-CAA-CBA
14	a	1111	CLA	CBA-CGA-O2A-C1
14	a	1111	CLA	O1A-CGA-O2A-C1
14	a	1112	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	a	1112	CLA	C2-C1-O2A-CGA
14	a	1114	CLA	C1A-C2A-CAA-CBA
14	a	1114	CLA	C3A-C2A-CAA-CBA
14	a	1114	CLA	CHA-CBD-CGD-O1D
14	a	1114	CLA	CHA-CBD-CGD-O2D
14	a	1115	CLA	C1A-C2A-CAA-CBA
14	a	1115	CLA	C3A-C2A-CAA-CBA
14	a	1115	CLA	CHA-CBD-CGD-O1D
14	a	1115	CLA	CHA-CBD-CGD-O2D
14	a	1116	CLA	C3A-C2A-CAA-CBA
14	a	1117	CLA	C1A-C2A-CAA-CBA
14	a	1117	CLA	C3A-C2A-CAA-CBA
14	a	1117	CLA	CBD-CGD-O2D-CED
14	a	1118	CLA	C2-C1-O2A-CGA
14	a	1119	CLA	CBD-CGD-O2D-CED
14	a	1120	CLA	C1A-C2A-CAA-CBA
14	a	1120	CLA	C3A-C2A-CAA-CBA
14	a	1120	CLA	CHA-CBD-CGD-O1D
14	a	1120	CLA	CHA-CBD-CGD-O2D
14	a	1122	CLA	C4-C3-C5-C6
14	a	1124	CLA	C1A-C2A-CAA-CBA
14	a	1125	CLA	C1A-C2A-CAA-CBA
14	a	1127	CLA	C1A-C2A-CAA-CBA
14	a	1128	CLA	CHA-CBD-CGD-O1D
14	a	1128	CLA	CHA-CBD-CGD-O2D
14	a	1130	CLA	C1A-C2A-CAA-CBA
14	a	1131	CLA	C2-C1-O2A-CGA
14	a	1131	CLA	C2B-C3B-CAB-CBB
14	a	1131	CLA	C4B-C3B-CAB-CBB
14	a	1132	CLA	CHA-CBD-CGD-O1D
14	a	1132	CLA	CHA-CBD-CGD-O2D
14	a	1132	CLA	CBD-CGD-O2D-CED
14	a	1133	CLA	O1A-CGA-O2A-C1
14	a	1135	CLA	C3A-C2A-CAA-CBA
14	a	1135	CLA	CHA-CBD-CGD-O2D
14	a	1137	CLA	C2-C1-O2A-CGA
14	a	1138	CLA	C1A-C2A-CAA-CBA
14	a	1140	CLA	C1A-C2A-CAA-CBA
14	a	1140	CLA	C3A-C2A-CAA-CBA
14	a	1140	CLA	C6-C7-C8-C9
14	b	1201	CLA	CHA-CBD-CGD-O1D
14	b	1201	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	b	1202	CLA	CHA-CBD-CGD-O1D
14	b	1202	CLA	CHA-CBD-CGD-O2D
14	b	1203	CLA	C1A-C2A-CAA-CBA
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	1209	CLA	C1A-C2A-CAA-CBA
14	b	1210	CLA	C1A-C2A-CAA-CBA
14	b	1210	CLA	C2-C1-O2A-CGA
14	b	1211	CLA	C2-C1-O2A-CGA
14	b	1213	CLA	CHA-CBD-CGD-O1D
14	b	1213	CLA	CHA-CBD-CGD-O2D
14	b	1213	CLA	C6-C7-C8-C9
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	1216	CLA	C1A-C2A-CAA-CBA
14	b	1216	CLA	C3A-C2A-CAA-CBA
14	b	1217	CLA	C1A-C2A-CAA-CBA
14	b	1217	CLA	C3A-C2A-CAA-CBA
14	b	1217	CLA	CBD-CGD-O2D-CED
14	b	1218	CLA	CHA-CBD-CGD-O1D
14	b	1218	CLA	CHA-CBD-CGD-O2D
14	b	1221	CLA	C1A-C2A-CAA-CBA
14	b	1222	CLA	CHA-CBD-CGD-O1D
14	b	1222	CLA	CHA-CBD-CGD-O2D
14	b	1225	CLA	C1A-C2A-CAA-CBA
14	b	1225	CLA	C3A-C2A-CAA-CBA
14	b	1226	CLA	C2-C1-O2A-CGA
14	b	1227	CLA	C3A-C2A-CAA-CBA
14	b	1228	CLA	C1A-C2A-CAA-CBA
14	b	1229	CLA	C2-C1-O2A-CGA
14	b	1234	CLA	C2B-C3B-CAB-CBB
14	b	1234	CLA	C4B-C3B-CAB-CBB
14	k	1401	CLA	C1A-C2A-CAA-CBA
14	k	1401	CLA	C3A-C2A-CAA-CBA
14	k	1401	CLA	CHA-CBD-CGD-O1D
14	k	1401	CLA	CHA-CBD-CGD-O2D
14	l	1502	CLA	C2B-C3B-CAB-CBB
14	l	1502	CLA	C4B-C3B-CAB-CBB
14	l	1503	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	l	1503	CLA	CBA-CGA-O2A-C1
14	l	1503	CLA	O1A-CGA-O2A-C1
14	l	1503	CLA	C4-C3-C5-C6
14	A	1013	CLA	C1A-C2A-CAA-CBA
14	A	1013	CLA	C3A-C2A-CAA-CBA
14	A	1013	CLA	C11-C10-C8-C9
14	A	1101	CLA	CHA-CBD-CGD-O1D
14	A	1101	CLA	CHA-CBD-CGD-O2D
14	A	1102	CLA	C1A-C2A-CAA-CBA
14	A	1102	CLA	CBA-CGA-O2A-C1
14	A	1102	CLA	O1A-CGA-O2A-C1
14	A	1103	CLA	CAD-CBD-CGD-O1D
14	A	1103	CLA	CAD-CBD-CGD-O2D
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	1107	CLA	CBD-CGD-O2D-CED
14	A	1108	CLA	CBD-CGD-O2D-CED
14	A	1109	CLA	C1A-C2A-CAA-CBA
14	A	1109	CLA	C3A-C2A-CAA-CBA
14	A	1111	CLA	CBA-CGA-O2A-C1
14	A	1111	CLA	O1A-CGA-O2A-C1
14	A	1112	CLA	C1A-C2A-CAA-CBA
14	A	1112	CLA	C2-C1-O2A-CGA
14	A	1114	CLA	C1A-C2A-CAA-CBA
14	A	1114	CLA	C3A-C2A-CAA-CBA
14	A	1114	CLA	CHA-CBD-CGD-O1D
14	A	1114	CLA	CHA-CBD-CGD-O2D
14	A	1115	CLA	C1A-C2A-CAA-CBA
14	A	1115	CLA	C3A-C2A-CAA-CBA
14	A	1115	CLA	CHA-CBD-CGD-O1D
14	A	1115	CLA	CHA-CBD-CGD-O2D
14	A	1116	CLA	C3A-C2A-CAA-CBA
14	A	1117	CLA	C1A-C2A-CAA-CBA
14	A	1117	CLA	C3A-C2A-CAA-CBA
14	A	1117	CLA	CBD-CGD-O2D-CED
14	A	1118	CLA	C2-C1-O2A-CGA
14	A	1119	CLA	CBD-CGD-O2D-CED
14	A	1120	CLA	C1A-C2A-CAA-CBA
14	A	1120	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	A	1120	CLA	CHA-CBD-CGD-O1D
14	A	1120	CLA	CHA-CBD-CGD-O2D
14	A	1122	CLA	C4-C3-C5-C6
14	A	1124	CLA	C1A-C2A-CAA-CBA
14	A	1125	CLA	C1A-C2A-CAA-CBA
14	A	1127	CLA	C1A-C2A-CAA-CBA
14	A	1128	CLA	CHA-CBD-CGD-O1D
14	A	1128	CLA	CHA-CBD-CGD-O2D
14	A	1130	CLA	C1A-C2A-CAA-CBA
14	A	1131	CLA	C2-C1-O2A-CGA
14	A	1131	CLA	C2B-C3B-CAB-CBB
14	A	1131	CLA	C4B-C3B-CAB-CBB
14	A	1132	CLA	CHA-CBD-CGD-O1D
14	A	1132	CLA	CHA-CBD-CGD-O2D
14	A	1132	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	O1A-CGA-O2A-C1
14	A	1135	CLA	C3A-C2A-CAA-CBA
14	A	1135	CLA	CHA-CBD-CGD-O2D
14	A	1137	CLA	C2-C1-O2A-CGA
14	A	1138	CLA	C1A-C2A-CAA-CBA
14	A	1140	CLA	C1A-C2A-CAA-CBA
14	A	1140	CLA	C3A-C2A-CAA-CBA
14	A	1140	CLA	C6-C7-C8-C9
14	B	1201	CLA	CHA-CBD-CGD-O1D
14	B	1201	CLA	CHA-CBD-CGD-O2D
14	B	1202	CLA	CHA-CBD-CGD-O1D
14	B	1202	CLA	CHA-CBD-CGD-O2D
14	B	1203	CLA	C1A-C2A-CAA-CBA
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	1209	CLA	C1A-C2A-CAA-CBA
14	B	1210	CLA	C1A-C2A-CAA-CBA
14	B	1210	CLA	C2-C1-O2A-CGA
14	B	1211	CLA	C2-C1-O2A-CGA
14	B	1213	CLA	CHA-CBD-CGD-O1D
14	B	1213	CLA	CHA-CBD-CGD-O2D
14	B	1213	CLA	C6-C7-C8-C9
14	B	1214	CLA	C2B-C3B-CAB-CBB
14	B	1214	CLA	C4B-C3B-CAB-CBB
14	B	1215	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	B	1216	CLA	C1A-C2A-CAA-CBA
14	B	1216	CLA	C3A-C2A-CAA-CBA
14	B	1217	CLA	C1A-C2A-CAA-CBA
14	B	1217	CLA	C3A-C2A-CAA-CBA
14	B	1217	CLA	CBD-CGD-O2D-CED
14	B	1218	CLA	CHA-CBD-CGD-O1D
14	B	1218	CLA	CHA-CBD-CGD-O2D
14	B	1221	CLA	C1A-C2A-CAA-CBA
14	B	1222	CLA	CHA-CBD-CGD-O1D
14	B	1222	CLA	CHA-CBD-CGD-O2D
14	B	1225	CLA	C1A-C2A-CAA-CBA
14	B	1225	CLA	C3A-C2A-CAA-CBA
14	B	1226	CLA	C2-C1-O2A-CGA
14	B	1227	CLA	C3A-C2A-CAA-CBA
14	B	1228	CLA	C1A-C2A-CAA-CBA
14	B	1229	CLA	C2-C1-O2A-CGA
14	B	1234	CLA	C2B-C3B-CAB-CBB
14	B	1234	CLA	C4B-C3B-CAB-CBB
14	K	1401	CLA	C1A-C2A-CAA-CBA
14	K	1401	CLA	C3A-C2A-CAA-CBA
14	K	1401	CLA	CHA-CBD-CGD-O1D
14	K	1401	CLA	CHA-CBD-CGD-O2D
14	L	1502	CLA	C2B-C3B-CAB-CBB
14	L	1502	CLA	C4B-C3B-CAB-CBB
14	L	1503	CLA	C1A-C2A-CAA-CBA
14	L	1503	CLA	CBA-CGA-O2A-C1
14	L	1503	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	C4-C3-C5-C6
15	G	1121	F6C	C1A-C2A-CAA-CBA
15	G	1121	F6C	C3A-C2A-CAA-CBA
15	G	1121	F6C	CBD-CGD-O2D-CED
15	H	1207	F6C	CAD-CBD-CGD-O1D
15	H	1207	F6C	CAD-CBD-CGD-O2D
15	H	1207	F6C	C1B-C2B-CMB-OMB
15	H	1207	F6C	C3B-C2B-CMB-OMB
15	H	1230	F6C	CHA-CBD-CGD-O1D
15	H	1230	F6C	CHA-CBD-CGD-O2D
15	H	1230	F6C	C1B-C2B-CMB-OMB
15	H	1230	F6C	C3B-C2B-CMB-OMB
15	H	1237	F6C	CBA-CGA-O2A-C1
15	H	1237	F6C	O1A-CGA-O2A-C1
15	H	1237	F6C	C1B-C2B-CMB-OMB

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

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Mol	Chain	Res	Type	Atoms
18	G	4001	BCR	C17-C18-C19-C20
18	G	4001	BCR	C21-C22-C23-C24
18	G	4002	BCR	C1-C6-C7-C8
18	G	4002	BCR	C5-C6-C7-C8
18	G	4003	BCR	C7-C8-C9-C10
18	G	4003	BCR	C11-C10-C9-C8
18	G	4003	BCR	C11-C10-C9-C34
18	G	4003	BCR	C10-C11-C12-C13
18	G	4003	BCR	C21-C22-C23-C24
18	G	4003	BCR	C37-C22-C23-C24
18	G	4007	BCR	C11-C10-C9-C8
18	G	4007	BCR	C11-C10-C9-C34
18	G	4007	BCR	C17-C18-C19-C20
18	G	4007	BCR	C21-C22-C23-C24
18	G	4007	BCR	C37-C22-C23-C24
18	G	4008	BCR	C7-C8-C9-C10
18	G	4008	BCR	C7-C8-C9-C34
18	G	4008	BCR	C11-C10-C9-C8
18	G	4008	BCR	C11-C10-C9-C34
18	G	4008	BCR	C10-C11-C12-C13
18	G	4008	BCR	C17-C18-C19-C20
18	G	4011	BCR	C7-C8-C9-C10
18	G	4011	BCR	C10-C11-C12-C13
18	G	4011	BCR	C11-C12-C13-C14
18	G	4011	BCR	C11-C12-C13-C35
18	G	4011	BCR	C23-C24-C25-C26
18	G	4011	BCR	C23-C24-C25-C30
18	H	4004	BCR	C7-C8-C9-C10
18	H	4004	BCR	C7-C8-C9-C34
18	H	4004	BCR	C11-C10-C9-C8
18	H	4004	BCR	C11-C10-C9-C34
18	H	4005	BCR	C11-C10-C9-C8
18	H	4005	BCR	C11-C10-C9-C34
18	H	4006	BCR	C5-C6-C7-C8
18	H	4009	BCR	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	4013	BCR	C11-C10-C9-C8
18	H	4013	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
18	H	4013	BCR	C11-C12-C13-C14
18	H	4013	BCR	C17-C18-C19-C20
18	H	4013	BCR	C36-C18-C19-C20
18	H	4013	BCR	C19-C20-C21-C22
18	H	4013	BCR	C23-C24-C25-C26
18	H	4014	BCR	C7-C8-C9-C10
18	H	4014	BCR	C11-C10-C9-C8
18	H	4014	BCR	C11-C10-C9-C34
18	H	4014	BCR	C17-C18-C19-C20
18	H	4016	BCR	C15-C16-C17-C18
18	H	4016	BCR	C36-C18-C19-C20
18	H	4017	BCR	C7-C8-C9-C10
18	H	4017	BCR	C7-C8-C9-C34
18	H	4017	BCR	C11-C10-C9-C8
18	H	4017	BCR	C11-C10-C9-C34
18	H	4017	BCR	C9-C10-C11-C12
18	H	4017	BCR	C10-C11-C12-C13
18	H	4017	BCR	C18-C19-C20-C21
18	H	4017	BCR	C21-C22-C23-C24
18	R	4018	BCR	C7-C8-C9-C10
18	R	4018	BCR	C7-C8-C9-C34
18	R	4018	BCR	C15-C16-C17-C18
18	R	4020	BCR	C10-C11-C12-C13
18	R	4020	BCR	C19-C20-C21-C22
18	U	4019	BCR	C11-C10-C9-C8
18	U	4019	BCR	C11-C10-C9-C34
18	U	4019	BCR	C10-C11-C12-C13
18	U	4019	BCR	C17-C18-C19-C20
18	U	4019	BCR	C36-C18-C19-C20
18	U	4019	BCR	C21-C22-C23-C24
18	U	4022	BCR	C7-C8-C9-C34
18	U	4022	BCR	C11-C10-C9-C8
18	U	4022	BCR	C11-C10-C9-C34
18	U	4022	BCR	C10-C11-C12-C13
18	V	4021	BCR	C7-C8-C9-C34
18	V	4021	BCR	C11-C10-C9-C8
18	V	4021	BCR	C11-C10-C9-C34
18	V	4021	BCR	C10-C11-C12-C13
18	V	4021	BCR	C15-C16-C17-C18
18	V	4021	BCR	C17-C18-C19-C20
18	V	4021	BCR	C36-C18-C19-C20
18	V	4021	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
18	a	4001	BCR	C11-C10-C9-C8
18	a	4001	BCR	C11-C10-C9-C34
18	a	4001	BCR	C17-C18-C19-C20
18	a	4001	BCR	C21-C22-C23-C24
18	a	4002	BCR	C1-C6-C7-C8
18	a	4002	BCR	C5-C6-C7-C8
18	a	4003	BCR	C7-C8-C9-C10
18	a	4003	BCR	C11-C10-C9-C8
18	a	4003	BCR	C11-C10-C9-C34
18	a	4003	BCR	C10-C11-C12-C13
18	a	4003	BCR	C21-C22-C23-C24
18	a	4003	BCR	C37-C22-C23-C24
18	a	4007	BCR	C11-C10-C9-C8
18	a	4007	BCR	C11-C10-C9-C34
18	a	4007	BCR	C17-C18-C19-C20
18	a	4007	BCR	C21-C22-C23-C24
18	a	4007	BCR	C37-C22-C23-C24
18	a	4008	BCR	C7-C8-C9-C10
18	a	4008	BCR	C7-C8-C9-C34
18	a	4008	BCR	C11-C10-C9-C8
18	a	4008	BCR	C11-C10-C9-C34
18	a	4008	BCR	C10-C11-C12-C13
18	a	4008	BCR	C17-C18-C19-C20
18	a	4011	BCR	C7-C8-C9-C10
18	a	4011	BCR	C10-C11-C12-C13
18	a	4011	BCR	C11-C12-C13-C14
18	a	4011	BCR	C11-C12-C13-C35
18	a	4011	BCR	C23-C24-C25-C26
18	a	4011	BCR	C23-C24-C25-C30
18	b	4004	BCR	C7-C8-C9-C10
18	b	4004	BCR	C7-C8-C9-C34
18	b	4004	BCR	C11-C10-C9-C8
18	b	4004	BCR	C11-C10-C9-C34
18	b	4005	BCR	C11-C10-C9-C8
18	b	4005	BCR	C11-C10-C9-C34
18	b	4006	BCR	C5-C6-C7-C8
18	b	4009	BCR	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	4013	BCR	C11-C10-C9-C8
18	b	4013	BCR	C11-C10-C9-C34
18	b	4013	BCR	C11-C12-C13-C14
18	b	4013	BCR	C17-C18-C19-C20
18	b	4013	BCR	C36-C18-C19-C20
18	b	4013	BCR	C19-C20-C21-C22
18	b	4013	BCR	C23-C24-C25-C26
18	b	4014	BCR	C7-C8-C9-C10
18	b	4014	BCR	C11-C10-C9-C8
18	b	4014	BCR	C11-C10-C9-C34
18	b	4014	BCR	C17-C18-C19-C20
18	b	4016	BCR	C15-C16-C17-C18
18	b	4016	BCR	C36-C18-C19-C20
18	b	4017	BCR	C7-C8-C9-C10
18	b	4017	BCR	C7-C8-C9-C34
18	b	4017	BCR	C11-C10-C9-C8
18	b	4017	BCR	C11-C10-C9-C34
18	b	4017	BCR	C9-C10-C11-C12
18	b	4017	BCR	C10-C11-C12-C13
18	b	4017	BCR	C18-C19-C20-C21
18	b	4017	BCR	C21-C22-C23-C24
18	i	4018	BCR	C7-C8-C9-C10
18	i	4018	BCR	C7-C8-C9-C34
18	i	4018	BCR	C15-C16-C17-C18
18	i	4020	BCR	C10-C11-C12-C13
18	i	4020	BCR	C19-C20-C21-C22
18	l	4019	BCR	C11-C10-C9-C8
18	l	4019	BCR	C11-C10-C9-C34
18	l	4019	BCR	C10-C11-C12-C13
18	l	4019	BCR	C17-C18-C19-C20
18	l	4019	BCR	C36-C18-C19-C20
18	l	4019	BCR	C21-C22-C23-C24
18	l	4022	BCR	C7-C8-C9-C34
18	l	4022	BCR	C11-C10-C9-C8
18	l	4022	BCR	C11-C10-C9-C34
18	l	4022	BCR	C10-C11-C12-C13
18	m	4021	BCR	C7-C8-C9-C34
18	m	4021	BCR	C11-C10-C9-C8
18	m	4021	BCR	C11-C10-C9-C34
18	m	4021	BCR	C10-C11-C12-C13
18	m	4021	BCR	C15-C16-C17-C18
18	m	4021	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	m	4021	BCR	C36-C18-C19-C20
18	m	4021	BCR	C19-C20-C21-C22
18	A	4001	BCR	C11-C10-C9-C8
18	A	4001	BCR	C11-C10-C9-C34
18	A	4001	BCR	C17-C18-C19-C20
18	A	4001	BCR	C21-C22-C23-C24
18	A	4002	BCR	C1-C6-C7-C8
18	A	4002	BCR	C5-C6-C7-C8
18	A	4003	BCR	C7-C8-C9-C10
18	A	4003	BCR	C11-C10-C9-C8
18	A	4003	BCR	C11-C10-C9-C34
18	A	4003	BCR	C10-C11-C12-C13
18	A	4003	BCR	C21-C22-C23-C24
18	A	4003	BCR	C37-C22-C23-C24
18	A	4007	BCR	C11-C10-C9-C8
18	A	4007	BCR	C11-C10-C9-C34
18	A	4007	BCR	C17-C18-C19-C20
18	A	4007	BCR	C21-C22-C23-C24
18	A	4007	BCR	C37-C22-C23-C24
18	A	4008	BCR	C7-C8-C9-C10
18	A	4008	BCR	C7-C8-C9-C34
18	A	4008	BCR	C11-C10-C9-C8
18	A	4008	BCR	C11-C10-C9-C34
18	A	4008	BCR	C10-C11-C12-C13
18	A	4008	BCR	C17-C18-C19-C20
18	A	4011	BCR	C7-C8-C9-C10
18	A	4011	BCR	C10-C11-C12-C13
18	A	4011	BCR	C11-C12-C13-C14
18	A	4011	BCR	C11-C12-C13-C35
18	A	4011	BCR	C23-C24-C25-C26
18	A	4011	BCR	C23-C24-C25-C30
18	B	4004	BCR	C7-C8-C9-C10
18	B	4004	BCR	C7-C8-C9-C34
18	B	4004	BCR	C11-C10-C9-C8
18	B	4004	BCR	C11-C10-C9-C34
18	B	4005	BCR	C11-C10-C9-C8
18	B	4005	BCR	C11-C10-C9-C34
18	B	4006	BCR	C5-C6-C7-C8
18	B	4009	BCR	C11-C10-C9-C8
18	B	4009	BCR	C11-C10-C9-C34
18	B	4009	BCR	C10-C11-C12-C13
18	B	4010	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	B	4010	BCR	C11-C10-C9-C34
18	B	4010	BCR	C17-C18-C19-C20
18	B	4013	BCR	C11-C10-C9-C8
18	B	4013	BCR	C11-C10-C9-C34
18	B	4013	BCR	C11-C12-C13-C14
18	B	4013	BCR	C17-C18-C19-C20
18	B	4013	BCR	C36-C18-C19-C20
18	B	4013	BCR	C19-C20-C21-C22
18	B	4013	BCR	C23-C24-C25-C26
18	B	4014	BCR	C7-C8-C9-C10
18	B	4014	BCR	C11-C10-C9-C8
18	B	4014	BCR	C11-C10-C9-C34
18	B	4014	BCR	C17-C18-C19-C20
18	B	4016	BCR	C15-C16-C17-C18
18	B	4016	BCR	C36-C18-C19-C20
18	B	4017	BCR	C7-C8-C9-C10
18	B	4017	BCR	C7-C8-C9-C34
18	B	4017	BCR	C11-C10-C9-C8
18	B	4017	BCR	C11-C10-C9-C34
18	B	4017	BCR	C9-C10-C11-C12
18	B	4017	BCR	C10-C11-C12-C13
18	B	4017	BCR	C18-C19-C20-C21
18	B	4017	BCR	C21-C22-C23-C24
18	I	4018	BCR	C7-C8-C9-C10
18	I	4018	BCR	C7-C8-C9-C34
18	I	4018	BCR	C15-C16-C17-C18
18	I	4020	BCR	C10-C11-C12-C13
18	I	4020	BCR	C19-C20-C21-C22
18	L	4019	BCR	C11-C10-C9-C8
18	L	4019	BCR	C11-C10-C9-C34
18	L	4019	BCR	C10-C11-C12-C13
18	L	4019	BCR	C17-C18-C19-C20
18	L	4019	BCR	C36-C18-C19-C20
18	L	4019	BCR	C21-C22-C23-C24
18	L	4022	BCR	C7-C8-C9-C34
18	L	4022	BCR	C11-C10-C9-C8
18	L	4022	BCR	C11-C10-C9-C34
18	L	4022	BCR	C10-C11-C12-C13
18	M	4021	BCR	C7-C8-C9-C34
18	M	4021	BCR	C11-C10-C9-C8
18	M	4021	BCR	C11-C10-C9-C34
18	M	4021	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
18	M	4021	BCR	C15-C16-C17-C18
18	M	4021	BCR	C17-C18-C19-C20
18	M	4021	BCR	C36-C18-C19-C20
18	M	4021	BCR	C19-C20-C21-C22
19	G	5001	LHG	O1-C1-C2-C3
19	G	5001	LHG	C1-C2-C3-O3
19	G	5001	LHG	C3-O3-P-O6
19	G	5001	LHG	C4-O6-P-O3
19	H	5004	LHG	O1-C1-C2-C3
19	H	5004	LHG	C4-O6-P-O3
19	a	5001	LHG	O1-C1-C2-C3
19	a	5001	LHG	C1-C2-C3-O3
19	a	5001	LHG	C3-O3-P-O6
19	a	5001	LHG	C4-O6-P-O3
19	b	5004	LHG	O1-C1-C2-C3
19	b	5004	LHG	C4-O6-P-O3
19	A	5001	LHG	O1-C1-C2-C3
19	A	5001	LHG	C1-C2-C3-O3
19	A	5001	LHG	C3-O3-P-O6
19	A	5001	LHG	C4-O6-P-O3
19	B	5004	LHG	O1-C1-C2-C3
19	B	5004	LHG	C4-O6-P-O3
20	G	5005	LMG	O6-C1-O1-C7
20	H	5002	LMG	C2-C1-O1-C7
20	H	5002	LMG	O6-C1-O1-C7
20	H	5002	LMG	C11-C10-O7-C8
20	a	5005	LMG	O6-C1-O1-C7
20	b	5002	LMG	C2-C1-O1-C7
20	b	5002	LMG	O6-C1-O1-C7
20	b	5002	LMG	C11-C10-O7-C8
20	A	5005	LMG	O6-C1-O1-C7
20	B	5002	LMG	C2-C1-O1-C7
20	B	5002	LMG	O6-C1-O1-C7
20	B	5002	LMG	C11-C10-O7-C8
14	G	1138	CLA	O1D-CGD-O2D-CED
14	H	1217	CLA	O1D-CGD-O2D-CED
14	H	1232	CLA	O1D-CGD-O2D-CED
14	a	1138	CLA	O1D-CGD-O2D-CED
14	b	1217	CLA	O1D-CGD-O2D-CED
14	b	1232	CLA	O1D-CGD-O2D-CED
14	A	1138	CLA	O1D-CGD-O2D-CED
14	B	1217	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	1232	CLA	O1D-CGD-O2D-CED
14	H	1239	CLA	C2C-C3C-CAC-CBC
14	b	1239	CLA	C2C-C3C-CAC-CBC
14	B	1239	CLA	C2C-C3C-CAC-CBC
14	H	1021	CLA	O1D-CGD-O2D-CED
14	b	1021	CLA	O1D-CGD-O2D-CED
14	B	1021	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	CBD-CGD-O2D-CED
14	G	1115	CLA	CBD-CGD-O2D-CED
14	G	1116	CLA	CBD-CGD-O2D-CED
14	G	1122	CLA	CBD-CGD-O2D-CED
14	G	1126	CLA	CBD-CGD-O2D-CED
14	G	1130	CLA	CBD-CGD-O2D-CED
14	G	1131	CLA	CBD-CGD-O2D-CED
14	G	1133	CLA	CBD-CGD-O2D-CED
14	G	1134	CLA	CBD-CGD-O2D-CED
14	G	1138	CLA	CBD-CGD-O2D-CED
14	G	1139	CLA	CBD-CGD-O2D-CED
14	G	1140	CLA	CBD-CGD-O2D-CED
14	H	1021	CLA	CBD-CGD-O2D-CED
14	H	1206	CLA	CBD-CGD-O2D-CED
14	H	1208	CLA	CBD-CGD-O2D-CED
14	H	1211	CLA	CBD-CGD-O2D-CED
14	H	1215	CLA	CBD-CGD-O2D-CED
14	H	1216	CLA	CBD-CGD-O2D-CED
14	H	1219	CLA	CBD-CGD-O2D-CED
14	H	1220	CLA	CBD-CGD-O2D-CED
14	H	1224	CLA	CBD-CGD-O2D-CED
14	H	1226	CLA	CBD-CGD-O2D-CED
14	H	1228	CLA	CBD-CGD-O2D-CED
14	H	1229	CLA	CBD-CGD-O2D-CED
14	H	1232	CLA	CBD-CGD-O2D-CED
14	H	1233	CLA	CBD-CGD-O2D-CED
14	H	1234	CLA	CBD-CGD-O2D-CED
14	H	1239	CLA	CBD-CGD-O2D-CED
14	T	1401	CLA	CBD-CGD-O2D-CED
14	W	1701	CLA	CBD-CGD-O2D-CED
14	a	1109	CLA	CBD-CGD-O2D-CED
14	a	1115	CLA	CBD-CGD-O2D-CED
14	a	1116	CLA	CBD-CGD-O2D-CED
14	a	1122	CLA	CBD-CGD-O2D-CED
14	a	1126	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	1130	CLA	CBD-CGD-O2D-CED
14	a	1131	CLA	CBD-CGD-O2D-CED
14	a	1133	CLA	CBD-CGD-O2D-CED
14	a	1134	CLA	CBD-CGD-O2D-CED
14	a	1138	CLA	CBD-CGD-O2D-CED
14	a	1139	CLA	CBD-CGD-O2D-CED
14	a	1140	CLA	CBD-CGD-O2D-CED
14	b	1021	CLA	CBD-CGD-O2D-CED
14	b	1206	CLA	CBD-CGD-O2D-CED
14	b	1208	CLA	CBD-CGD-O2D-CED
14	b	1211	CLA	CBD-CGD-O2D-CED
14	b	1215	CLA	CBD-CGD-O2D-CED
14	b	1216	CLA	CBD-CGD-O2D-CED
14	b	1219	CLA	CBD-CGD-O2D-CED
14	b	1220	CLA	CBD-CGD-O2D-CED
14	b	1224	CLA	CBD-CGD-O2D-CED
14	b	1226	CLA	CBD-CGD-O2D-CED
14	b	1228	CLA	CBD-CGD-O2D-CED
14	b	1229	CLA	CBD-CGD-O2D-CED
14	b	1232	CLA	CBD-CGD-O2D-CED
14	b	1233	CLA	CBD-CGD-O2D-CED
14	b	1234	CLA	CBD-CGD-O2D-CED
14	b	1239	CLA	CBD-CGD-O2D-CED
14	k	1401	CLA	CBD-CGD-O2D-CED
14	l	1503	CLA	CBD-CGD-O2D-CED
14	x	1701	CLA	CBD-CGD-O2D-CED
14	A	1109	CLA	CBD-CGD-O2D-CED
14	A	1115	CLA	CBD-CGD-O2D-CED
14	A	1116	CLA	CBD-CGD-O2D-CED
14	A	1122	CLA	CBD-CGD-O2D-CED
14	A	1126	CLA	CBD-CGD-O2D-CED
14	A	1130	CLA	CBD-CGD-O2D-CED
14	A	1131	CLA	CBD-CGD-O2D-CED
14	A	1133	CLA	CBD-CGD-O2D-CED
14	A	1134	CLA	CBD-CGD-O2D-CED
14	A	1138	CLA	CBD-CGD-O2D-CED
14	A	1139	CLA	CBD-CGD-O2D-CED
14	A	1140	CLA	CBD-CGD-O2D-CED
14	B	1021	CLA	CBD-CGD-O2D-CED
14	B	1206	CLA	CBD-CGD-O2D-CED
14	B	1208	CLA	CBD-CGD-O2D-CED
14	B	1211	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	1215	CLA	CBD-CGD-O2D-CED
14	B	1216	CLA	CBD-CGD-O2D-CED
14	B	1219	CLA	CBD-CGD-O2D-CED
14	B	1220	CLA	CBD-CGD-O2D-CED
14	B	1224	CLA	CBD-CGD-O2D-CED
14	B	1226	CLA	CBD-CGD-O2D-CED
14	B	1228	CLA	CBD-CGD-O2D-CED
14	B	1229	CLA	CBD-CGD-O2D-CED
14	B	1232	CLA	CBD-CGD-O2D-CED
14	B	1233	CLA	CBD-CGD-O2D-CED
14	B	1234	CLA	CBD-CGD-O2D-CED
14	B	1239	CLA	CBD-CGD-O2D-CED
14	K	1401	CLA	CBD-CGD-O2D-CED
14	L	1503	CLA	CBD-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
15	H	1230	F6C	CBD-CGD-O2D-CED
15	H	1237	F6C	CBD-CGD-O2D-CED
15	b	1230	F6C	CBD-CGD-O2D-CED
15	b	1237	F6C	CBD-CGD-O2D-CED
15	B	1230	F6C	CBD-CGD-O2D-CED
15	B	1237	F6C	CBD-CGD-O2D-CED
21	G	6002	LMT	O5B-C1B-O1B-C4'
21	a	6002	LMT	O5B-C1B-O1B-C4'
21	A	6002	LMT	O5B-C1B-O1B-C4'
14	G	1122	CLA	O1A-CGA-O2A-C1
14	H	1235	CLA	O1A-CGA-O2A-C1
14	a	1122	CLA	O1A-CGA-O2A-C1
14	b	1235	CLA	O1A-CGA-O2A-C1
14	A	1122	CLA	O1A-CGA-O2A-C1
14	B	1235	CLA	O1A-CGA-O2A-C1
14	H	1239	CLA	C4C-C3C-CAC-CBC
14	b	1239	CLA	C4C-C3C-CAC-CBC
14	B	1239	CLA	C4C-C3C-CAC-CBC
14	H	1211	CLA	O1D-CGD-O2D-CED
14	H	1216	CLA	O1D-CGD-O2D-CED
14	H	1224	CLA	O1D-CGD-O2D-CED
14	W	1701	CLA	O1D-CGD-O2D-CED
14	b	1211	CLA	O1D-CGD-O2D-CED
14	b	1216	CLA	O1D-CGD-O2D-CED
14	b	1224	CLA	O1D-CGD-O2D-CED
14	x	1701	CLA	O1D-CGD-O2D-CED
14	B	1211	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	1216	CLA	O1D-CGD-O2D-CED
14	B	1224	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
14	G	1118	CLA	CBA-CGA-O2A-C1
14	G	1133	CLA	CBA-CGA-O2A-C1
14	a	1118	CLA	CBA-CGA-O2A-C1
14	a	1133	CLA	CBA-CGA-O2A-C1
14	A	1118	CLA	CBA-CGA-O2A-C1
14	A	1133	CLA	CBA-CGA-O2A-C1
14	G	1101	CLA	CBD-CGD-O2D-CED
14	G	1112	CLA	CBD-CGD-O2D-CED
14	H	1218	CLA	CBD-CGD-O2D-CED
14	H	1227	CLA	CBD-CGD-O2D-CED
14	U	1503	CLA	CBD-CGD-O2D-CED
14	a	1101	CLA	CBD-CGD-O2D-CED
14	a	1112	CLA	CBD-CGD-O2D-CED
14	b	1218	CLA	CBD-CGD-O2D-CED
14	b	1227	CLA	CBD-CGD-O2D-CED
14	A	1101	CLA	CBD-CGD-O2D-CED
14	A	1112	CLA	CBD-CGD-O2D-CED
14	B	1218	CLA	CBD-CGD-O2D-CED
14	B	1227	CLA	CBD-CGD-O2D-CED
14	G	1106	CLA	O1A-CGA-O2A-C1
14	G	1118	CLA	O1A-CGA-O2A-C1
14	G	1138	CLA	O1A-CGA-O2A-C1
14	H	1203	CLA	O1A-CGA-O2A-C1
14	H	1222	CLA	O1A-CGA-O2A-C1
14	H	1224	CLA	O1A-CGA-O2A-C1
14	a	1106	CLA	O1A-CGA-O2A-C1
14	a	1118	CLA	O1A-CGA-O2A-C1
14	a	1138	CLA	O1A-CGA-O2A-C1
14	b	1203	CLA	O1A-CGA-O2A-C1
14	b	1222	CLA	O1A-CGA-O2A-C1
14	b	1224	CLA	O1A-CGA-O2A-C1
14	A	1106	CLA	O1A-CGA-O2A-C1
14	A	1118	CLA	O1A-CGA-O2A-C1
14	A	1138	CLA	O1A-CGA-O2A-C1
14	B	1203	CLA	O1A-CGA-O2A-C1
14	B	1222	CLA	O1A-CGA-O2A-C1
14	B	1224	CLA	O1A-CGA-O2A-C1
20	G	5005	LMG	O10-C28-O8-C9
20	H	5002	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
20	R	5006	LMG	O10-C28-O8-C9
20	a	5005	LMG	O10-C28-O8-C9
20	b	5002	LMG	O10-C28-O8-C9
20	i	5006	LMG	O10-C28-O8-C9
20	A	5005	LMG	O10-C28-O8-C9
20	B	5002	LMG	O10-C28-O8-C9
20	I	5006	LMG	O10-C28-O8-C9
14	G	1108	CLA	O1D-CGD-O2D-CED
14	G	1119	CLA	O1D-CGD-O2D-CED
14	H	1234	CLA	O1D-CGD-O2D-CED
14	a	1108	CLA	O1D-CGD-O2D-CED
14	a	1119	CLA	O1D-CGD-O2D-CED
14	b	1234	CLA	O1D-CGD-O2D-CED
14	A	1108	CLA	O1D-CGD-O2D-CED
14	A	1119	CLA	O1D-CGD-O2D-CED
14	B	1234	CLA	O1D-CGD-O2D-CED
14	G	1107	CLA	O1D-CGD-O2D-CED
14	a	1107	CLA	O1D-CGD-O2D-CED
14	A	1107	CLA	O1D-CGD-O2D-CED
15	G	1121	F6C	O1D-CGD-O2D-CED
15	a	1121	F6C	O1D-CGD-O2D-CED
15	A	1121	F6C	O1D-CGD-O2D-CED
14	G	1012	CLA	CBD-CGD-O2D-CED
14	a	1012	CLA	CBD-CGD-O2D-CED
14	A	1012	CLA	CBD-CGD-O2D-CED
20	H	5002	LMG	O9-C10-O7-C8
20	b	5002	LMG	O9-C10-O7-C8
20	B	5002	LMG	O9-C10-O7-C8
14	G	1102	CLA	C3-C5-C6-C7
14	H	1202	CLA	C3-C5-C6-C7
14	H	1205	CLA	C3-C5-C6-C7
14	H	1208	CLA	C3-C5-C6-C7
14	H	1214	CLA	C3-C5-C6-C7
14	H	1217	CLA	C3-C5-C6-C7
14	H	1223	CLA	C3-C5-C6-C7
14	H	1228	CLA	C3-C5-C6-C7
14	H	1239	CLA	C3-C5-C6-C7
14	a	1102	CLA	C3-C5-C6-C7
14	b	1202	CLA	C3-C5-C6-C7
14	b	1205	CLA	C3-C5-C6-C7
14	b	1208	CLA	C3-C5-C6-C7
14	b	1214	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	b	1217	CLA	C3-C5-C6-C7
14	b	1223	CLA	C3-C5-C6-C7
14	b	1228	CLA	C3-C5-C6-C7
14	b	1239	CLA	C3-C5-C6-C7
14	A	1102	CLA	C3-C5-C6-C7
14	B	1202	CLA	C3-C5-C6-C7
14	B	1205	CLA	C3-C5-C6-C7
14	B	1208	CLA	C3-C5-C6-C7
14	B	1214	CLA	C3-C5-C6-C7
14	B	1217	CLA	C3-C5-C6-C7
14	B	1223	CLA	C3-C5-C6-C7
14	B	1228	CLA	C3-C5-C6-C7
14	B	1239	CLA	C3-C5-C6-C7
15	H	1238	F6C	C3-C5-C6-C7
15	b	1238	F6C	C3-C5-C6-C7
15	B	1238	F6C	C3-C5-C6-C7
14	G	1106	CLA	CBA-CGA-O2A-C1
14	G	1117	CLA	CBA-CGA-O2A-C1
14	G	1122	CLA	CBA-CGA-O2A-C1
14	G	1137	CLA	CBA-CGA-O2A-C1
14	H	1222	CLA	CBA-CGA-O2A-C1
14	H	1226	CLA	CBA-CGA-O2A-C1
14	H	1235	CLA	CBA-CGA-O2A-C1
14	H	1239	CLA	CBA-CGA-O2A-C1
14	a	1106	CLA	CBA-CGA-O2A-C1
14	a	1117	CLA	CBA-CGA-O2A-C1
14	a	1122	CLA	CBA-CGA-O2A-C1
14	a	1137	CLA	CBA-CGA-O2A-C1
14	b	1222	CLA	CBA-CGA-O2A-C1
14	b	1226	CLA	CBA-CGA-O2A-C1
14	b	1235	CLA	CBA-CGA-O2A-C1
14	b	1239	CLA	CBA-CGA-O2A-C1
14	A	1106	CLA	CBA-CGA-O2A-C1
14	A	1117	CLA	CBA-CGA-O2A-C1
14	A	1122	CLA	CBA-CGA-O2A-C1
14	A	1137	CLA	CBA-CGA-O2A-C1
14	B	1222	CLA	CBA-CGA-O2A-C1
14	B	1226	CLA	CBA-CGA-O2A-C1
14	B	1235	CLA	CBA-CGA-O2A-C1
14	B	1239	CLA	CBA-CGA-O2A-C1
20	G	5005	LMG	C29-C28-O8-C9
20	H	5002	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
20	R	5006	LMG	C29-C28-O8-C9
20	a	5005	LMG	C29-C28-O8-C9
20	b	5002	LMG	C29-C28-O8-C9
20	i	5006	LMG	C29-C28-O8-C9
20	A	5005	LMG	C29-C28-O8-C9
20	B	5002	LMG	C29-C28-O8-C9
20	I	5006	LMG	C29-C28-O8-C9
14	G	1013	CLA	CBD-CGD-O2D-CED
14	G	1102	CLA	CBD-CGD-O2D-CED
14	G	1105	CLA	CBD-CGD-O2D-CED
14	G	1106	CLA	CBD-CGD-O2D-CED
14	G	1111	CLA	CBD-CGD-O2D-CED
14	G	1114	CLA	CBD-CGD-O2D-CED
14	G	1123	CLA	CBD-CGD-O2D-CED
14	G	1124	CLA	CBD-CGD-O2D-CED
14	H	1023	CLA	CBD-CGD-O2D-CED
14	H	1204	CLA	CBD-CGD-O2D-CED
14	H	1205	CLA	CBD-CGD-O2D-CED
14	H	1212	CLA	CBD-CGD-O2D-CED
14	H	1213	CLA	CBD-CGD-O2D-CED
14	H	1214	CLA	CBD-CGD-O2D-CED
14	H	1231	CLA	CBD-CGD-O2D-CED
14	U	1501	CLA	CBD-CGD-O2D-CED
14	a	1013	CLA	CBD-CGD-O2D-CED
14	a	1102	CLA	CBD-CGD-O2D-CED
14	a	1105	CLA	CBD-CGD-O2D-CED
14	a	1106	CLA	CBD-CGD-O2D-CED
14	a	1111	CLA	CBD-CGD-O2D-CED
14	a	1114	CLA	CBD-CGD-O2D-CED
14	a	1123	CLA	CBD-CGD-O2D-CED
14	a	1124	CLA	CBD-CGD-O2D-CED
14	b	1023	CLA	CBD-CGD-O2D-CED
14	b	1204	CLA	CBD-CGD-O2D-CED
14	b	1205	CLA	CBD-CGD-O2D-CED
14	b	1212	CLA	CBD-CGD-O2D-CED
14	b	1213	CLA	CBD-CGD-O2D-CED
14	b	1214	CLA	CBD-CGD-O2D-CED
14	b	1231	CLA	CBD-CGD-O2D-CED
14	l	1501	CLA	CBD-CGD-O2D-CED
14	A	1013	CLA	CBD-CGD-O2D-CED
14	A	1102	CLA	CBD-CGD-O2D-CED
14	A	1105	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	1106	CLA	CBD-CGD-O2D-CED
14	A	1111	CLA	CBD-CGD-O2D-CED
14	A	1114	CLA	CBD-CGD-O2D-CED
14	A	1123	CLA	CBD-CGD-O2D-CED
14	A	1124	CLA	CBD-CGD-O2D-CED
14	B	1023	CLA	CBD-CGD-O2D-CED
14	B	1204	CLA	CBD-CGD-O2D-CED
14	B	1205	CLA	CBD-CGD-O2D-CED
14	B	1212	CLA	CBD-CGD-O2D-CED
14	B	1213	CLA	CBD-CGD-O2D-CED
14	B	1214	CLA	CBD-CGD-O2D-CED
14	B	1231	CLA	CBD-CGD-O2D-CED
14	L	1501	CLA	CBD-CGD-O2D-CED
14	H	1023	CLA	C2C-C3C-CAC-CBC
14	b	1023	CLA	C2C-C3C-CAC-CBC
14	B	1023	CLA	C2C-C3C-CAC-CBC
14	G	1117	CLA	O1D-CGD-O2D-CED
14	G	1131	CLA	O1D-CGD-O2D-CED
14	G	1132	CLA	O1D-CGD-O2D-CED
14	H	1208	CLA	O1D-CGD-O2D-CED
14	H	1219	CLA	O1D-CGD-O2D-CED
14	a	1117	CLA	O1D-CGD-O2D-CED
14	a	1131	CLA	O1D-CGD-O2D-CED
14	a	1132	CLA	O1D-CGD-O2D-CED
14	b	1208	CLA	O1D-CGD-O2D-CED
14	b	1219	CLA	O1D-CGD-O2D-CED
14	A	1117	CLA	O1D-CGD-O2D-CED
14	A	1131	CLA	O1D-CGD-O2D-CED
14	A	1132	CLA	O1D-CGD-O2D-CED
14	B	1208	CLA	O1D-CGD-O2D-CED
14	B	1219	CLA	O1D-CGD-O2D-CED
14	H	1217	CLA	O1A-CGA-O2A-C1
14	b	1217	CLA	O1A-CGA-O2A-C1
14	B	1217	CLA	O1A-CGA-O2A-C1
14	G	1109	CLA	O1D-CGD-O2D-CED
14	G	1139	CLA	O1D-CGD-O2D-CED
14	G	1140	CLA	O1D-CGD-O2D-CED
14	a	1139	CLA	O1D-CGD-O2D-CED
14	a	1140	CLA	O1D-CGD-O2D-CED
14	A	1109	CLA	O1D-CGD-O2D-CED
14	A	1139	CLA	O1D-CGD-O2D-CED
14	A	1140	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	G	1128	CLA	C4-C3-C5-C6
14	H	1201	CLA	C4-C3-C5-C6
14	H	1213	CLA	C4-C3-C5-C6
14	H	1216	CLA	C4-C3-C5-C6
14	H	1229	CLA	C4-C3-C5-C6
14	W	1701	CLA	C4-C3-C5-C6
14	a	1128	CLA	C4-C3-C5-C6
14	b	1201	CLA	C4-C3-C5-C6
14	b	1213	CLA	C4-C3-C5-C6
14	b	1216	CLA	C4-C3-C5-C6
14	b	1229	CLA	C4-C3-C5-C6
14	x	1701	CLA	C4-C3-C5-C6
14	A	1128	CLA	C4-C3-C5-C6
14	B	1201	CLA	C4-C3-C5-C6
14	B	1213	CLA	C4-C3-C5-C6
14	B	1216	CLA	C4-C3-C5-C6
14	B	1229	CLA	C4-C3-C5-C6
14	X	1701	CLA	C4-C3-C5-C6
15	H	1237	F6C	C4-C3-C5-C6
15	b	1237	F6C	C4-C3-C5-C6
15	B	1237	F6C	C4-C3-C5-C6
14	G	1122	CLA	C2-C3-C5-C6
14	G	1128	CLA	C2-C3-C5-C6
14	H	1213	CLA	C2-C3-C5-C6
14	H	1216	CLA	C2-C3-C5-C6
14	H	1229	CLA	C2-C3-C5-C6
14	U	1503	CLA	C2-C3-C5-C6
14	a	1122	CLA	C2-C3-C5-C6
14	a	1128	CLA	C2-C3-C5-C6
14	b	1213	CLA	C2-C3-C5-C6
14	b	1216	CLA	C2-C3-C5-C6
14	b	1229	CLA	C2-C3-C5-C6
14	l	1503	CLA	C2-C3-C5-C6
14	A	1122	CLA	C2-C3-C5-C6
14	A	1128	CLA	C2-C3-C5-C6
14	B	1213	CLA	C2-C3-C5-C6
14	B	1216	CLA	C2-C3-C5-C6
14	B	1229	CLA	C2-C3-C5-C6
14	L	1503	CLA	C2-C3-C5-C6
15	H	1237	F6C	C2-C3-C5-C6
15	b	1237	F6C	C2-C3-C5-C6
15	B	1237	F6C	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	G	1113	CLA	CBD-CGD-O2D-CED
14	a	1113	CLA	CBD-CGD-O2D-CED
14	A	1113	CLA	CBD-CGD-O2D-CED
14	G	1116	CLA	O1D-CGD-O2D-CED
14	G	1133	CLA	O1D-CGD-O2D-CED
14	H	1206	CLA	O1D-CGD-O2D-CED
14	H	1226	CLA	O1D-CGD-O2D-CED
14	H	1233	CLA	O1D-CGD-O2D-CED
14	a	1109	CLA	O1D-CGD-O2D-CED
14	a	1116	CLA	O1D-CGD-O2D-CED
14	a	1133	CLA	O1D-CGD-O2D-CED
14	b	1206	CLA	O1D-CGD-O2D-CED
14	b	1226	CLA	O1D-CGD-O2D-CED
14	b	1233	CLA	O1D-CGD-O2D-CED
14	A	1116	CLA	O1D-CGD-O2D-CED
14	A	1133	CLA	O1D-CGD-O2D-CED
14	B	1206	CLA	O1D-CGD-O2D-CED
14	B	1226	CLA	O1D-CGD-O2D-CED
14	B	1233	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	C2A-CAA-CBA-CGA
14	G	1127	CLA	C2A-CAA-CBA-CGA
14	H	1216	CLA	C2A-CAA-CBA-CGA
14	a	1109	CLA	C2A-CAA-CBA-CGA
14	a	1127	CLA	C2A-CAA-CBA-CGA
14	b	1216	CLA	C2A-CAA-CBA-CGA
14	A	1109	CLA	C2A-CAA-CBA-CGA
14	A	1127	CLA	C2A-CAA-CBA-CGA
14	B	1216	CLA	C2A-CAA-CBA-CGA
14	G	1115	CLA	C3-C5-C6-C7
14	H	1204	CLA	C3-C5-C6-C7
14	H	1220	CLA	C3-C5-C6-C7
14	a	1115	CLA	C3-C5-C6-C7
14	b	1204	CLA	C3-C5-C6-C7
14	b	1220	CLA	C3-C5-C6-C7
14	A	1115	CLA	C3-C5-C6-C7
14	B	1204	CLA	C3-C5-C6-C7
14	B	1220	CLA	C3-C5-C6-C7
14	G	1104	CLA	CBA-CGA-O2A-C1
14	G	1130	CLA	CBA-CGA-O2A-C1
14	G	1138	CLA	CBA-CGA-O2A-C1
14	H	1202	CLA	CBA-CGA-O2A-C1
14	H	1203	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	H	1208	CLA	CBA-CGA-O2A-C1
14	H	1214	CLA	CBA-CGA-O2A-C1
14	H	1224	CLA	CBA-CGA-O2A-C1
14	a	1104	CLA	CBA-CGA-O2A-C1
14	a	1130	CLA	CBA-CGA-O2A-C1
14	a	1138	CLA	CBA-CGA-O2A-C1
14	b	1202	CLA	CBA-CGA-O2A-C1
14	b	1203	CLA	CBA-CGA-O2A-C1
14	b	1208	CLA	CBA-CGA-O2A-C1
14	b	1214	CLA	CBA-CGA-O2A-C1
14	b	1224	CLA	CBA-CGA-O2A-C1
14	A	1104	CLA	CBA-CGA-O2A-C1
14	A	1130	CLA	CBA-CGA-O2A-C1
14	A	1138	CLA	CBA-CGA-O2A-C1
14	B	1202	CLA	CBA-CGA-O2A-C1
14	B	1203	CLA	CBA-CGA-O2A-C1
14	B	1208	CLA	CBA-CGA-O2A-C1
14	B	1214	CLA	CBA-CGA-O2A-C1
14	B	1224	CLA	CBA-CGA-O2A-C1
20	H	5002	LMG	C17-C18-C19-C20
14	G	1104	CLA	O1A-CGA-O2A-C1
14	G	1128	CLA	O1A-CGA-O2A-C1
14	G	1130	CLA	O1A-CGA-O2A-C1
14	G	1137	CLA	O1A-CGA-O2A-C1
14	H	1202	CLA	O1A-CGA-O2A-C1
14	H	1208	CLA	O1A-CGA-O2A-C1
14	H	1214	CLA	O1A-CGA-O2A-C1
14	H	1226	CLA	O1A-CGA-O2A-C1
14	H	1239	CLA	O1A-CGA-O2A-C1
14	a	1104	CLA	O1A-CGA-O2A-C1
14	a	1128	CLA	O1A-CGA-O2A-C1
14	a	1130	CLA	O1A-CGA-O2A-C1
14	a	1137	CLA	O1A-CGA-O2A-C1
14	b	1202	CLA	O1A-CGA-O2A-C1
14	b	1208	CLA	O1A-CGA-O2A-C1
14	b	1214	CLA	O1A-CGA-O2A-C1
14	b	1226	CLA	O1A-CGA-O2A-C1
14	b	1239	CLA	O1A-CGA-O2A-C1
14	A	1104	CLA	O1A-CGA-O2A-C1
14	A	1128	CLA	O1A-CGA-O2A-C1
14	A	1130	CLA	O1A-CGA-O2A-C1
14	A	1137	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1202	CLA	O1A-CGA-O2A-C1
14	B	1208	CLA	O1A-CGA-O2A-C1
14	B	1214	CLA	O1A-CGA-O2A-C1
14	B	1226	CLA	O1A-CGA-O2A-C1
14	B	1239	CLA	O1A-CGA-O2A-C1
15	H	1230	F6C	C1A-C2A-CAA-CBA
15	b	1230	F6C	C1A-C2A-CAA-CBA
15	B	1230	F6C	C1A-C2A-CAA-CBA
20	b	5002	LMG	C17-C18-C19-C20
20	B	5002	LMG	C17-C18-C19-C20
20	L	5007	LMG	C35-C36-C37-C38
14	G	1140	CLA	C8-C10-C11-C12
14	H	1021	CLA	C5-C6-C7-C8
14	a	1140	CLA	C8-C10-C11-C12
14	b	1021	CLA	C5-C6-C7-C8
14	A	1140	CLA	C8-C10-C11-C12
14	B	1021	CLA	C5-C6-C7-C8
20	U	5007	LMG	C35-C36-C37-C38
20	l	5007	LMG	C35-C36-C37-C38
14	G	1134	CLA	O1D-CGD-O2D-CED
14	T	1401	CLA	O1D-CGD-O2D-CED
14	a	1134	CLA	O1D-CGD-O2D-CED
14	k	1401	CLA	O1D-CGD-O2D-CED
14	A	1134	CLA	O1D-CGD-O2D-CED
14	K	1401	CLA	O1D-CGD-O2D-CED
14	G	1135	CLA	C3-C5-C6-C7
14	G	1136	CLA	C3-C5-C6-C7
14	H	1235	CLA	C3-C5-C6-C7
14	a	1135	CLA	C3-C5-C6-C7
14	a	1136	CLA	C3-C5-C6-C7
14	b	1235	CLA	C3-C5-C6-C7
14	A	1135	CLA	C3-C5-C6-C7
14	A	1136	CLA	C3-C5-C6-C7
14	B	1235	CLA	C3-C5-C6-C7
14	G	1125	CLA	CBD-CGD-O2D-CED
14	G	1135	CLA	CBD-CGD-O2D-CED
14	H	1235	CLA	CBD-CGD-O2D-CED
14	a	1125	CLA	CBD-CGD-O2D-CED
14	a	1135	CLA	CBD-CGD-O2D-CED
14	b	1235	CLA	CBD-CGD-O2D-CED
14	A	1125	CLA	CBD-CGD-O2D-CED
14	A	1135	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	1235	CLA	CBD-CGD-O2D-CED
20	G	5005	LMG	C35-C36-C37-C38
20	a	5005	LMG	C35-C36-C37-C38
20	A	5005	LMG	C35-C36-C37-C38
19	G	5001	LHG	O2-C2-C3-O3
19	a	5001	LHG	O2-C2-C3-O3
19	A	5001	LHG	O2-C2-C3-O3
14	G	1122	CLA	O1D-CGD-O2D-CED
14	G	1126	CLA	O1D-CGD-O2D-CED
14	H	1228	CLA	O1D-CGD-O2D-CED
14	a	1122	CLA	O1D-CGD-O2D-CED
14	b	1228	CLA	O1D-CGD-O2D-CED
14	A	1122	CLA	O1D-CGD-O2D-CED
14	B	1228	CLA	O1D-CGD-O2D-CED
15	H	1237	F6C	O1D-CGD-O2D-CED
15	b	1237	F6C	O1D-CGD-O2D-CED
15	B	1237	F6C	O1D-CGD-O2D-CED
14	G	1131	CLA	CBA-CGA-O2A-C1
14	H	1217	CLA	CBA-CGA-O2A-C1
14	H	1223	CLA	CBA-CGA-O2A-C1
14	a	1131	CLA	CBA-CGA-O2A-C1
14	b	1217	CLA	CBA-CGA-O2A-C1
14	b	1223	CLA	CBA-CGA-O2A-C1
14	A	1131	CLA	CBA-CGA-O2A-C1
14	B	1217	CLA	CBA-CGA-O2A-C1
14	B	1223	CLA	CBA-CGA-O2A-C1
14	G	1117	CLA	O1A-CGA-O2A-C1
14	a	1117	CLA	O1A-CGA-O2A-C1
14	A	1117	CLA	O1A-CGA-O2A-C1
14	a	1126	CLA	O1D-CGD-O2D-CED
14	A	1126	CLA	O1D-CGD-O2D-CED
14	B	1220	CLA	O1D-CGD-O2D-CED
14	G	1120	CLA	CBD-CGD-O2D-CED
14	H	1222	CLA	CBD-CGD-O2D-CED
14	a	1120	CLA	CBD-CGD-O2D-CED
14	b	1222	CLA	CBD-CGD-O2D-CED
14	A	1120	CLA	CBD-CGD-O2D-CED
14	B	1222	CLA	CBD-CGD-O2D-CED
14	H	1220	CLA	O1D-CGD-O2D-CED
14	b	1220	CLA	O1D-CGD-O2D-CED
14	G	1130	CLA	O1D-CGD-O2D-CED
14	a	1130	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	1130	CLA	O1D-CGD-O2D-CED
14	G	1138	CLA	C3-C5-C6-C7
14	a	1138	CLA	C3-C5-C6-C7
14	b	1226	CLA	C3-C5-C6-C7
14	A	1138	CLA	C3-C5-C6-C7
14	B	1226	CLA	C3-C5-C6-C7
16	H	2002	PQN	C13-C15-C16-C17
16	b	2002	PQN	C13-C15-C16-C17
16	B	2002	PQN	C13-C15-C16-C17
14	G	1104	CLA	CBD-CGD-O2D-CED
14	G	1118	CLA	CBD-CGD-O2D-CED
14	G	1136	CLA	CBD-CGD-O2D-CED
14	a	1104	CLA	CBD-CGD-O2D-CED
14	a	1118	CLA	CBD-CGD-O2D-CED
14	a	1136	CLA	CBD-CGD-O2D-CED
14	A	1104	CLA	CBD-CGD-O2D-CED
14	A	1118	CLA	CBD-CGD-O2D-CED
14	A	1136	CLA	CBD-CGD-O2D-CED
14	H	1215	CLA	O1D-CGD-O2D-CED
14	H	1229	CLA	O1D-CGD-O2D-CED
14	b	1215	CLA	O1D-CGD-O2D-CED
14	b	1229	CLA	O1D-CGD-O2D-CED
14	B	1215	CLA	O1D-CGD-O2D-CED
14	B	1229	CLA	O1D-CGD-O2D-CED
15	H	1230	F6C	O1D-CGD-O2D-CED
15	b	1230	F6C	O1D-CGD-O2D-CED
15	B	1230	F6C	O1D-CGD-O2D-CED
14	G	1128	CLA	CBA-CGA-O2A-C1
14	a	1128	CLA	CBA-CGA-O2A-C1
14	A	1128	CLA	CBA-CGA-O2A-C1
14	G	1103	CLA	C4-C3-C5-C6
14	G	1136	CLA	C4-C3-C5-C6
14	G	1140	CLA	C4-C3-C5-C6
14	H	1022	CLA	C4-C3-C5-C6
14	H	1203	CLA	C4-C3-C5-C6
14	H	1210	CLA	C4-C3-C5-C6
14	a	1103	CLA	C4-C3-C5-C6
14	a	1136	CLA	C4-C3-C5-C6
14	a	1140	CLA	C4-C3-C5-C6
14	b	1022	CLA	C4-C3-C5-C6
14	b	1203	CLA	C4-C3-C5-C6
14	b	1210	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	1103	CLA	C4-C3-C5-C6
14	A	1136	CLA	C4-C3-C5-C6
14	A	1140	CLA	C4-C3-C5-C6
14	B	1022	CLA	C4-C3-C5-C6
14	B	1203	CLA	C4-C3-C5-C6
14	B	1210	CLA	C4-C3-C5-C6
14	G	1109	CLA	C2-C3-C5-C6
14	G	1136	CLA	C2-C3-C5-C6
14	G	1140	CLA	C2-C3-C5-C6
14	H	1022	CLA	C2-C3-C5-C6
14	H	1201	CLA	C2-C3-C5-C6
14	H	1203	CLA	C2-C3-C5-C6
14	H	1210	CLA	C2-C3-C5-C6
14	W	1701	CLA	C2-C3-C5-C6
14	a	1109	CLA	C2-C3-C5-C6
14	a	1136	CLA	C2-C3-C5-C6
14	a	1140	CLA	C2-C3-C5-C6
14	b	1022	CLA	C2-C3-C5-C6
14	b	1201	CLA	C2-C3-C5-C6
14	b	1203	CLA	C2-C3-C5-C6
14	b	1210	CLA	C2-C3-C5-C6
14	x	1701	CLA	C2-C3-C5-C6
14	A	1109	CLA	C2-C3-C5-C6
14	A	1136	CLA	C2-C3-C5-C6
14	A	1140	CLA	C2-C3-C5-C6
14	B	1022	CLA	C2-C3-C5-C6
14	B	1201	CLA	C2-C3-C5-C6
14	B	1203	CLA	C2-C3-C5-C6
14	B	1210	CLA	C2-C3-C5-C6
14	X	1701	CLA	C2-C3-C5-C6
14	G	1131	CLA	O1A-CGA-O2A-C1
14	a	1131	CLA	O1A-CGA-O2A-C1
14	A	1131	CLA	O1A-CGA-O2A-C1
21	G	6001	LMT	O5'-C5'-C6'-O6'
21	a	6001	LMT	O5'-C5'-C6'-O6'
21	A	6001	LMT	O5'-C5'-C6'-O6'
14	b	1218	CLA	O1D-CGD-O2D-CED
14	G	1115	CLA	O1D-CGD-O2D-CED
14	H	1218	CLA	O1D-CGD-O2D-CED
14	a	1115	CLA	O1D-CGD-O2D-CED
14	A	1115	CLA	O1D-CGD-O2D-CED
14	B	1218	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
15	H	1207	F6C	C2A-CAA-CBA-CGA
15	b	1207	F6C	C2A-CAA-CBA-CGA
15	B	1207	F6C	C2A-CAA-CBA-CGA
14	G	1106	CLA	C2A-CAA-CBA-CGA
14	G	1123	CLA	C2A-CAA-CBA-CGA
14	G	1139	CLA	C2A-CAA-CBA-CGA
14	H	1214	CLA	C2A-CAA-CBA-CGA
14	H	1228	CLA	C2A-CAA-CBA-CGA
14	a	1106	CLA	C2A-CAA-CBA-CGA
14	a	1123	CLA	C2A-CAA-CBA-CGA
14	a	1139	CLA	C2A-CAA-CBA-CGA
14	b	1214	CLA	C2A-CAA-CBA-CGA
14	b	1228	CLA	C2A-CAA-CBA-CGA
14	A	1106	CLA	C2A-CAA-CBA-CGA
14	A	1123	CLA	C2A-CAA-CBA-CGA
14	A	1139	CLA	C2A-CAA-CBA-CGA
14	B	1214	CLA	C2A-CAA-CBA-CGA
14	B	1228	CLA	C2A-CAA-CBA-CGA
14	H	1239	CLA	O1D-CGD-O2D-CED
14	b	1239	CLA	O1D-CGD-O2D-CED
14	B	1239	CLA	O1D-CGD-O2D-CED
14	H	1226	CLA	C3-C5-C6-C7
20	R	5006	LMG	O6-C1-O1-C7
20	i	5006	LMG	O6-C1-O1-C7
20	I	5006	LMG	O6-C1-O1-C7
21	G	6002	LMT	O5'-C1'-O1'-C1
21	a	6002	LMT	O5'-C1'-O1'-C1
21	A	6002	LMT	O5'-C1'-O1'-C1
14	H	1227	CLA	O1D-CGD-O2D-CED
14	U	1503	CLA	O1D-CGD-O2D-CED
14	b	1227	CLA	O1D-CGD-O2D-CED
14	l	1503	CLA	O1D-CGD-O2D-CED
14	B	1227	CLA	O1D-CGD-O2D-CED
14	L	1503	CLA	O1D-CGD-O2D-CED
14	G	1115	CLA	CBA-CGA-O2A-C1
14	H	1229	CLA	CBA-CGA-O2A-C1
14	a	1115	CLA	CBA-CGA-O2A-C1
14	b	1229	CLA	CBA-CGA-O2A-C1
14	A	1115	CLA	CBA-CGA-O2A-C1
14	B	1229	CLA	CBA-CGA-O2A-C1
14	H	1223	CLA	O1A-CGA-O2A-C1
14	b	1223	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1223	CLA	O1A-CGA-O2A-C1
14	G	1112	CLA	O1D-CGD-O2D-CED
14	a	1112	CLA	O1D-CGD-O2D-CED
19	H	5004	LHG	C28-C29-C30-C31
19	b	5004	LHG	C28-C29-C30-C31
19	B	5004	LHG	C28-C29-C30-C31
15	H	1207	F6C	CBD-CGD-O2D-CED
15	b	1207	F6C	CBD-CGD-O2D-CED
15	B	1207	F6C	CBD-CGD-O2D-CED
14	G	1140	CLA	C3-C5-C6-C7
14	a	1140	CLA	C3-C5-C6-C7
14	A	1140	CLA	C3-C5-C6-C7
14	A	1112	CLA	O1D-CGD-O2D-CED
18	H	4017	BCR	C19-C20-C21-C22
18	b	4017	BCR	C19-C20-C21-C22
18	B	4017	BCR	C19-C20-C21-C22
14	G	1112	CLA	O1A-CGA-O2A-C1
14	a	1112	CLA	O1A-CGA-O2A-C1
14	A	1112	CLA	O1A-CGA-O2A-C1
14	G	1112	CLA	CBA-CGA-O2A-C1
14	G	1124	CLA	CBA-CGA-O2A-C1
14	H	1021	CLA	CBA-CGA-O2A-C1
14	H	1231	CLA	CBA-CGA-O2A-C1
14	H	1234	CLA	CBA-CGA-O2A-C1
14	a	1112	CLA	CBA-CGA-O2A-C1
14	a	1124	CLA	CBA-CGA-O2A-C1
14	b	1021	CLA	CBA-CGA-O2A-C1
14	b	1231	CLA	CBA-CGA-O2A-C1
14	b	1234	CLA	CBA-CGA-O2A-C1
14	A	1112	CLA	CBA-CGA-O2A-C1
14	A	1124	CLA	CBA-CGA-O2A-C1
14	B	1021	CLA	CBA-CGA-O2A-C1
14	B	1231	CLA	CBA-CGA-O2A-C1
14	B	1234	CLA	CBA-CGA-O2A-C1
15	H	1207	F6C	CBA-CGA-O2A-C1
15	H	1238	F6C	CBA-CGA-O2A-C1
15	b	1207	F6C	CBA-CGA-O2A-C1
15	b	1238	F6C	CBA-CGA-O2A-C1
15	B	1207	F6C	CBA-CGA-O2A-C1
15	B	1238	F6C	CBA-CGA-O2A-C1
14	H	1023	CLA	C4C-C3C-CAC-CBC
19	G	5001	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	a	5001	LHG	C11-C12-C13-C14
19	A	5001	LHG	C11-C12-C13-C14
14	G	1101	CLA	O1D-CGD-O2D-CED
14	G	1123	CLA	O1D-CGD-O2D-CED
14	a	1101	CLA	O1D-CGD-O2D-CED
14	A	1101	CLA	O1D-CGD-O2D-CED
14	L	1501	CLA	O1D-CGD-O2D-CED
14	b	1023	CLA	C4C-C3C-CAC-CBC
14	B	1023	CLA	C4C-C3C-CAC-CBC
14	U	1501	CLA	O1D-CGD-O2D-CED
14	l	1501	CLA	O1D-CGD-O2D-CED
14	A	1123	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	C4-C3-C5-C6
14	G	1116	CLA	C4-C3-C5-C6
14	a	1109	CLA	C4-C3-C5-C6
14	a	1116	CLA	C4-C3-C5-C6
14	A	1109	CLA	C4-C3-C5-C6
14	A	1116	CLA	C4-C3-C5-C6
14	G	1116	CLA	C2-C3-C5-C6
14	a	1116	CLA	C2-C3-C5-C6
14	A	1116	CLA	C2-C3-C5-C6
14	G	1104	CLA	C6-C7-C8-C9
14	G	1109	CLA	C14-C13-C15-C16
14	G	1123	CLA	C6-C7-C8-C9
14	G	1126	CLA	C6-C7-C8-C9
14	G	1138	CLA	C11-C10-C8-C9
14	H	1021	CLA	C14-C13-C15-C16
14	H	1022	CLA	C11-C10-C8-C9
14	H	1208	CLA	C14-C13-C15-C16
14	H	1213	CLA	C14-C13-C15-C16
14	H	1222	CLA	C6-C7-C8-C9
14	H	1234	CLA	C6-C7-C8-C9
14	U	1501	CLA	C11-C10-C8-C9
14	U	1503	CLA	C14-C13-C15-C16
14	a	1104	CLA	C6-C7-C8-C9
14	a	1109	CLA	C14-C13-C15-C16
14	a	1123	CLA	C6-C7-C8-C9
14	a	1126	CLA	C6-C7-C8-C9
14	a	1138	CLA	C11-C10-C8-C9
14	b	1021	CLA	C14-C13-C15-C16
14	b	1022	CLA	C11-C10-C8-C9
14	b	1208	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	b	1213	CLA	C14-C13-C15-C16
14	b	1222	CLA	C6-C7-C8-C9
14	b	1234	CLA	C6-C7-C8-C9
14	l	1501	CLA	C11-C10-C8-C9
14	l	1503	CLA	C14-C13-C15-C16
14	A	1104	CLA	C6-C7-C8-C9
14	A	1109	CLA	C14-C13-C15-C16
14	A	1123	CLA	C6-C7-C8-C9
14	A	1126	CLA	C6-C7-C8-C9
14	A	1138	CLA	C11-C10-C8-C9
14	B	1021	CLA	C14-C13-C15-C16
14	B	1022	CLA	C11-C10-C8-C9
14	B	1208	CLA	C14-C13-C15-C16
14	B	1213	CLA	C14-C13-C15-C16
14	B	1222	CLA	C6-C7-C8-C9
14	B	1234	CLA	C6-C7-C8-C9
14	L	1501	CLA	C11-C10-C8-C9
14	L	1503	CLA	C14-C13-C15-C16
15	H	1207	F6C	C14-C13-C15-C16
15	H	1237	F6C	C11-C12-C13-C14
15	b	1207	F6C	C14-C13-C15-C16
15	b	1237	F6C	C11-C12-C13-C14
15	B	1207	F6C	C14-C13-C15-C16
15	B	1237	F6C	C11-C12-C13-C14
14	G	1012	CLA	O1D-CGD-O2D-CED
14	G	1013	CLA	O1D-CGD-O2D-CED
14	H	1214	CLA	O1D-CGD-O2D-CED
14	a	1012	CLA	O1D-CGD-O2D-CED
14	a	1013	CLA	O1D-CGD-O2D-CED
14	a	1123	CLA	O1D-CGD-O2D-CED
14	b	1214	CLA	O1D-CGD-O2D-CED
14	A	1012	CLA	O1D-CGD-O2D-CED
14	A	1013	CLA	O1D-CGD-O2D-CED
14	B	1214	CLA	O1D-CGD-O2D-CED
20	R	5006	LMG	C2-C1-O1-C7
20	i	5006	LMG	C2-C1-O1-C7
20	I	5006	LMG	C2-C1-O1-C7
21	G	6001	LMT	C2'-C1'-O1'-C1
21	a	6001	LMT	C2'-C1'-O1'-C1
21	A	6001	LMT	C2'-C1'-O1'-C1
14	H	1021	CLA	O1A-CGA-O2A-C1
14	H	1234	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	b	1021	CLA	O1A-CGA-O2A-C1
14	b	1234	CLA	O1A-CGA-O2A-C1
14	B	1021	CLA	O1A-CGA-O2A-C1
14	B	1234	CLA	O1A-CGA-O2A-C1
14	H	1231	CLA	O1D-CGD-O2D-CED
14	b	1231	CLA	O1D-CGD-O2D-CED
18	G	4001	BCR	C7-C8-C9-C34
18	G	4001	BCR	C36-C18-C19-C20
18	G	4001	BCR	C37-C22-C23-C24
18	G	4002	BCR	C7-C8-C9-C34
18	G	4003	BCR	C7-C8-C9-C34
18	G	4007	BCR	C36-C18-C19-C20
18	G	4008	BCR	C36-C18-C19-C20
18	G	4011	BCR	C7-C8-C9-C34
18	G	4011	BCR	C37-C22-C23-C24
18	H	4004	BCR	C37-C22-C23-C24
18	H	4006	BCR	C37-C22-C23-C24
18	H	4010	BCR	C36-C18-C19-C20
18	H	4013	BCR	C11-C12-C13-C35
18	H	4014	BCR	C7-C8-C9-C34
18	H	4014	BCR	C36-C18-C19-C20
18	H	4016	BCR	C7-C8-C9-C34
18	H	4017	BCR	C37-C22-C23-C24
18	U	4019	BCR	C37-C22-C23-C24
18	a	4001	BCR	C7-C8-C9-C34
18	a	4001	BCR	C36-C18-C19-C20
18	a	4001	BCR	C37-C22-C23-C24
18	a	4002	BCR	C7-C8-C9-C34
18	a	4003	BCR	C7-C8-C9-C34
18	a	4007	BCR	C36-C18-C19-C20
18	a	4008	BCR	C36-C18-C19-C20
18	a	4011	BCR	C7-C8-C9-C34
18	a	4011	BCR	C37-C22-C23-C24
18	b	4004	BCR	C37-C22-C23-C24
18	b	4006	BCR	C37-C22-C23-C24
18	b	4010	BCR	C36-C18-C19-C20
18	b	4013	BCR	C11-C12-C13-C35
18	b	4014	BCR	C7-C8-C9-C34
18	b	4014	BCR	C36-C18-C19-C20
18	b	4016	BCR	C7-C8-C9-C34
18	b	4017	BCR	C37-C22-C23-C24
18	l	4019	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
18	A	4001	BCR	C7-C8-C9-C34
18	A	4001	BCR	C36-C18-C19-C20
18	A	4001	BCR	C37-C22-C23-C24
18	A	4002	BCR	C7-C8-C9-C34
18	A	4003	BCR	C7-C8-C9-C34
18	A	4007	BCR	C36-C18-C19-C20
18	A	4008	BCR	C36-C18-C19-C20
18	A	4011	BCR	C7-C8-C9-C34
18	A	4011	BCR	C37-C22-C23-C24
18	B	4004	BCR	C37-C22-C23-C24
18	B	4006	BCR	C37-C22-C23-C24
18	B	4010	BCR	C36-C18-C19-C20
18	B	4013	BCR	C11-C12-C13-C35
18	B	4014	BCR	C7-C8-C9-C34
18	B	4014	BCR	C36-C18-C19-C20
18	B	4016	BCR	C7-C8-C9-C34
18	B	4017	BCR	C37-C22-C23-C24
18	L	4019	BCR	C37-C22-C23-C24
18	G	4001	BCR	C7-C8-C9-C10
18	G	4002	BCR	C7-C8-C9-C10
18	G	4011	BCR	C21-C22-C23-C24
18	H	4004	BCR	C21-C22-C23-C24
18	H	4006	BCR	C21-C22-C23-C24
18	H	4009	BCR	C7-C8-C9-C10
18	H	4016	BCR	C17-C18-C19-C20
18	U	4022	BCR	C7-C8-C9-C10
18	V	4021	BCR	C7-C8-C9-C10
18	a	4001	BCR	C7-C8-C9-C10
18	a	4002	BCR	C7-C8-C9-C10
18	a	4011	BCR	C21-C22-C23-C24
18	b	4004	BCR	C21-C22-C23-C24
18	b	4006	BCR	C21-C22-C23-C24
18	b	4009	BCR	C7-C8-C9-C10
18	b	4016	BCR	C17-C18-C19-C20
18	l	4022	BCR	C7-C8-C9-C10
18	m	4021	BCR	C7-C8-C9-C10
18	A	4001	BCR	C7-C8-C9-C10
18	A	4002	BCR	C7-C8-C9-C10
18	A	4011	BCR	C21-C22-C23-C24
18	B	4004	BCR	C21-C22-C23-C24
18	B	4006	BCR	C21-C22-C23-C24
18	B	4009	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
18	B	4016	BCR	C17-C18-C19-C20
18	L	4022	BCR	C7-C8-C9-C10
18	M	4021	BCR	C7-C8-C9-C10
14	G	1111	CLA	C2A-CAA-CBA-CGA
14	G	1131	CLA	C2A-CAA-CBA-CGA
14	H	1022	CLA	C2A-CAA-CBA-CGA
14	a	1111	CLA	C2A-CAA-CBA-CGA
14	b	1022	CLA	C2A-CAA-CBA-CGA
14	A	1111	CLA	C2A-CAA-CBA-CGA
14	B	1022	CLA	C2A-CAA-CBA-CGA
19	H	5004	LHG	C23-C24-C25-C26
19	b	5004	LHG	C23-C24-C25-C26
19	B	5004	LHG	C23-C24-C25-C26
14	B	1231	CLA	O1D-CGD-O2D-CED
14	G	1124	CLA	O1A-CGA-O2A-C1
14	a	1124	CLA	O1A-CGA-O2A-C1
14	A	1124	CLA	O1A-CGA-O2A-C1
19	H	5004	LHG	O7-C5-C6-O8
19	b	5004	LHG	O7-C5-C6-O8
19	B	5004	LHG	O7-C5-C6-O8
14	H	1215	CLA	CBA-CGA-O2A-C1
14	b	1215	CLA	CBA-CGA-O2A-C1
14	B	1215	CLA	CBA-CGA-O2A-C1
14	H	1221	CLA	C15-C16-C17-C18
14	b	1221	CLA	C15-C16-C17-C18
14	A	1109	CLA	C8-C10-C11-C12
14	B	1221	CLA	C15-C16-C17-C18
14	G	1122	CLA	C2-C1-O2A-CGA
14	G	1128	CLA	C2-C1-O2A-CGA
14	G	1140	CLA	C2-C1-O2A-CGA
14	H	1202	CLA	C2-C1-O2A-CGA
14	H	1214	CLA	C2-C1-O2A-CGA
14	W	1701	CLA	C2-C1-O2A-CGA
14	a	1122	CLA	C2-C1-O2A-CGA
14	a	1128	CLA	C2-C1-O2A-CGA
14	a	1140	CLA	C2-C1-O2A-CGA
14	b	1202	CLA	C2-C1-O2A-CGA
14	b	1214	CLA	C2-C1-O2A-CGA
14	x	1701	CLA	C2-C1-O2A-CGA
14	A	1122	CLA	C2-C1-O2A-CGA
14	A	1128	CLA	C2-C1-O2A-CGA
14	A	1140	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	B	1202	CLA	C2-C1-O2A-CGA
14	B	1214	CLA	C2-C1-O2A-CGA
14	X	1701	CLA	C2-C1-O2A-CGA
15	H	1207	F6C	C2-C1-O2A-CGA
15	b	1207	F6C	C2-C1-O2A-CGA
15	B	1207	F6C	C2-C1-O2A-CGA
14	G	1105	CLA	O1D-CGD-O2D-CED
14	G	1111	CLA	O1D-CGD-O2D-CED
14	G	1114	CLA	O1D-CGD-O2D-CED
14	H	1204	CLA	O1D-CGD-O2D-CED
14	a	1105	CLA	O1D-CGD-O2D-CED
14	a	1111	CLA	O1D-CGD-O2D-CED
14	a	1114	CLA	O1D-CGD-O2D-CED
14	b	1204	CLA	O1D-CGD-O2D-CED
14	A	1105	CLA	O1D-CGD-O2D-CED
14	A	1111	CLA	O1D-CGD-O2D-CED
14	A	1114	CLA	O1D-CGD-O2D-CED
14	B	1204	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	C8-C10-C11-C12
14	G	1132	CLA	C5-C6-C7-C8
14	H	1204	CLA	C10-C11-C12-C13
14	H	1205	CLA	C10-C11-C12-C13
14	a	1109	CLA	C8-C10-C11-C12
14	a	1132	CLA	C5-C6-C7-C8
14	b	1204	CLA	C10-C11-C12-C13
14	b	1205	CLA	C10-C11-C12-C13
14	A	1132	CLA	C5-C6-C7-C8
14	B	1204	CLA	C10-C11-C12-C13
14	B	1205	CLA	C10-C11-C12-C13
14	H	1211	CLA	C3-C5-C6-C7
14	H	1213	CLA	C3-C5-C6-C7
14	b	1211	CLA	C3-C5-C6-C7
14	b	1213	CLA	C3-C5-C6-C7
14	B	1211	CLA	C3-C5-C6-C7
14	B	1213	CLA	C3-C5-C6-C7
14	G	1106	CLA	O1D-CGD-O2D-CED
14	H	1212	CLA	O1D-CGD-O2D-CED
14	a	1106	CLA	O1D-CGD-O2D-CED
14	b	1212	CLA	O1D-CGD-O2D-CED
14	A	1106	CLA	O1D-CGD-O2D-CED
14	B	1212	CLA	O1D-CGD-O2D-CED
14	G	1128	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	a	1128	CLA	CBD-CGD-O2D-CED
14	A	1128	CLA	CBD-CGD-O2D-CED
14	G	1125	CLA	C11-C12-C13-C15
14	G	1136	CLA	C6-C7-C8-C10
14	H	1021	CLA	C11-C12-C13-C15
14	H	1203	CLA	C11-C12-C13-C15
14	H	1216	CLA	C12-C13-C15-C16
14	H	1223	CLA	C11-C10-C8-C7
14	a	1125	CLA	C11-C12-C13-C15
14	a	1136	CLA	C6-C7-C8-C10
14	b	1021	CLA	C11-C12-C13-C15
14	b	1203	CLA	C11-C12-C13-C15
14	b	1216	CLA	C12-C13-C15-C16
14	b	1223	CLA	C11-C10-C8-C7
14	A	1125	CLA	C11-C12-C13-C15
14	A	1136	CLA	C6-C7-C8-C10
14	B	1021	CLA	C11-C12-C13-C15
14	B	1203	CLA	C11-C12-C13-C15
14	B	1216	CLA	C12-C13-C15-C16
14	B	1223	CLA	C11-C10-C8-C7
14	H	1201	CLA	CBA-CGA-O2A-C1
14	b	1201	CLA	CBA-CGA-O2A-C1
14	B	1201	CLA	CBA-CGA-O2A-C1
14	U	1503	CLA	C13-C15-C16-C17
19	H	5004	LHG	C7-C8-C9-C10
19	b	5004	LHG	C7-C8-C9-C10
19	B	5004	LHG	C7-C8-C9-C10
14	H	1213	CLA	O1D-CGD-O2D-CED
14	b	1213	CLA	O1D-CGD-O2D-CED
14	B	1213	CLA	O1D-CGD-O2D-CED
14	H	1224	CLA	C13-C15-C16-C17
14	b	1224	CLA	C13-C15-C16-C17
14	b	1234	CLA	C10-C11-C12-C13
14	l	1503	CLA	C13-C15-C16-C17
14	B	1224	CLA	C13-C15-C16-C17
14	B	1234	CLA	C10-C11-C12-C13
14	L	1503	CLA	C13-C15-C16-C17
14	G	1115	CLA	O1A-CGA-O2A-C1
14	H	1231	CLA	O1A-CGA-O2A-C1
14	b	1231	CLA	O1A-CGA-O2A-C1
14	B	1231	CLA	O1A-CGA-O2A-C1
20	G	5005	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
20	a	5005	LMG	C11-C10-O7-C8
20	A	5005	LMG	C11-C10-O7-C8
14	G	1124	CLA	O1D-CGD-O2D-CED
14	a	1124	CLA	O1D-CGD-O2D-CED
14	A	1124	CLA	O1D-CGD-O2D-CED
14	G	1123	CLA	C8-C10-C11-C12
14	G	1127	CLA	C8-C10-C11-C12
14	G	1140	CLA	C13-C15-C16-C17
14	H	1208	CLA	C15-C16-C17-C18
14	H	1211	CLA	C13-C15-C16-C17
14	H	1211	CLA	C15-C16-C17-C18
14	H	1234	CLA	C10-C11-C12-C13
14	U	1503	CLA	C8-C10-C11-C12
14	a	1123	CLA	C8-C10-C11-C12
14	a	1127	CLA	C8-C10-C11-C12
14	a	1140	CLA	C13-C15-C16-C17
14	b	1208	CLA	C15-C16-C17-C18
14	b	1211	CLA	C13-C15-C16-C17
14	b	1211	CLA	C15-C16-C17-C18
14	l	1503	CLA	C8-C10-C11-C12
14	A	1117	CLA	C15-C16-C17-C18
14	A	1123	CLA	C8-C10-C11-C12
14	A	1127	CLA	C8-C10-C11-C12
14	A	1140	CLA	C13-C15-C16-C17
14	B	1208	CLA	C15-C16-C17-C18
14	B	1211	CLA	C13-C15-C16-C17
14	B	1211	CLA	C15-C16-C17-C18
14	L	1503	CLA	C8-C10-C11-C12
15	H	1238	F6C	C2A-CAA-CBA-CGA
15	b	1238	F6C	C2A-CAA-CBA-CGA
15	B	1238	F6C	C2A-CAA-CBA-CGA
14	G	1132	CLA	C2A-CAA-CBA-CGA
14	G	1134	CLA	C2A-CAA-CBA-CGA
14	G	1140	CLA	C2A-CAA-CBA-CGA
14	H	1209	CLA	C2A-CAA-CBA-CGA
14	H	1211	CLA	C2A-CAA-CBA-CGA
14	H	1212	CLA	C2A-CAA-CBA-CGA
14	H	1213	CLA	C2A-CAA-CBA-CGA
14	H	1223	CLA	C2A-CAA-CBA-CGA
14	H	1225	CLA	C2A-CAA-CBA-CGA
14	H	1227	CLA	C2A-CAA-CBA-CGA
14	a	1131	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
14	a	1132	CLA	C2A-CAA-CBA-CGA
14	a	1134	CLA	C2A-CAA-CBA-CGA
14	a	1140	CLA	C2A-CAA-CBA-CGA
14	b	1209	CLA	C2A-CAA-CBA-CGA
14	b	1211	CLA	C2A-CAA-CBA-CGA
14	b	1212	CLA	C2A-CAA-CBA-CGA
14	b	1213	CLA	C2A-CAA-CBA-CGA
14	b	1223	CLA	C2A-CAA-CBA-CGA
14	b	1225	CLA	C2A-CAA-CBA-CGA
14	b	1227	CLA	C2A-CAA-CBA-CGA
14	A	1131	CLA	C2A-CAA-CBA-CGA
14	A	1132	CLA	C2A-CAA-CBA-CGA
14	A	1134	CLA	C2A-CAA-CBA-CGA
14	A	1140	CLA	C2A-CAA-CBA-CGA
14	B	1209	CLA	C2A-CAA-CBA-CGA
14	B	1211	CLA	C2A-CAA-CBA-CGA
14	B	1212	CLA	C2A-CAA-CBA-CGA
14	B	1213	CLA	C2A-CAA-CBA-CGA
14	B	1223	CLA	C2A-CAA-CBA-CGA
14	B	1225	CLA	C2A-CAA-CBA-CGA
14	B	1227	CLA	C2A-CAA-CBA-CGA
14	H	1205	CLA	O1D-CGD-O2D-CED
14	b	1205	CLA	O1D-CGD-O2D-CED
14	B	1205	CLA	O1D-CGD-O2D-CED
18	H	4010	BCR	C10-C11-C12-C13
18	R	4018	BCR	C10-C11-C12-C13
18	i	4018	BCR	C10-C11-C12-C13
18	I	4018	BCR	C10-C11-C12-C13
14	G	1013	CLA	C5-C6-C7-C8
14	G	1104	CLA	C10-C11-C12-C13
14	G	1115	CLA	C13-C15-C16-C17
14	G	1117	CLA	C15-C16-C17-C18
14	G	1119	CLA	C10-C11-C12-C13
14	G	1125	CLA	C8-C10-C11-C12
14	G	1128	CLA	C10-C11-C12-C13
14	G	1136	CLA	C10-C11-C12-C13
14	G	1140	CLA	C5-C6-C7-C8
14	H	1022	CLA	C5-C6-C7-C8
14	H	1022	CLA	C15-C16-C17-C18
14	H	1216	CLA	C5-C6-C7-C8
14	H	1234	CLA	C15-C16-C17-C18
14	a	1013	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	a	1104	CLA	C10-C11-C12-C13
14	a	1115	CLA	C13-C15-C16-C17
14	a	1117	CLA	C15-C16-C17-C18
14	a	1119	CLA	C10-C11-C12-C13
14	a	1125	CLA	C8-C10-C11-C12
14	a	1128	CLA	C10-C11-C12-C13
14	a	1136	CLA	C10-C11-C12-C13
14	a	1140	CLA	C5-C6-C7-C8
14	b	1022	CLA	C5-C6-C7-C8
14	b	1022	CLA	C15-C16-C17-C18
14	b	1234	CLA	C15-C16-C17-C18
14	A	1013	CLA	C5-C6-C7-C8
14	A	1104	CLA	C10-C11-C12-C13
14	A	1115	CLA	C13-C15-C16-C17
14	A	1119	CLA	C10-C11-C12-C13
14	A	1125	CLA	C8-C10-C11-C12
14	A	1128	CLA	C10-C11-C12-C13
14	A	1136	CLA	C10-C11-C12-C13
14	A	1140	CLA	C5-C6-C7-C8
14	B	1022	CLA	C5-C6-C7-C8
14	B	1022	CLA	C15-C16-C17-C18
14	B	1216	CLA	C5-C6-C7-C8
14	B	1234	CLA	C15-C16-C17-C18
16	H	2002	PQN	C18-C20-C21-C22
16	b	2002	PQN	C18-C20-C21-C22
16	B	2002	PQN	C18-C20-C21-C22
14	H	1023	CLA	O1D-CGD-O2D-CED
14	a	1115	CLA	O1A-CGA-O2A-C1
14	A	1115	CLA	O1A-CGA-O2A-C1
21	G	6001	LMT	O5'-C1'-O1'-C1
21	a	6001	LMT	O5'-C1'-O1'-C1
21	A	6001	LMT	O5'-C1'-O1'-C1
14	b	1023	CLA	O1D-CGD-O2D-CED
14	B	1023	CLA	O1D-CGD-O2D-CED
14	G	1117	CLA	C5-C6-C7-C8
14	G	1119	CLA	C8-C10-C11-C12
14	G	1122	CLA	C5-C6-C7-C8
14	G	1138	CLA	C5-C6-C7-C8
14	H	1021	CLA	C15-C16-C17-C18
14	H	1023	CLA	C13-C15-C16-C17
14	H	1215	CLA	C10-C11-C12-C13
14	H	1216	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	H	1222	CLA	C5-C6-C7-C8
14	H	1222	CLA	C13-C15-C16-C17
14	H	1222	CLA	C15-C16-C17-C18
14	H	1226	CLA	C13-C15-C16-C17
14	H	1234	CLA	C8-C10-C11-C12
14	H	1235	CLA	C10-C11-C12-C13
14	H	1239	CLA	C15-C16-C17-C18
14	a	1117	CLA	C5-C6-C7-C8
14	a	1119	CLA	C8-C10-C11-C12
14	a	1138	CLA	C5-C6-C7-C8
14	b	1021	CLA	C15-C16-C17-C18
14	b	1023	CLA	C13-C15-C16-C17
14	b	1215	CLA	C10-C11-C12-C13
14	b	1216	CLA	C5-C6-C7-C8
14	b	1216	CLA	C13-C15-C16-C17
14	b	1222	CLA	C5-C6-C7-C8
14	b	1222	CLA	C13-C15-C16-C17
14	b	1222	CLA	C15-C16-C17-C18
14	b	1234	CLA	C8-C10-C11-C12
14	b	1235	CLA	C10-C11-C12-C13
14	b	1239	CLA	C15-C16-C17-C18
14	A	1117	CLA	C5-C6-C7-C8
14	A	1119	CLA	C8-C10-C11-C12
14	A	1138	CLA	C5-C6-C7-C8
14	B	1021	CLA	C15-C16-C17-C18
14	B	1023	CLA	C13-C15-C16-C17
14	B	1215	CLA	C10-C11-C12-C13
14	B	1216	CLA	C13-C15-C16-C17
14	B	1222	CLA	C5-C6-C7-C8
14	B	1222	CLA	C13-C15-C16-C17
14	B	1222	CLA	C15-C16-C17-C18
14	B	1226	CLA	C13-C15-C16-C17
14	B	1234	CLA	C8-C10-C11-C12
14	B	1235	CLA	C10-C11-C12-C13
14	B	1239	CLA	C15-C16-C17-C18
15	H	1237	F6C	C8-C10-C11-C12
15	b	1237	F6C	C8-C10-C11-C12
15	B	1237	F6C	C8-C10-C11-C12
14	b	1225	CLA	CBD-CGD-O2D-CED
14	B	1225	CLA	CBD-CGD-O2D-CED
14	H	1229	CLA	O1A-CGA-O2A-C1
14	b	1229	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1229	CLA	O1A-CGA-O2A-C1
15	H	1207	F6C	O1A-CGA-O2A-C1
15	B	1207	F6C	O1A-CGA-O2A-C1
14	G	1104	CLA	C15-C16-C17-C18
14	H	1204	CLA	C13-C15-C16-C17
14	H	1225	CLA	C10-C11-C12-C13
14	H	1239	CLA	C10-C11-C12-C13
14	a	1104	CLA	C15-C16-C17-C18
14	a	1122	CLA	C5-C6-C7-C8
14	b	1204	CLA	C13-C15-C16-C17
14	b	1225	CLA	C10-C11-C12-C13
14	b	1226	CLA	C13-C15-C16-C17
14	b	1239	CLA	C10-C11-C12-C13
14	A	1104	CLA	C15-C16-C17-C18
14	A	1122	CLA	C5-C6-C7-C8
14	B	1204	CLA	C13-C15-C16-C17
14	B	1225	CLA	C10-C11-C12-C13
14	B	1239	CLA	C10-C11-C12-C13
16	H	2002	PQN	C20-C21-C22-C23
16	b	2002	PQN	C20-C21-C22-C23
16	B	2002	PQN	C20-C21-C22-C23
20	U	5007	LMG	C20-C21-C22-C23
20	l	5007	LMG	C20-C21-C22-C23
20	L	5007	LMG	C20-C21-C22-C23
14	A	1135	CLA	O1D-CGD-O2D-CED
14	G	1130	CLA	C3-C5-C6-C7
14	a	1130	CLA	C3-C5-C6-C7
14	A	1130	CLA	C3-C5-C6-C7
14	G	1102	CLA	O1D-CGD-O2D-CED
14	G	1113	CLA	O1D-CGD-O2D-CED
14	G	1125	CLA	O1D-CGD-O2D-CED
14	G	1135	CLA	O1D-CGD-O2D-CED
14	a	1113	CLA	O1D-CGD-O2D-CED
14	a	1125	CLA	O1D-CGD-O2D-CED
14	a	1135	CLA	O1D-CGD-O2D-CED
14	A	1102	CLA	O1D-CGD-O2D-CED
14	A	1113	CLA	O1D-CGD-O2D-CED
14	A	1125	CLA	O1D-CGD-O2D-CED
14	G	1106	CLA	C8-C10-C11-C12
14	G	1128	CLA	C5-C6-C7-C8
14	H	1021	CLA	C13-C15-C16-C17
14	a	1106	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	a	1128	CLA	C5-C6-C7-C8
14	b	1021	CLA	C13-C15-C16-C17
14	A	1012	CLA	C15-C16-C17-C18
14	A	1106	CLA	C8-C10-C11-C12
14	A	1128	CLA	C5-C6-C7-C8
14	B	1021	CLA	C13-C15-C16-C17
15	H	1207	F6C	C5-C6-C7-C8
15	H	1237	F6C	C13-C15-C16-C17
15	b	1207	F6C	C5-C6-C7-C8
15	b	1237	F6C	C13-C15-C16-C17
15	B	1207	F6C	C5-C6-C7-C8
15	B	1237	F6C	C13-C15-C16-C17
16	H	2002	PQN	C25-C26-C27-C28
16	b	2002	PQN	C25-C26-C27-C28
16	B	2002	PQN	C25-C26-C27-C28
14	H	1225	CLA	CBD-CGD-O2D-CED
15	b	1207	F6C	O1A-CGA-O2A-C1
14	a	1102	CLA	O1D-CGD-O2D-CED
14	G	1012	CLA	C15-C16-C17-C18
14	H	1235	CLA	C8-C10-C11-C12
14	a	1012	CLA	C15-C16-C17-C18
14	B	1235	CLA	C8-C10-C11-C12
14	G	1109	CLA	CBA-CGA-O2A-C1
14	a	1109	CLA	CBA-CGA-O2A-C1
14	A	1109	CLA	CBA-CGA-O2A-C1
19	G	5001	LHG	C8-C7-O7-C5
19	a	5001	LHG	C8-C7-O7-C5
19	A	5001	LHG	C8-C7-O7-C5
15	H	1238	F6C	O1A-CGA-O2A-C1
15	b	1238	F6C	O1A-CGA-O2A-C1
15	B	1238	F6C	O1A-CGA-O2A-C1
14	G	1132	CLA	C13-C15-C16-C17
14	a	1132	CLA	C13-C15-C16-C17
14	b	1235	CLA	C8-C10-C11-C12
14	A	1132	CLA	C13-C15-C16-C17
14	H	1215	CLA	C3-C5-C6-C7
14	b	1215	CLA	C3-C5-C6-C7
14	B	1215	CLA	C3-C5-C6-C7
18	G	4003	BCR	C9-C10-C11-C12
18	G	4007	BCR	C19-C20-C21-C22
18	R	4018	BCR	C19-C20-C21-C22
18	a	4007	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
18	i	4018	BCR	C19-C20-C21-C22
18	A	4007	BCR	C19-C20-C21-C22
18	I	4018	BCR	C19-C20-C21-C22
14	G	1102	CLA	C8-C10-C11-C12
14	H	1214	CLA	C8-C10-C11-C12
14	H	1223	CLA	C8-C10-C11-C12
14	H	1229	CLA	C8-C10-C11-C12
14	H	1234	CLA	C13-C15-C16-C17
14	b	1214	CLA	C8-C10-C11-C12
14	b	1223	CLA	C8-C10-C11-C12
14	b	1229	CLA	C8-C10-C11-C12
14	b	1234	CLA	C13-C15-C16-C17
14	B	1214	CLA	C8-C10-C11-C12
14	B	1223	CLA	C8-C10-C11-C12
14	B	1229	CLA	C8-C10-C11-C12
14	B	1234	CLA	C13-C15-C16-C17
20	G	5005	LMG	O9-C10-O7-C8
20	a	5005	LMG	O9-C10-O7-C8
20	A	5005	LMG	O9-C10-O7-C8
14	b	1235	CLA	O1D-CGD-O2D-CED
14	U	1502	CLA	CBA-CGA-O2A-C1
14	W	1701	CLA	CBA-CGA-O2A-C1
14	l	1502	CLA	CBA-CGA-O2A-C1
14	x	1701	CLA	CBA-CGA-O2A-C1
14	L	1502	CLA	CBA-CGA-O2A-C1
14	X	1701	CLA	CBA-CGA-O2A-C1
14	G	1106	CLA	C10-C11-C12-C13
14	G	1133	CLA	C5-C6-C7-C8
14	G	1136	CLA	C5-C6-C7-C8
14	H	1022	CLA	C8-C10-C11-C12
14	H	1203	CLA	C15-C16-C17-C18
14	W	1701	CLA	C5-C6-C7-C8
14	a	1102	CLA	C8-C10-C11-C12
14	a	1106	CLA	C10-C11-C12-C13
14	a	1133	CLA	C5-C6-C7-C8
14	b	1022	CLA	C8-C10-C11-C12
14	b	1203	CLA	C15-C16-C17-C18
14	x	1701	CLA	C5-C6-C7-C8
14	A	1102	CLA	C8-C10-C11-C12
14	A	1106	CLA	C10-C11-C12-C13
14	A	1133	CLA	C5-C6-C7-C8
14	A	1136	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	B	1022	CLA	C8-C10-C11-C12
14	B	1203	CLA	C15-C16-C17-C18
14	X	1701	CLA	C5-C6-C7-C8
14	G	1120	CLA	O1D-CGD-O2D-CED
14	H	1235	CLA	O1D-CGD-O2D-CED
14	a	1120	CLA	O1D-CGD-O2D-CED
14	A	1120	CLA	O1D-CGD-O2D-CED
14	B	1235	CLA	O1D-CGD-O2D-CED
14	H	1224	CLA	C15-C16-C17-C18
14	H	1229	CLA	C10-C11-C12-C13
14	H	1239	CLA	C5-C6-C7-C8
14	a	1136	CLA	C5-C6-C7-C8
14	b	1224	CLA	C15-C16-C17-C18
14	b	1229	CLA	C10-C11-C12-C13
14	b	1239	CLA	C5-C6-C7-C8
14	B	1224	CLA	C15-C16-C17-C18
14	B	1229	CLA	C10-C11-C12-C13
14	B	1239	CLA	C5-C6-C7-C8
14	G	1115	CLA	C15-C16-C17-C18
14	H	1204	CLA	C5-C6-C7-C8
14	H	1211	CLA	C10-C11-C12-C13
14	a	1115	CLA	C15-C16-C17-C18
14	b	1204	CLA	C5-C6-C7-C8
14	b	1211	CLA	C10-C11-C12-C13
14	A	1115	CLA	C15-C16-C17-C18
14	B	1204	CLA	C5-C6-C7-C8
14	B	1211	CLA	C10-C11-C12-C13
15	H	1207	F6C	C15-C16-C17-C18
15	b	1207	F6C	C15-C16-C17-C18
15	B	1207	F6C	C15-C16-C17-C18
14	H	1222	CLA	O1D-CGD-O2D-CED
14	a	1118	CLA	O1D-CGD-O2D-CED
14	b	1222	CLA	O1D-CGD-O2D-CED
14	H	1223	CLA	CBD-CGD-O2D-CED
14	b	1223	CLA	CBD-CGD-O2D-CED
14	B	1223	CLA	CBD-CGD-O2D-CED
20	G	5005	LMG	O6-C5-C6-O5
20	a	5005	LMG	O6-C5-C6-O5
20	A	5005	LMG	O6-C5-C6-O5
14	G	1104	CLA	O1D-CGD-O2D-CED
14	G	1118	CLA	O1D-CGD-O2D-CED
14	a	1104	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	A	1104	CLA	O1D-CGD-O2D-CED
14	A	1118	CLA	O1D-CGD-O2D-CED
14	B	1222	CLA	O1D-CGD-O2D-CED
19	G	5001	LHG	O9-C7-O7-C5
19	a	5001	LHG	O9-C7-O7-C5
19	A	5001	LHG	O9-C7-O7-C5
21	G	6002	LMT	C2'-C1'-O1'-C1
21	a	6002	LMT	C2'-C1'-O1'-C1
21	A	6002	LMT	C2'-C1'-O1'-C1
14	G	1123	CLA	C5-C6-C7-C8
14	A	1123	CLA	C5-C6-C7-C8
20	H	5002	LMG	C10-C11-C12-C13
20	b	5002	LMG	C10-C11-C12-C13
20	B	5002	LMG	C10-C11-C12-C13
14	G	1125	CLA	C16-C17-C18-C20
14	a	1125	CLA	C16-C17-C18-C20
14	A	1125	CLA	C16-C17-C18-C20
14	a	1123	CLA	C5-C6-C7-C8
15	H	1207	F6C	C8-C10-C11-C12
15	b	1207	F6C	C8-C10-C11-C12
15	B	1207	F6C	C8-C10-C11-C12
14	H	1201	CLA	O1A-CGA-O2A-C1
14	b	1201	CLA	O1A-CGA-O2A-C1
14	B	1201	CLA	O1A-CGA-O2A-C1
18	G	4011	BCR	C11-C10-C9-C34
18	R	4020	BCR	C11-C10-C9-C34
18	a	4011	BCR	C11-C10-C9-C34
18	i	4020	BCR	C11-C10-C9-C34
18	A	4011	BCR	C11-C10-C9-C34
18	I	4020	BCR	C11-C10-C9-C34
14	H	1225	CLA	C15-C16-C17-C18
14	b	1225	CLA	C15-C16-C17-C18
14	B	1225	CLA	C15-C16-C17-C18
18	H	4009	BCR	C7-C8-C9-C34
18	b	4009	BCR	C7-C8-C9-C34
18	B	4009	BCR	C7-C8-C9-C34
15	G	1121	F6C	C2A-CAA-CBA-CGA
15	a	1121	F6C	C2A-CAA-CBA-CGA
15	A	1121	F6C	C2A-CAA-CBA-CGA
14	G	1109	CLA	O1A-CGA-O2A-C1
14	W	1701	CLA	O1A-CGA-O2A-C1
14	a	1109	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	x	1701	CLA	O1A-CGA-O2A-C1
14	A	1109	CLA	O1A-CGA-O2A-C1
14	X	1701	CLA	O1A-CGA-O2A-C1
14	H	1206	CLA	C2A-CAA-CBA-CGA
14	H	1224	CLA	C2A-CAA-CBA-CGA
14	b	1206	CLA	C2A-CAA-CBA-CGA
14	b	1224	CLA	C2A-CAA-CBA-CGA
14	B	1206	CLA	C2A-CAA-CBA-CGA
14	B	1224	CLA	C2A-CAA-CBA-CGA
14	G	1102	CLA	C10-C11-C12-C13
14	U	1501	CLA	C13-C15-C16-C17
14	a	1102	CLA	C10-C11-C12-C13
14	l	1501	CLA	C13-C15-C16-C17
14	A	1102	CLA	C10-C11-C12-C13
14	L	1501	CLA	C13-C15-C16-C17
14	G	1103	CLA	C11-C12-C13-C14
14	G	1103	CLA	C11-C12-C13-C15
14	H	1215	CLA	C11-C12-C13-C15
14	H	1223	CLA	C16-C17-C18-C19
14	H	1225	CLA	C16-C17-C18-C19
14	a	1103	CLA	C11-C12-C13-C15
14	b	1215	CLA	C11-C12-C13-C15
14	b	1223	CLA	C16-C17-C18-C19
14	b	1225	CLA	C16-C17-C18-C19
14	A	1103	CLA	C11-C12-C13-C15
14	B	1215	CLA	C11-C12-C13-C15
14	B	1223	CLA	C16-C17-C18-C19
14	B	1225	CLA	C16-C17-C18-C19
14	G	1136	CLA	O1D-CGD-O2D-CED
14	a	1136	CLA	O1D-CGD-O2D-CED
14	A	1136	CLA	O1D-CGD-O2D-CED
14	G	1131	CLA	C3-C5-C6-C7
14	a	1131	CLA	C3-C5-C6-C7
14	b	1223	CLA	C5-C6-C7-C8
18	G	4011	BCR	C11-C10-C9-C8
18	R	4020	BCR	C11-C10-C9-C8
18	R	4020	BCR	C20-C21-C22-C23
18	a	4011	BCR	C11-C10-C9-C8
18	i	4020	BCR	C11-C10-C9-C8
18	i	4020	BCR	C20-C21-C22-C23
18	A	4011	BCR	C11-C10-C9-C8
18	I	4020	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
18	I	4020	BCR	C20-C21-C22-C23
14	H	1223	CLA	C5-C6-C7-C8
14	B	1223	CLA	C5-C6-C7-C8
15	b	1237	F6C	C15-C16-C17-C18
14	H	1234	CLA	C5-C6-C7-C8
14	b	1234	CLA	C5-C6-C7-C8
14	B	1234	CLA	C5-C6-C7-C8
15	H	1237	F6C	C15-C16-C17-C18
15	B	1237	F6C	C15-C16-C17-C18
14	A	1131	CLA	C3-C5-C6-C7
14	G	1012	CLA	C2-C1-O2A-CGA
14	G	1124	CLA	C2-C1-O2A-CGA
14	G	1136	CLA	C2-C1-O2A-CGA
14	H	1215	CLA	C2-C1-O2A-CGA
14	H	1239	CLA	C2-C1-O2A-CGA
14	a	1012	CLA	C2-C1-O2A-CGA
14	a	1124	CLA	C2-C1-O2A-CGA
14	a	1136	CLA	C2-C1-O2A-CGA
14	b	1215	CLA	C2-C1-O2A-CGA
14	b	1239	CLA	C2-C1-O2A-CGA
14	A	1012	CLA	C2-C1-O2A-CGA
14	A	1124	CLA	C2-C1-O2A-CGA
14	A	1136	CLA	C2-C1-O2A-CGA
14	B	1215	CLA	C2-C1-O2A-CGA
14	B	1239	CLA	C2-C1-O2A-CGA
14	G	1111	CLA	C11-C12-C13-C15
14	G	1112	CLA	C6-C7-C8-C10
14	G	1125	CLA	C16-C17-C18-C19
14	G	1126	CLA	C11-C12-C13-C14
14	H	1216	CLA	C16-C17-C18-C20
14	H	1221	CLA	C16-C17-C18-C20
14	a	1102	CLA	C11-C12-C13-C15
14	a	1103	CLA	C11-C12-C13-C14
14	a	1111	CLA	C11-C12-C13-C15
14	a	1112	CLA	C6-C7-C8-C10
14	a	1125	CLA	C16-C17-C18-C19
14	a	1126	CLA	C11-C12-C13-C14
14	b	1216	CLA	C16-C17-C18-C20
14	b	1221	CLA	C16-C17-C18-C20
14	A	1102	CLA	C11-C12-C13-C15
14	A	1103	CLA	C11-C12-C13-C14
14	A	1111	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	A	1112	CLA	C6-C7-C8-C10
14	A	1125	CLA	C16-C17-C18-C19
14	A	1126	CLA	C11-C12-C13-C14
14	B	1216	CLA	C16-C17-C18-C20
14	B	1221	CLA	C16-C17-C18-C20
19	H	5004	LHG	C11-C10-C9-C8
19	b	5004	LHG	C11-C10-C9-C8
19	B	5004	LHG	C11-C10-C9-C8
14	H	1215	CLA	O1A-CGA-O2A-C1
14	b	1215	CLA	O1A-CGA-O2A-C1
14	B	1215	CLA	O1A-CGA-O2A-C1
14	G	1140	CLA	CBA-CGA-O2A-C1
14	a	1140	CLA	CBA-CGA-O2A-C1
14	A	1140	CLA	CBA-CGA-O2A-C1
19	G	5001	LHG	O1-C1-C2-O2
19	a	5001	LHG	O1-C1-C2-O2
19	A	5001	LHG	O1-C1-C2-O2
14	G	1115	CLA	C5-C6-C7-C8
14	a	1115	CLA	C5-C6-C7-C8
14	A	1115	CLA	C5-C6-C7-C8
14	G	1012	CLA	C4B-C3B-CAB-CBB
14	G	1114	CLA	C4B-C3B-CAB-CBB
14	G	1116	CLA	C4B-C3B-CAB-CBB
14	G	1120	CLA	C4B-C3B-CAB-CBB
14	G	1129	CLA	C4B-C3B-CAB-CBB
14	G	1132	CLA	C4B-C3B-CAB-CBB
14	H	1204	CLA	C4B-C3B-CAB-CBB
14	H	1209	CLA	C4B-C3B-CAB-CBB
14	H	1215	CLA	C4B-C3B-CAB-CBB
14	H	1217	CLA	C4B-C3B-CAB-CBB
14	H	1219	CLA	C4B-C3B-CAB-CBB
14	H	1224	CLA	C4B-C3B-CAB-CBB
14	H	1233	CLA	C4B-C3B-CAB-CBB
14	H	1239	CLA	C4B-C3B-CAB-CBB
14	T	1401	CLA	C4B-C3B-CAB-CBB
14	a	1012	CLA	C4B-C3B-CAB-CBB
14	a	1114	CLA	C4B-C3B-CAB-CBB
14	a	1116	CLA	C4B-C3B-CAB-CBB
14	a	1120	CLA	C4B-C3B-CAB-CBB
14	a	1129	CLA	C4B-C3B-CAB-CBB
14	a	1132	CLA	C4B-C3B-CAB-CBB
14	b	1204	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	1209	CLA	C4B-C3B-CAB-CBB
14	b	1215	CLA	C4B-C3B-CAB-CBB
14	b	1217	CLA	C4B-C3B-CAB-CBB
14	b	1219	CLA	C4B-C3B-CAB-CBB
14	b	1224	CLA	C4B-C3B-CAB-CBB
14	b	1233	CLA	C4B-C3B-CAB-CBB
14	b	1239	CLA	C4B-C3B-CAB-CBB
14	k	1401	CLA	C4B-C3B-CAB-CBB
14	A	1012	CLA	C4B-C3B-CAB-CBB
14	A	1114	CLA	C4B-C3B-CAB-CBB
14	A	1116	CLA	C4B-C3B-CAB-CBB
14	A	1120	CLA	C4B-C3B-CAB-CBB
14	A	1129	CLA	C4B-C3B-CAB-CBB
14	A	1132	CLA	C4B-C3B-CAB-CBB
14	B	1204	CLA	C4B-C3B-CAB-CBB
14	B	1209	CLA	C4B-C3B-CAB-CBB
14	B	1215	CLA	C4B-C3B-CAB-CBB
14	B	1217	CLA	C4B-C3B-CAB-CBB
14	B	1219	CLA	C4B-C3B-CAB-CBB
14	B	1224	CLA	C4B-C3B-CAB-CBB
14	B	1233	CLA	C4B-C3B-CAB-CBB
14	B	1239	CLA	C4B-C3B-CAB-CBB
14	K	1401	CLA	C4B-C3B-CAB-CBB
15	H	1207	F6C	C3A-C2A-CAA-CBA
15	b	1207	F6C	C3A-C2A-CAA-CBA
15	B	1207	F6C	C3A-C2A-CAA-CBA
14	G	1102	CLA	C11-C12-C13-C15
14	G	1112	CLA	C6-C7-C8-C9
14	G	1126	CLA	C11-C12-C13-C15
14	H	1202	CLA	C11-C12-C13-C15
14	H	1216	CLA	C16-C17-C18-C19
14	H	1225	CLA	C16-C17-C18-C20
14	H	1239	CLA	C16-C17-C18-C19
14	a	1112	CLA	C6-C7-C8-C9
14	a	1126	CLA	C11-C12-C13-C15
14	b	1202	CLA	C11-C12-C13-C15
14	b	1216	CLA	C16-C17-C18-C19
14	b	1225	CLA	C16-C17-C18-C20
14	b	1239	CLA	C16-C17-C18-C19
14	A	1112	CLA	C6-C7-C8-C9
14	A	1126	CLA	C11-C12-C13-C15
14	B	1202	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
14	B	1216	CLA	C16-C17-C18-C19
14	B	1225	CLA	C16-C17-C18-C20
14	B	1239	CLA	C16-C17-C18-C19
14	G	1113	CLA	C2A-CAA-CBA-CGA
14	G	1135	CLA	C2A-CAA-CBA-CGA
14	T	1401	CLA	C2A-CAA-CBA-CGA
14	a	1113	CLA	C2A-CAA-CBA-CGA
14	a	1135	CLA	C2A-CAA-CBA-CGA
14	k	1401	CLA	C2A-CAA-CBA-CGA
14	A	1113	CLA	C2A-CAA-CBA-CGA
14	A	1135	CLA	C2A-CAA-CBA-CGA
14	K	1401	CLA	C2A-CAA-CBA-CGA
14	G	1109	CLA	C13-C15-C16-C17
14	G	1124	CLA	C5-C6-C7-C8
14	H	1229	CLA	C5-C6-C7-C8
14	a	1109	CLA	C13-C15-C16-C17
14	a	1124	CLA	C5-C6-C7-C8
14	b	1229	CLA	C5-C6-C7-C8
14	A	1109	CLA	C13-C15-C16-C17
14	A	1124	CLA	C5-C6-C7-C8
14	B	1229	CLA	C5-C6-C7-C8
14	G	1109	CLA	C11-C12-C13-C15
14	a	1109	CLA	C11-C12-C13-C15
14	A	1109	CLA	C11-C12-C13-C15
19	H	5004	LHG	C33-C34-C35-C36
19	b	5004	LHG	C33-C34-C35-C36
19	B	5004	LHG	C33-C34-C35-C36
19	G	5001	LHG	C23-C24-C25-C26
19	a	5001	LHG	C23-C24-C25-C26
19	A	5001	LHG	C23-C24-C25-C26
20	R	5006	LMG	C28-C29-C30-C31
20	i	5006	LMG	C28-C29-C30-C31
20	I	5006	LMG	C28-C29-C30-C31
14	H	1228	CLA	C5-C6-C7-C8
14	b	1228	CLA	C5-C6-C7-C8
14	B	1228	CLA	C5-C6-C7-C8
20	G	5005	LMG	C30-C31-C32-C33
20	a	5005	LMG	C30-C31-C32-C33
20	A	5005	LMG	C30-C31-C32-C33
14	G	1125	CLA	C3-C5-C6-C7
14	a	1125	CLA	C3-C5-C6-C7
14	A	1125	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	G	1102	CLA	C3A-C2A-CAA-CBA
14	G	1103	CLA	C3A-C2A-CAA-CBA
14	G	1125	CLA	C3A-C2A-CAA-CBA
14	G	1127	CLA	C3A-C2A-CAA-CBA
14	G	1138	CLA	C3A-C2A-CAA-CBA
14	H	1210	CLA	C3A-C2A-CAA-CBA
14	H	1220	CLA	C3A-C2A-CAA-CBA
14	H	1221	CLA	C3A-C2A-CAA-CBA
14	H	1229	CLA	C3A-C2A-CAA-CBA
14	U	1503	CLA	C3A-C2A-CAA-CBA
14	a	1102	CLA	C3A-C2A-CAA-CBA
14	a	1103	CLA	C3A-C2A-CAA-CBA
14	a	1125	CLA	C3A-C2A-CAA-CBA
14	a	1127	CLA	C3A-C2A-CAA-CBA
14	a	1138	CLA	C3A-C2A-CAA-CBA
14	b	1210	CLA	C3A-C2A-CAA-CBA
14	b	1220	CLA	C3A-C2A-CAA-CBA
14	b	1221	CLA	C3A-C2A-CAA-CBA
14	b	1229	CLA	C3A-C2A-CAA-CBA
14	l	1503	CLA	C3A-C2A-CAA-CBA
14	A	1102	CLA	C3A-C2A-CAA-CBA
14	A	1103	CLA	C3A-C2A-CAA-CBA
14	A	1125	CLA	C3A-C2A-CAA-CBA
14	A	1127	CLA	C3A-C2A-CAA-CBA
14	A	1138	CLA	C3A-C2A-CAA-CBA
14	B	1210	CLA	C3A-C2A-CAA-CBA
14	B	1220	CLA	C3A-C2A-CAA-CBA
14	B	1221	CLA	C3A-C2A-CAA-CBA
14	B	1229	CLA	C3A-C2A-CAA-CBA
14	L	1503	CLA	C3A-C2A-CAA-CBA
21	G	6001	LMT	C3-C4-C5-C6
21	A	6001	LMT	C3-C4-C5-C6
21	G	6002	LMT	C1-C2-C3-C4
21	a	6002	LMT	C1-C2-C3-C4
21	A	6002	LMT	C1-C2-C3-C4
21	a	6001	LMT	C3-C4-C5-C6
14	G	1138	CLA	C8-C10-C11-C12
14	H	1211	CLA	C8-C10-C11-C12
14	a	1138	CLA	C8-C10-C11-C12
14	b	1211	CLA	C8-C10-C11-C12
14	A	1138	CLA	C8-C10-C11-C12
14	B	1211	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
16	G	2001	PQN	C23-C25-C26-C27
16	a	2001	PQN	C23-C25-C26-C27
16	A	2001	PQN	C23-C25-C26-C27
18	a	4003	BCR	C9-C10-C11-C12
18	A	4003	BCR	C9-C10-C11-C12
14	G	1102	CLA	C11-C12-C13-C14
14	H	1215	CLA	C11-C12-C13-C14
14	a	1102	CLA	C11-C12-C13-C14
14	b	1215	CLA	C11-C12-C13-C14
14	A	1102	CLA	C11-C12-C13-C14
14	B	1215	CLA	C11-C12-C13-C14
20	B	5002	LMG	C19-C20-C21-C22
14	G	1126	CLA	CBA-CGA-O2A-C1
14	a	1126	CLA	CBA-CGA-O2A-C1
14	A	1126	CLA	CBA-CGA-O2A-C1
19	a	5001	LHG	C29-C30-C31-C32
19	A	5001	LHG	C29-C30-C31-C32
20	G	5005	LMG	C13-C14-C15-C16
20	H	5002	LMG	C19-C20-C21-C22
20	a	5005	LMG	C13-C14-C15-C16
20	b	5002	LMG	C19-C20-C21-C22
20	A	5005	LMG	C13-C14-C15-C16
14	b	1210	CLA	C5-C6-C7-C8
14	B	1210	CLA	C5-C6-C7-C8
19	G	5001	LHG	C29-C30-C31-C32
14	U	1502	CLA	O1A-CGA-O2A-C1
14	l	1502	CLA	O1A-CGA-O2A-C1
14	L	1502	CLA	O1A-CGA-O2A-C1
14	H	1210	CLA	C5-C6-C7-C8
14	G	1111	CLA	C11-C12-C13-C14
14	a	1111	CLA	C11-C12-C13-C14
14	A	1111	CLA	C11-C12-C13-C14
14	G	1114	CLA	C2B-C3B-CAB-CBB
14	G	1120	CLA	C2B-C3B-CAB-CBB
14	H	1209	CLA	C2B-C3B-CAB-CBB
14	H	1217	CLA	C2B-C3B-CAB-CBB
14	H	1219	CLA	C2B-C3B-CAB-CBB
14	H	1233	CLA	C2B-C3B-CAB-CBB
14	H	1239	CLA	C2B-C3B-CAB-CBB
14	T	1401	CLA	C2B-C3B-CAB-CBB
14	a	1114	CLA	C2B-C3B-CAB-CBB
14	a	1120	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	b	1209	CLA	C2B-C3B-CAB-CBB
14	b	1217	CLA	C2B-C3B-CAB-CBB
14	b	1219	CLA	C2B-C3B-CAB-CBB
14	b	1233	CLA	C2B-C3B-CAB-CBB
14	b	1239	CLA	C2B-C3B-CAB-CBB
14	k	1401	CLA	C2B-C3B-CAB-CBB
14	A	1114	CLA	C2B-C3B-CAB-CBB
14	A	1120	CLA	C2B-C3B-CAB-CBB
14	B	1209	CLA	C2B-C3B-CAB-CBB
14	B	1217	CLA	C2B-C3B-CAB-CBB
14	B	1219	CLA	C2B-C3B-CAB-CBB
14	B	1233	CLA	C2B-C3B-CAB-CBB
14	B	1239	CLA	C2B-C3B-CAB-CBB
14	K	1401	CLA	C2B-C3B-CAB-CBB
18	G	4003	BCR	C1-C6-C7-C8
18	G	4003	BCR	C5-C6-C7-C8
18	G	4007	BCR	C23-C24-C25-C26
18	G	4007	BCR	C23-C24-C25-C30
18	G	4008	BCR	C1-C6-C7-C8
18	G	4008	BCR	C5-C6-C7-C8
18	G	4008	BCR	C23-C24-C25-C26
18	G	4008	BCR	C23-C24-C25-C30
18	H	4006	BCR	C1-C6-C7-C8
18	H	4006	BCR	C23-C24-C25-C26
18	H	4006	BCR	C23-C24-C25-C30
18	H	4009	BCR	C1-C6-C7-C8
18	H	4009	BCR	C5-C6-C7-C8
18	H	4013	BCR	C23-C24-C25-C30
18	H	4016	BCR	C1-C6-C7-C8
18	H	4016	BCR	C5-C6-C7-C8
18	H	4017	BCR	C23-C24-C25-C30
18	a	4003	BCR	C1-C6-C7-C8
18	a	4003	BCR	C5-C6-C7-C8
18	a	4007	BCR	C23-C24-C25-C26
18	a	4007	BCR	C23-C24-C25-C30
18	a	4008	BCR	C1-C6-C7-C8
18	a	4008	BCR	C5-C6-C7-C8
18	a	4008	BCR	C23-C24-C25-C26
18	a	4008	BCR	C23-C24-C25-C30
18	b	4006	BCR	C1-C6-C7-C8
18	b	4006	BCR	C23-C24-C25-C26
18	b	4006	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
18	b	4009	BCR	C1-C6-C7-C8
18	b	4009	BCR	C5-C6-C7-C8
18	b	4013	BCR	C23-C24-C25-C30
18	b	4016	BCR	C1-C6-C7-C8
18	b	4016	BCR	C5-C6-C7-C8
18	b	4017	BCR	C23-C24-C25-C30
18	A	4003	BCR	C1-C6-C7-C8
18	A	4003	BCR	C5-C6-C7-C8
18	A	4007	BCR	C23-C24-C25-C26
18	A	4007	BCR	C23-C24-C25-C30
18	A	4008	BCR	C1-C6-C7-C8
18	A	4008	BCR	C5-C6-C7-C8
18	A	4008	BCR	C23-C24-C25-C26
18	A	4008	BCR	C23-C24-C25-C30
18	B	4006	BCR	C1-C6-C7-C8
18	B	4006	BCR	C23-C24-C25-C26
18	B	4006	BCR	C23-C24-C25-C30
18	B	4009	BCR	C1-C6-C7-C8
18	B	4009	BCR	C5-C6-C7-C8
18	B	4013	BCR	C23-C24-C25-C30
18	B	4016	BCR	C1-C6-C7-C8
18	B	4016	BCR	C5-C6-C7-C8
18	B	4017	BCR	C23-C24-C25-C30
18	L	4019	BCR	C23-C24-C25-C30
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	G	1130	CLA	C4-C3-C5-C6
14	a	1130	CLA	C4-C3-C5-C6
14	A	1130	CLA	C4-C3-C5-C6
18	G	4007	BCR	C10-C11-C12-C13
18	H	4004	BCR	C10-C11-C12-C13
18	V	4021	BCR	C18-C19-C20-C21
18	a	4007	BCR	C10-C11-C12-C13
18	b	4004	BCR	C10-C11-C12-C13
18	b	4010	BCR	C10-C11-C12-C13
18	m	4021	BCR	C18-C19-C20-C21
18	A	4007	BCR	C10-C11-C12-C13
18	B	4004	BCR	C10-C11-C12-C13
18	B	4010	BCR	C10-C11-C12-C13
18	M	4021	BCR	C18-C19-C20-C21
14	b	1210	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	B	1210	CLA	C10-C11-C12-C13
14	G	1103	CLA	C2-C3-C5-C6
14	a	1103	CLA	C2-C3-C5-C6
14	A	1103	CLA	C2-C3-C5-C6
16	b	2002	PQN	C12-C13-C15-C16
16	B	2002	PQN	C12-C13-C15-C16
14	H	1223	CLA	C16-C17-C18-C20
14	b	1223	CLA	C16-C17-C18-C20
14	B	1223	CLA	C16-C17-C18-C20
19	H	5004	LHG	C13-C14-C15-C16
14	G	1013	CLA	CBA-CGA-O2A-C1
14	G	1127	CLA	CBA-CGA-O2A-C1
14	G	1136	CLA	CBA-CGA-O2A-C1
14	H	1228	CLA	CBA-CGA-O2A-C1
14	U	1501	CLA	CBA-CGA-O2A-C1
14	a	1013	CLA	CBA-CGA-O2A-C1
14	a	1136	CLA	CBA-CGA-O2A-C1
14	b	1228	CLA	CBA-CGA-O2A-C1
14	l	1501	CLA	CBA-CGA-O2A-C1
14	A	1013	CLA	CBA-CGA-O2A-C1
14	A	1136	CLA	CBA-CGA-O2A-C1
14	B	1228	CLA	CBA-CGA-O2A-C1
14	L	1501	CLA	CBA-CGA-O2A-C1
15	H	1237	F6C	C6-C7-C8-C9
15	b	1237	F6C	C6-C7-C8-C9
15	B	1237	F6C	C6-C7-C8-C9
19	b	5004	LHG	C13-C14-C15-C16
19	B	5004	LHG	C13-C14-C15-C16
14	G	1115	CLA	C10-C11-C12-C13
14	H	1210	CLA	C10-C11-C12-C13
14	H	1211	CLA	C5-C6-C7-C8
14	a	1115	CLA	C10-C11-C12-C13
14	b	1211	CLA	C5-C6-C7-C8
14	A	1115	CLA	C10-C11-C12-C13
14	B	1211	CLA	C5-C6-C7-C8
14	G	1012	CLA	C10-C11-C12-C13
14	G	1102	CLA	C5-C6-C7-C8
14	G	1126	CLA	C5-C6-C7-C8
14	a	1012	CLA	C10-C11-C12-C13
14	a	1102	CLA	C5-C6-C7-C8
14	a	1126	CLA	C5-C6-C7-C8
14	A	1012	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	A	1102	CLA	C5-C6-C7-C8
14	A	1126	CLA	C5-C6-C7-C8
14	a	1127	CLA	CBA-CGA-O2A-C1
14	A	1127	CLA	CBA-CGA-O2A-C1
14	A	1126	CLA	C10-C11-C12-C13
14	G	1126	CLA	C10-C11-C12-C13
15	H	1237	F6C	C3-C5-C6-C7
15	b	1237	F6C	C3-C5-C6-C7
15	B	1237	F6C	C3-C5-C6-C7
18	H	4016	BCR	C7-C8-C9-C10
18	b	4016	BCR	C7-C8-C9-C10
18	B	4016	BCR	C7-C8-C9-C10
14	a	1126	CLA	C10-C11-C12-C13
14	H	1023	CLA	C2A-CAA-CBA-CGA
14	b	1023	CLA	C2A-CAA-CBA-CGA
14	B	1023	CLA	C2A-CAA-CBA-CGA
14	H	1208	CLA	C16-C17-C18-C19
14	b	1208	CLA	C16-C17-C18-C19
14	B	1208	CLA	C16-C17-C18-C19
14	H	1225	CLA	C4-C3-C5-C6
14	b	1225	CLA	C4-C3-C5-C6
14	B	1225	CLA	C4-C3-C5-C6
14	G	1130	CLA	C2-C3-C5-C6
15	G	1121	F6C	C2B-C3B-CAB-CBB
15	a	1121	F6C	C2B-C3B-CAB-CBB
15	A	1121	F6C	C2B-C3B-CAB-CBB
16	H	2002	PQN	C12-C13-C15-C16
19	H	5004	LHG	C25-C26-C27-C28
19	b	5004	LHG	C25-C26-C27-C28
14	A	1135	CLA	C5-C6-C7-C8
19	B	5004	LHG	C25-C26-C27-C28
14	G	1135	CLA	C5-C6-C7-C8
14	U	1501	CLA	C5-C6-C7-C8
14	a	1135	CLA	C5-C6-C7-C8
14	l	1501	CLA	C5-C6-C7-C8
14	L	1501	CLA	C5-C6-C7-C8
16	G	2001	PQN	C25-C26-C27-C28
16	H	2002	PQN	C15-C16-C17-C18
16	a	2001	PQN	C25-C26-C27-C28
16	b	2002	PQN	C15-C16-C17-C18
16	A	2001	PQN	C25-C26-C27-C28
16	B	2002	PQN	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	U	1502	CLA	C8-C10-C11-C12
14	l	1502	CLA	C8-C10-C11-C12
14	L	1502	CLA	C8-C10-C11-C12
14	G	1126	CLA	O1A-CGA-O2A-C1
14	a	1126	CLA	O1A-CGA-O2A-C1
14	A	1126	CLA	O1A-CGA-O2A-C1
15	H	1238	F6C	C8-C10-C11-C12
15	b	1238	F6C	C8-C10-C11-C12
15	B	1238	F6C	C8-C10-C11-C12
14	H	1225	CLA	O1D-CGD-O2D-CED
14	b	1225	CLA	O1D-CGD-O2D-CED
14	B	1225	CLA	O1D-CGD-O2D-CED
20	A	5005	LMG	C29-C30-C31-C32
14	G	1123	CLA	C2-C1-O2A-CGA
14	G	1129	CLA	C2-C1-O2A-CGA
14	a	1123	CLA	C2-C1-O2A-CGA
14	a	1129	CLA	C2-C1-O2A-CGA
14	A	1123	CLA	C2-C1-O2A-CGA
14	A	1129	CLA	C2-C1-O2A-CGA
20	G	5005	LMG	C29-C30-C31-C32
20	a	5005	LMG	C29-C30-C31-C32
15	H	1238	F6C	C1A-C2A-CAA-CBA
15	b	1238	F6C	C1A-C2A-CAA-CBA
15	B	1238	F6C	C1A-C2A-CAA-CBA
16	H	2002	PQN	C14-C13-C15-C16
16	b	2002	PQN	C14-C13-C15-C16
16	B	2002	PQN	C14-C13-C15-C16
14	a	1130	CLA	C2-C3-C5-C6
16	G	2001	PQN	C15-C16-C17-C18
16	A	2001	PQN	C15-C16-C17-C18
14	G	1012	CLA	C2A-CAA-CBA-CGA
14	G	1126	CLA	C2A-CAA-CBA-CGA
14	a	1012	CLA	C2A-CAA-CBA-CGA
14	a	1126	CLA	C2A-CAA-CBA-CGA
14	A	1012	CLA	C2A-CAA-CBA-CGA
14	A	1126	CLA	C2A-CAA-CBA-CGA
14	G	1110	CLA	CBD-CGD-O2D-CED
14	a	1110	CLA	CBD-CGD-O2D-CED
14	A	1110	CLA	CBD-CGD-O2D-CED
15	H	1207	F6C	O1D-CGD-O2D-CED
15	b	1207	F6C	O1D-CGD-O2D-CED
15	B	1207	F6C	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	G	1111	CLA	C5-C6-C7-C8
14	H	1221	CLA	C8-C10-C11-C12
14	a	1111	CLA	C5-C6-C7-C8
14	b	1221	CLA	C8-C10-C11-C12
14	A	1111	CLA	C5-C6-C7-C8
14	B	1221	CLA	C8-C10-C11-C12
16	a	2001	PQN	C15-C16-C17-C18
19	H	5004	LHG	O1-C1-C2-O2
19	b	5004	LHG	O1-C1-C2-O2
19	B	5004	LHG	O1-C1-C2-O2
14	G	1127	CLA	O1A-CGA-O2A-C1
14	U	1501	CLA	O1A-CGA-O2A-C1
14	a	1127	CLA	O1A-CGA-O2A-C1
14	l	1501	CLA	O1A-CGA-O2A-C1
14	A	1127	CLA	O1A-CGA-O2A-C1
14	L	1501	CLA	O1A-CGA-O2A-C1
19	G	5001	LHG	C13-C14-C15-C16
14	G	1103	CLA	C1A-C2A-CAA-CBA
14	G	1105	CLA	C1A-C2A-CAA-CBA
14	G	1106	CLA	C1A-C2A-CAA-CBA
14	G	1107	CLA	C1A-C2A-CAA-CBA
14	G	1110	CLA	C1A-C2A-CAA-CBA
14	G	1113	CLA	C1A-C2A-CAA-CBA
14	G	1116	CLA	C1A-C2A-CAA-CBA
14	G	1118	CLA	C1A-C2A-CAA-CBA
14	G	1132	CLA	C1A-C2A-CAA-CBA
14	G	1135	CLA	C1A-C2A-CAA-CBA
14	G	1137	CLA	C1A-C2A-CAA-CBA
14	H	1215	CLA	C1A-C2A-CAA-CBA
14	H	1220	CLA	C1A-C2A-CAA-CBA
14	H	1227	CLA	C1A-C2A-CAA-CBA
14	H	1229	CLA	C1A-C2A-CAA-CBA
14	H	1236	CLA	C1A-C2A-CAA-CBA
14	a	1103	CLA	C1A-C2A-CAA-CBA
14	a	1105	CLA	C1A-C2A-CAA-CBA
14	a	1106	CLA	C1A-C2A-CAA-CBA
14	a	1107	CLA	C1A-C2A-CAA-CBA
14	a	1110	CLA	C1A-C2A-CAA-CBA
14	a	1113	CLA	C1A-C2A-CAA-CBA
14	a	1116	CLA	C1A-C2A-CAA-CBA
14	a	1118	CLA	C1A-C2A-CAA-CBA
14	a	1132	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	a	1135	CLA	C1A-C2A-CAA-CBA
14	a	1137	CLA	C1A-C2A-CAA-CBA
14	b	1215	CLA	C1A-C2A-CAA-CBA
14	b	1220	CLA	C1A-C2A-CAA-CBA
14	b	1227	CLA	C1A-C2A-CAA-CBA
14	b	1229	CLA	C1A-C2A-CAA-CBA
14	b	1236	CLA	C1A-C2A-CAA-CBA
14	A	1103	CLA	C1A-C2A-CAA-CBA
14	A	1105	CLA	C1A-C2A-CAA-CBA
14	A	1106	CLA	C1A-C2A-CAA-CBA
14	A	1107	CLA	C1A-C2A-CAA-CBA
14	A	1110	CLA	C1A-C2A-CAA-CBA
14	A	1113	CLA	C1A-C2A-CAA-CBA
14	A	1116	CLA	C1A-C2A-CAA-CBA
14	A	1118	CLA	C1A-C2A-CAA-CBA
14	A	1132	CLA	C1A-C2A-CAA-CBA
14	A	1135	CLA	C1A-C2A-CAA-CBA
14	A	1137	CLA	C1A-C2A-CAA-CBA
14	B	1215	CLA	C1A-C2A-CAA-CBA
14	B	1220	CLA	C1A-C2A-CAA-CBA
14	B	1227	CLA	C1A-C2A-CAA-CBA
14	B	1229	CLA	C1A-C2A-CAA-CBA
14	B	1236	CLA	C1A-C2A-CAA-CBA
19	a	5001	LHG	C13-C14-C15-C16
19	A	5001	LHG	C13-C14-C15-C16
15	H	1207	F6C	C13-C15-C16-C17
15	b	1207	F6C	C13-C15-C16-C17
15	B	1207	F6C	C13-C15-C16-C17
14	G	1102	CLA	C6-C7-C8-C10
14	G	1115	CLA	C12-C13-C15-C16
14	G	1117	CLA	C6-C7-C8-C10
14	G	1123	CLA	C6-C7-C8-C10
14	G	1131	CLA	C6-C7-C8-C10
14	H	1022	CLA	C11-C12-C13-C15
14	H	1023	CLA	C11-C10-C8-C7
14	H	1210	CLA	C6-C7-C8-C10
14	H	1213	CLA	C6-C7-C8-C10
14	H	1214	CLA	C11-C12-C13-C15
14	H	1215	CLA	C6-C7-C8-C10
14	H	1216	CLA	C11-C12-C13-C15
14	H	1221	CLA	C11-C12-C13-C15
14	H	1224	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	H	1234	CLA	C11-C12-C13-C15
14	H	1239	CLA	C11-C10-C8-C7
14	a	1102	CLA	C6-C7-C8-C10
14	a	1115	CLA	C12-C13-C15-C16
14	a	1117	CLA	C6-C7-C8-C10
14	a	1123	CLA	C6-C7-C8-C10
14	a	1131	CLA	C6-C7-C8-C10
14	b	1022	CLA	C11-C12-C13-C15
14	b	1023	CLA	C11-C10-C8-C7
14	b	1210	CLA	C6-C7-C8-C10
14	b	1213	CLA	C6-C7-C8-C10
14	b	1214	CLA	C11-C12-C13-C15
14	b	1215	CLA	C6-C7-C8-C10
14	b	1216	CLA	C11-C12-C13-C15
14	b	1221	CLA	C11-C12-C13-C15
14	b	1224	CLA	C12-C13-C15-C16
14	b	1234	CLA	C11-C12-C13-C15
14	b	1239	CLA	C11-C10-C8-C7
14	A	1102	CLA	C6-C7-C8-C10
14	A	1115	CLA	C12-C13-C15-C16
14	A	1117	CLA	C6-C7-C8-C10
14	A	1123	CLA	C6-C7-C8-C10
14	A	1131	CLA	C6-C7-C8-C10
14	B	1022	CLA	C11-C12-C13-C15
14	B	1023	CLA	C11-C10-C8-C7
14	B	1210	CLA	C6-C7-C8-C10
14	B	1213	CLA	C6-C7-C8-C10
14	B	1214	CLA	C11-C12-C13-C15
14	B	1215	CLA	C6-C7-C8-C10
14	B	1216	CLA	C11-C12-C13-C15
14	B	1221	CLA	C11-C12-C13-C15
14	B	1224	CLA	C12-C13-C15-C16
14	B	1234	CLA	C11-C12-C13-C15
14	B	1239	CLA	C11-C10-C8-C7
15	H	1238	F6C	C6-C7-C8-C10
15	b	1238	F6C	C6-C7-C8-C10
15	B	1238	F6C	C6-C7-C8-C10
14	G	1131	CLA	C5-C6-C7-C8
14	G	1135	CLA	C8-C10-C11-C12
14	H	1224	CLA	C10-C11-C12-C13
14	a	1131	CLA	C5-C6-C7-C8
14	a	1135	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	b	1224	CLA	C10-C11-C12-C13
14	A	1131	CLA	C5-C6-C7-C8
14	A	1135	CLA	C8-C10-C11-C12
14	B	1224	CLA	C10-C11-C12-C13
14	a	1136	CLA	O1A-CGA-O2A-C1
14	G	1112	CLA	C2-C3-C5-C6
14	a	1112	CLA	C2-C3-C5-C6
14	A	1112	CLA	C2-C3-C5-C6
14	A	1130	CLA	C2-C3-C5-C6
19	b	5004	LHG	C11-C12-C13-C14
14	G	1136	CLA	O1A-CGA-O2A-C1
14	A	1136	CLA	O1A-CGA-O2A-C1
19	H	5004	LHG	C11-C12-C13-C14
19	B	5004	LHG	C11-C12-C13-C14
14	G	1116	CLA	C2A-CAA-CBA-CGA
14	a	1116	CLA	C2A-CAA-CBA-CGA
14	A	1116	CLA	C2A-CAA-CBA-CGA
14	G	1111	CLA	C6-C7-C8-C9
14	G	1125	CLA	C6-C7-C8-C9
14	G	1131	CLA	C6-C7-C8-C9
14	H	1022	CLA	C11-C12-C13-C14
14	H	1023	CLA	C11-C10-C8-C9
14	H	1210	CLA	C6-C7-C8-C9
14	H	1214	CLA	C11-C12-C13-C14
14	H	1215	CLA	C6-C7-C8-C9
14	H	1216	CLA	C11-C12-C13-C14
14	H	1216	CLA	C14-C13-C15-C16
14	H	1234	CLA	C11-C12-C13-C14
14	a	1111	CLA	C6-C7-C8-C9
14	a	1125	CLA	C6-C7-C8-C9
14	a	1131	CLA	C6-C7-C8-C9
14	b	1022	CLA	C11-C12-C13-C14
14	b	1023	CLA	C11-C10-C8-C9
14	b	1210	CLA	C6-C7-C8-C9
14	b	1214	CLA	C11-C12-C13-C14
14	b	1215	CLA	C6-C7-C8-C9
14	b	1216	CLA	C11-C12-C13-C14
14	b	1216	CLA	C14-C13-C15-C16
14	b	1234	CLA	C11-C12-C13-C14
14	A	1111	CLA	C6-C7-C8-C9
14	A	1125	CLA	C6-C7-C8-C9
14	A	1131	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	B	1022	CLA	C11-C12-C13-C14
14	B	1023	CLA	C11-C10-C8-C9
14	B	1210	CLA	C6-C7-C8-C9
14	B	1214	CLA	C11-C12-C13-C14
14	B	1215	CLA	C6-C7-C8-C9
14	B	1216	CLA	C11-C12-C13-C14
14	B	1216	CLA	C14-C13-C15-C16
14	B	1234	CLA	C11-C12-C13-C14
18	U	4019	BCR	C15-C16-C17-C18
18	l	4019	BCR	C15-C16-C17-C18
18	L	4019	BCR	C15-C16-C17-C18
20	U	5007	LMG	C18-C19-C20-C21
20	l	5007	LMG	C18-C19-C20-C21
20	L	5007	LMG	C18-C19-C20-C21
14	b	1211	CLA	CBA-CGA-O2A-C1
14	B	1211	CLA	CBA-CGA-O2A-C1
14	G	1118	CLA	C5-C6-C7-C8
14	a	1118	CLA	C5-C6-C7-C8
20	R	5006	LMG	O6-C5-C6-O5
20	i	5006	LMG	O6-C5-C6-O5
20	I	5006	LMG	O6-C5-C6-O5
15	H	1237	F6C	C1A-C2A-CAA-CBA
15	b	1237	F6C	C1A-C2A-CAA-CBA
15	B	1237	F6C	C1A-C2A-CAA-CBA
14	A	1118	CLA	C5-C6-C7-C8
19	H	5004	LHG	C4-C5-C6-O8
19	b	5004	LHG	C4-C5-C6-O8
19	B	5004	LHG	C4-C5-C6-O8
20	U	5007	LMG	O6-C5-C6-O5
20	l	5007	LMG	O6-C5-C6-O5
20	L	5007	LMG	O6-C5-C6-O5
19	G	5001	LHG	C30-C31-C32-C33
19	a	5001	LHG	C30-C31-C32-C33
19	A	5001	LHG	C30-C31-C32-C33
14	H	1211	CLA	CBA-CGA-O2A-C1
14	H	1225	CLA	CBA-CGA-O2A-C1
14	b	1225	CLA	CBA-CGA-O2A-C1
14	B	1225	CLA	CBA-CGA-O2A-C1
14	H	1221	CLA	C16-C17-C18-C19
14	b	1221	CLA	C16-C17-C18-C19
14	B	1221	CLA	C16-C17-C18-C19
18	R	4020	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
18	i	4020	BCR	C20-C21-C22-C37
18	I	4020	BCR	C20-C21-C22-C37
18	V	4021	BCR	C14-C15-C16-C17
18	m	4021	BCR	C14-C15-C16-C17
18	M	4021	BCR	C14-C15-C16-C17
14	H	1228	CLA	O1A-CGA-O2A-C1
14	b	1228	CLA	O1A-CGA-O2A-C1
14	B	1228	CLA	O1A-CGA-O2A-C1
14	H	1225	CLA	C2-C3-C5-C6
14	b	1225	CLA	C2-C3-C5-C6
14	B	1225	CLA	C2-C3-C5-C6
14	H	1021	CLA	C10-C11-C12-C13
14	b	1021	CLA	C10-C11-C12-C13
14	B	1021	CLA	C10-C11-C12-C13
21	G	6002	LMT	O5B-C5B-C6B-O6B
21	a	6002	LMT	O5B-C5B-C6B-O6B
21	A	6002	LMT	O5B-C5B-C6B-O6B
14	b	1211	CLA	O1A-CGA-O2A-C1
14	G	1126	CLA	C8-C10-C11-C12
14	A	1136	CLA	C2A-CAA-CBA-CGA
14	H	1213	CLA	C13-C15-C16-C17
14	a	1126	CLA	C8-C10-C11-C12
14	b	1213	CLA	C13-C15-C16-C17
14	A	1126	CLA	C8-C10-C11-C12
14	B	1213	CLA	C13-C15-C16-C17
14	H	1211	CLA	O1A-CGA-O2A-C1
14	H	1213	CLA	CBA-CGA-O2A-C1
14	a	1119	CLA	CBA-CGA-O2A-C1
14	b	1213	CLA	CBA-CGA-O2A-C1
14	A	1119	CLA	CBA-CGA-O2A-C1
14	B	1213	CLA	CBA-CGA-O2A-C1
18	H	4013	BCR	C10-C11-C12-C13
18	b	4013	BCR	C10-C11-C12-C13
18	B	4013	BCR	C10-C11-C12-C13
18	G	4011	BCR	C19-C20-C21-C22
18	a	4011	BCR	C19-C20-C21-C22
18	A	4011	BCR	C19-C20-C21-C22
15	H	1207	F6C	C16-C17-C18-C19
15	b	1207	F6C	C16-C17-C18-C19
15	B	1207	F6C	C16-C17-C18-C19
14	B	1211	CLA	O1A-CGA-O2A-C1
19	H	5004	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	b	5004	LHG	C9-C10-C11-C12
19	B	5004	LHG	C9-C10-C11-C12
14	a	1128	CLA	O1D-CGD-O2D-CED
14	G	1119	CLA	CBA-CGA-O2A-C1
14	A	1128	CLA	O1D-CGD-O2D-CED
14	H	1235	CLA	C4-C3-C5-C6
14	b	1235	CLA	C4-C3-C5-C6
14	B	1235	CLA	C4-C3-C5-C6
13	G	1011	CL0	C16-C17-C18-C20
13	a	1011	CL0	C16-C17-C18-C20
13	A	1011	CL0	C16-C17-C18-C20
14	G	1128	CLA	O1D-CGD-O2D-CED
14	H	1208	CLA	CAA-CBA-CGA-O2A
14	b	1208	CLA	CAA-CBA-CGA-O2A
14	B	1208	CLA	CAA-CBA-CGA-O2A
20	R	5006	LMG	O7-C10-C11-C12
20	i	5006	LMG	O7-C10-C11-C12
20	I	5006	LMG	O7-C10-C11-C12
14	G	1136	CLA	C2A-CAA-CBA-CGA
14	a	1136	CLA	C2A-CAA-CBA-CGA
14	G	1012	CLA	C13-C15-C16-C17
14	H	1203	CLA	C10-C11-C12-C13
14	H	1214	CLA	C5-C6-C7-C8
14	a	1012	CLA	C13-C15-C16-C17
14	b	1203	CLA	C10-C11-C12-C13
14	b	1214	CLA	C5-C6-C7-C8
14	A	1012	CLA	C13-C15-C16-C17
14	B	1203	CLA	C10-C11-C12-C13
14	B	1214	CLA	C5-C6-C7-C8
18	G	4001	BCR	C15-C16-C17-C18
18	a	4001	BCR	C15-C16-C17-C18
18	A	4001	BCR	C15-C16-C17-C18
14	G	1109	CLA	C16-C17-C18-C20
14	a	1109	CLA	C16-C17-C18-C20
14	A	1109	CLA	C16-C17-C18-C20
14	H	1220	CLA	C4-C3-C5-C6
14	b	1220	CLA	C4-C3-C5-C6
14	B	1220	CLA	C4-C3-C5-C6
14	H	1210	CLA	CBA-CGA-O2A-C1
14	b	1210	CLA	CBA-CGA-O2A-C1
14	B	1210	CLA	CBA-CGA-O2A-C1
14	G	1102	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	G	1109	CLA	C11-C12-C13-C14
14	G	1115	CLA	C14-C13-C15-C16
14	G	1117	CLA	C6-C7-C8-C9
14	G	1117	CLA	C11-C12-C13-C14
14	G	1117	CLA	C14-C13-C15-C16
14	G	1127	CLA	C14-C13-C15-C16
14	G	1128	CLA	C6-C7-C8-C9
14	G	1135	CLA	C11-C10-C8-C9
14	G	1136	CLA	C6-C7-C8-C9
14	H	1203	CLA	C11-C10-C8-C9
14	H	1204	CLA	C14-C13-C15-C16
14	H	1221	CLA	C11-C12-C13-C14
14	H	1224	CLA	C11-C12-C13-C14
14	H	1224	CLA	C14-C13-C15-C16
14	H	1239	CLA	C11-C10-C8-C9
14	a	1102	CLA	C6-C7-C8-C9
14	a	1109	CLA	C11-C12-C13-C14
14	a	1115	CLA	C14-C13-C15-C16
14	a	1117	CLA	C6-C7-C8-C9
14	a	1117	CLA	C11-C12-C13-C14
14	a	1117	CLA	C14-C13-C15-C16
14	a	1127	CLA	C14-C13-C15-C16
14	a	1128	CLA	C6-C7-C8-C9
14	a	1135	CLA	C11-C10-C8-C9
14	a	1136	CLA	C6-C7-C8-C9
14	b	1203	CLA	C11-C10-C8-C9
14	b	1204	CLA	C14-C13-C15-C16
14	b	1221	CLA	C11-C12-C13-C14
14	b	1224	CLA	C11-C12-C13-C14
14	b	1224	CLA	C14-C13-C15-C16
14	b	1239	CLA	C11-C10-C8-C9
14	A	1102	CLA	C6-C7-C8-C9
14	A	1109	CLA	C11-C12-C13-C14
14	A	1115	CLA	C14-C13-C15-C16
14	A	1117	CLA	C6-C7-C8-C9
14	A	1117	CLA	C11-C12-C13-C14
14	A	1117	CLA	C14-C13-C15-C16
14	A	1127	CLA	C14-C13-C15-C16
14	A	1128	CLA	C6-C7-C8-C9
14	A	1135	CLA	C11-C10-C8-C9
14	A	1136	CLA	C6-C7-C8-C9
14	B	1203	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
14	B	1204	CLA	C14-C13-C15-C16
14	B	1221	CLA	C11-C12-C13-C14
14	B	1224	CLA	C11-C12-C13-C14
14	B	1224	CLA	C14-C13-C15-C16
14	B	1239	CLA	C11-C10-C8-C9
15	H	1238	F6C	C6-C7-C8-C9
15	b	1238	F6C	C6-C7-C8-C9
15	B	1238	F6C	C6-C7-C8-C9
14	G	1013	CLA	C8-C10-C11-C12
14	A	1013	CLA	C8-C10-C11-C12
14	G	1101	CLA	C4B-C3B-CAB-CBB
14	G	1124	CLA	C4B-C3B-CAB-CBB
14	H	1022	CLA	C4B-C3B-CAB-CBB
14	H	1023	CLA	C4B-C3B-CAB-CBB
14	H	1227	CLA	C4B-C3B-CAB-CBB
14	a	1101	CLA	C4B-C3B-CAB-CBB
14	a	1124	CLA	C4B-C3B-CAB-CBB
14	b	1022	CLA	C4B-C3B-CAB-CBB
14	b	1023	CLA	C4B-C3B-CAB-CBB
14	b	1227	CLA	C4B-C3B-CAB-CBB
14	A	1124	CLA	C4B-C3B-CAB-CBB
14	B	1022	CLA	C4B-C3B-CAB-CBB
14	B	1023	CLA	C4B-C3B-CAB-CBB
14	B	1227	CLA	C4B-C3B-CAB-CBB
14	H	1224	CLA	C5-C6-C7-C8
14	a	1013	CLA	C8-C10-C11-C12
14	b	1224	CLA	C5-C6-C7-C8
14	B	1224	CLA	C5-C6-C7-C8
13	G	1011	CL0	C16-C17-C18-C19
13	a	1011	CL0	C16-C17-C18-C19
13	A	1011	CL0	C16-C17-C18-C19
19	H	5004	LHG	C32-C33-C34-C35
19	b	5004	LHG	C32-C33-C34-C35
20	a	5005	LMG	C32-C33-C34-C35
19	B	5004	LHG	C32-C33-C34-C35
20	G	5005	LMG	C32-C33-C34-C35
20	A	5005	LMG	C32-C33-C34-C35
14	G	1117	CLA	C11-C12-C13-C15
14	G	1117	CLA	C12-C13-C15-C16
14	G	1125	CLA	C6-C7-C8-C10
14	G	1126	CLA	C11-C10-C8-C7
14	G	1127	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	G	1128	CLA	C6-C7-C8-C10
14	G	1135	CLA	C11-C10-C8-C7
14	G	1140	CLA	C6-C7-C8-C10
14	H	1021	CLA	C12-C13-C15-C16
14	H	1022	CLA	C6-C7-C8-C10
14	H	1203	CLA	C12-C13-C15-C16
14	H	1208	CLA	C12-C13-C15-C16
14	H	1224	CLA	C11-C12-C13-C15
14	a	1117	CLA	C11-C12-C13-C15
14	a	1117	CLA	C12-C13-C15-C16
14	a	1125	CLA	C6-C7-C8-C10
14	a	1126	CLA	C11-C10-C8-C7
14	a	1128	CLA	C6-C7-C8-C10
14	a	1135	CLA	C11-C10-C8-C7
14	b	1021	CLA	C12-C13-C15-C16
14	b	1022	CLA	C6-C7-C8-C10
14	b	1203	CLA	C12-C13-C15-C16
14	b	1208	CLA	C12-C13-C15-C16
14	b	1224	CLA	C11-C12-C13-C15
14	A	1117	CLA	C11-C12-C13-C15
14	A	1117	CLA	C12-C13-C15-C16
14	A	1125	CLA	C6-C7-C8-C10
14	A	1126	CLA	C11-C10-C8-C7
14	A	1128	CLA	C6-C7-C8-C10
14	A	1135	CLA	C11-C10-C8-C7
14	B	1021	CLA	C12-C13-C15-C16
14	B	1022	CLA	C6-C7-C8-C10
14	B	1203	CLA	C12-C13-C15-C16
14	B	1208	CLA	C12-C13-C15-C16
14	B	1224	CLA	C11-C12-C13-C15
15	H	1237	F6C	C11-C12-C13-C15
15	b	1237	F6C	C11-C12-C13-C15
15	B	1237	F6C	C11-C12-C13-C15
16	a	2001	PQN	C21-C22-C23-C25
15	B	1238	F6C	C13-C15-C16-C17
15	H	1238	F6C	C13-C15-C16-C17
15	b	1238	F6C	C13-C15-C16-C17
14	H	1202	CLA	C11-C12-C13-C14
14	b	1202	CLA	C11-C12-C13-C14
14	A	1133	CLA	C11-C12-C13-C15
14	B	1202	CLA	C11-C12-C13-C14
14	G	1013	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	A	1013	CLA	O1A-CGA-O2A-C1
14	G	1111	CLA	C4-C3-C5-C6
14	G	1112	CLA	C3A-C2A-CAA-CBA
14	G	1112	CLA	C4-C3-C5-C6
14	G	1124	CLA	C3A-C2A-CAA-CBA
14	G	1138	CLA	C4-C3-C5-C6
14	H	1203	CLA	C3A-C2A-CAA-CBA
14	a	1111	CLA	C4-C3-C5-C6
14	a	1112	CLA	C3A-C2A-CAA-CBA
14	a	1112	CLA	C4-C3-C5-C6
14	a	1124	CLA	C3A-C2A-CAA-CBA
14	a	1126	CLA	C4-C3-C5-C6
14	a	1138	CLA	C4-C3-C5-C6
14	b	1203	CLA	C3A-C2A-CAA-CBA
14	A	1111	CLA	C4-C3-C5-C6
14	A	1112	CLA	C3A-C2A-CAA-CBA
14	A	1112	CLA	C4-C3-C5-C6
14	A	1124	CLA	C3A-C2A-CAA-CBA
14	A	1138	CLA	C4-C3-C5-C6
14	B	1203	CLA	C3A-C2A-CAA-CBA
14	H	1202	CLA	C8-C10-C11-C12
14	B	1202	CLA	C8-C10-C11-C12
14	H	1205	CLA	C2-C3-C5-C6
14	b	1205	CLA	C2-C3-C5-C6
14	B	1205	CLA	C2-C3-C5-C6
14	H	1225	CLA	O1A-CGA-O2A-C1
14	a	1013	CLA	O1A-CGA-O2A-C1
14	b	1225	CLA	O1A-CGA-O2A-C1
14	B	1225	CLA	O1A-CGA-O2A-C1
14	H	1208	CLA	C5-C6-C7-C8
14	b	1202	CLA	C8-C10-C11-C12
14	B	1208	CLA	C5-C6-C7-C8
18	G	4003	BCR	C19-C20-C21-C22
18	G	4008	BCR	C9-C10-C11-C12
18	G	4011	BCR	C9-C10-C11-C12
18	H	4014	BCR	C19-C20-C21-C22
18	a	4003	BCR	C19-C20-C21-C22
18	a	4008	BCR	C9-C10-C11-C12
18	a	4011	BCR	C9-C10-C11-C12
18	b	4014	BCR	C19-C20-C21-C22
18	A	4003	BCR	C19-C20-C21-C22
18	A	4008	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
18	A	4011	BCR	C9-C10-C11-C12
18	B	4014	BCR	C19-C20-C21-C22
14	G	1133	CLA	C11-C12-C13-C15
14	a	1133	CLA	C11-C12-C13-C15
14	b	1208	CLA	C5-C6-C7-C8
14	G	1119	CLA	O1A-CGA-O2A-C1
14	a	1119	CLA	O1A-CGA-O2A-C1
14	H	1214	CLA	C15-C16-C17-C18
14	b	1214	CLA	C15-C16-C17-C18
14	B	1214	CLA	C15-C16-C17-C18
16	a	2001	PQN	C18-C20-C21-C22
16	A	2001	PQN	C18-C20-C21-C22
14	H	1217	CLA	C2A-CAA-CBA-CGA
14	b	1217	CLA	C2A-CAA-CBA-CGA
14	B	1217	CLA	C2A-CAA-CBA-CGA
20	G	5005	LMG	C7-C8-C9-O8
20	a	5005	LMG	C7-C8-C9-O8
20	A	5005	LMG	C7-C8-C9-O8
20	U	5007	LMG	C39-C40-C41-C42
14	a	1133	CLA	C11-C12-C13-C14
14	A	1133	CLA	C11-C12-C13-C14
14	a	1136	CLA	C13-C15-C16-C17
14	A	1136	CLA	C13-C15-C16-C17
16	G	2001	PQN	C18-C20-C21-C22
20	l	5007	LMG	C39-C40-C41-C42
20	L	5007	LMG	C39-C40-C41-C42
14	A	1119	CLA	O1A-CGA-O2A-C1
14	G	1136	CLA	C13-C15-C16-C17
14	H	1226	CLA	C5-C6-C7-C8
14	b	1226	CLA	C5-C6-C7-C8
14	B	1226	CLA	C5-C6-C7-C8
14	G	1126	CLA	C4-C3-C5-C6
14	H	1205	CLA	C4-C3-C5-C6
14	A	1126	CLA	C4-C3-C5-C6
14	b	1202	CLA	CAA-CBA-CGA-O2A
14	H	1201	CLA	C3-C5-C6-C7
14	b	1201	CLA	C3-C5-C6-C7
14	B	1201	CLA	C3-C5-C6-C7
14	G	1133	CLA	C11-C12-C13-C14
19	H	5004	LHG	O6-C4-C5-O7
19	b	5004	LHG	O6-C4-C5-O7
19	B	5004	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
14	H	1215	CLA	C2B-C3B-CAB-CBB
14	b	1215	CLA	C2B-C3B-CAB-CBB
14	B	1215	CLA	C2B-C3B-CAB-CBB
18	G	4001	BCR	C1-C6-C7-C8
18	G	4001	BCR	C23-C24-C25-C30
18	R	4020	BCR	C23-C24-C25-C30
18	U	4019	BCR	C23-C24-C25-C30
18	V	4021	BCR	C1-C6-C7-C8
18	V	4021	BCR	C23-C24-C25-C30
18	a	4001	BCR	C1-C6-C7-C8
18	a	4001	BCR	C23-C24-C25-C30
18	i	4020	BCR	C23-C24-C25-C30
18	l	4019	BCR	C23-C24-C25-C30
18	m	4021	BCR	C1-C6-C7-C8
18	m	4021	BCR	C23-C24-C25-C30
18	A	4001	BCR	C1-C6-C7-C8
18	A	4001	BCR	C23-C24-C25-C30
18	I	4020	BCR	C23-C24-C25-C30
18	M	4021	BCR	C1-C6-C7-C8
18	M	4021	BCR	C23-C24-C25-C30
14	H	1021	CLA	CAA-CBA-CGA-O2A
14	H	1202	CLA	CAA-CBA-CGA-O2A
14	b	1021	CLA	CAA-CBA-CGA-O2A
14	B	1021	CLA	CAA-CBA-CGA-O2A
14	B	1202	CLA	CAA-CBA-CGA-O2A
19	H	5004	LHG	C2-C3-O3-P
19	b	5004	LHG	C2-C3-O3-P
19	B	5004	LHG	C2-C3-O3-P
14	H	1217	CLA	C5-C6-C7-C8
14	b	1217	CLA	C5-C6-C7-C8
14	B	1217	CLA	C5-C6-C7-C8
15	H	1237	F6C	C3A-C2A-CAA-CBA
15	b	1237	F6C	C3A-C2A-CAA-CBA
15	B	1237	F6C	C3A-C2A-CAA-CBA
14	H	1239	CLA	C16-C17-C18-C20
14	b	1239	CLA	C16-C17-C18-C20
14	B	1239	CLA	C16-C17-C18-C20
14	G	1137	CLA	C2A-CAA-CBA-CGA
14	a	1137	CLA	C2A-CAA-CBA-CGA
14	A	1137	CLA	C2A-CAA-CBA-CGA
14	H	1214	CLA	C10-C11-C12-C13
14	b	1214	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	B	1214	CLA	C10-C11-C12-C13
20	G	5005	LMG	O7-C8-C9-O8
20	a	5005	LMG	O7-C8-C9-O8
20	A	5005	LMG	O7-C8-C9-O8
14	a	1111	CLA	C3-C5-C6-C7
14	G	1132	CLA	C4-C3-C5-C6
14	a	1132	CLA	C4-C3-C5-C6
14	b	1205	CLA	C4-C3-C5-C6
14	A	1132	CLA	C4-C3-C5-C6
14	B	1205	CLA	C4-C3-C5-C6
14	G	1117	CLA	C10-C11-C12-C13
14	G	1125	CLA	C15-C16-C17-C18
14	a	1117	CLA	C10-C11-C12-C13
14	a	1125	CLA	C15-C16-C17-C18
14	A	1117	CLA	C10-C11-C12-C13
14	A	1125	CLA	C15-C16-C17-C18
14	G	1138	CLA	C2-C3-C5-C6
14	H	1220	CLA	C2-C3-C5-C6
14	a	1138	CLA	C2-C3-C5-C6
14	b	1220	CLA	C2-C3-C5-C6
14	A	1138	CLA	C2-C3-C5-C6
14	B	1220	CLA	C2-C3-C5-C6
14	b	1208	CLA	C16-C17-C18-C20
14	H	1213	CLA	O1A-CGA-O2A-C1
14	b	1213	CLA	O1A-CGA-O2A-C1
14	B	1213	CLA	O1A-CGA-O2A-C1
14	G	1111	CLA	C3-C5-C6-C7
14	G	1124	CLA	C3-C5-C6-C7
14	a	1124	CLA	C3-C5-C6-C7
14	A	1111	CLA	C3-C5-C6-C7
14	A	1124	CLA	C3-C5-C6-C7
14	G	1126	CLA	C11-C10-C8-C9
14	a	1126	CLA	C11-C10-C8-C9
14	A	1126	CLA	C11-C10-C8-C9
14	H	1208	CLA	C16-C17-C18-C20
14	B	1208	CLA	C16-C17-C18-C20
14	H	1022	CLA	C3-C5-C6-C7
14	b	1022	CLA	C3-C5-C6-C7
14	B	1022	CLA	C3-C5-C6-C7
15	H	1238	F6C	C3A-C2A-CAA-CBA
15	b	1238	F6C	C3A-C2A-CAA-CBA
15	B	1238	F6C	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	G	5005	LMG	C42-C43-C44-C45
20	A	5005	LMG	C42-C43-C44-C45
20	a	5005	LMG	C42-C43-C44-C45
14	H	1023	CLA	CBA-CGA-O2A-C1
14	b	1023	CLA	CBA-CGA-O2A-C1
14	B	1023	CLA	CBA-CGA-O2A-C1
18	U	4019	BCR	C19-C20-C21-C22
18	l	4019	BCR	C19-C20-C21-C22
18	L	4019	BCR	C19-C20-C21-C22
14	A	1140	CLA	CAA-CBA-CGA-O2A
14	B	1223	CLA	O1D-CGD-O2D-CED
14	G	1125	CLA	C5-C6-C7-C8
14	b	1223	CLA	O1D-CGD-O2D-CED
14	a	1125	CLA	C5-C6-C7-C8
14	G	1140	CLA	CAA-CBA-CGA-O2A
14	a	1140	CLA	CAA-CBA-CGA-O2A
20	U	5007	LMG	C29-C28-O8-C9
20	l	5007	LMG	C29-C28-O8-C9
20	L	5007	LMG	C29-C28-O8-C9
13	G	1011	CL0	C10-C11-C12-C13
13	a	1011	CL0	C10-C11-C12-C13
14	A	1125	CLA	C5-C6-C7-C8
14	H	1223	CLA	O1D-CGD-O2D-CED
14	G	1109	CLA	C16-C17-C18-C19
14	a	1109	CLA	C16-C17-C18-C19
14	A	1109	CLA	C16-C17-C18-C19
13	A	1011	CL0	C10-C11-C12-C13
18	V	4021	BCR	C37-C22-C23-C24
18	m	4021	BCR	C37-C22-C23-C24
18	M	4021	BCR	C37-C22-C23-C24
14	G	1109	CLA	C12-C13-C15-C16
14	G	1138	CLA	C11-C10-C8-C7
14	H	1022	CLA	C11-C10-C8-C7
14	H	1204	CLA	C12-C13-C15-C16
14	H	1208	CLA	C6-C7-C8-C10
14	H	1234	CLA	C6-C7-C8-C10
14	a	1109	CLA	C12-C13-C15-C16
14	a	1127	CLA	C12-C13-C15-C16
14	a	1138	CLA	C11-C10-C8-C7
14	a	1140	CLA	C6-C7-C8-C10
14	b	1022	CLA	C11-C10-C8-C7
14	b	1204	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	b	1208	CLA	C6-C7-C8-C10
14	b	1234	CLA	C6-C7-C8-C10
14	A	1109	CLA	C12-C13-C15-C16
14	A	1127	CLA	C12-C13-C15-C16
14	A	1138	CLA	C11-C10-C8-C7
14	A	1140	CLA	C6-C7-C8-C10
14	B	1022	CLA	C11-C10-C8-C7
14	B	1204	CLA	C12-C13-C15-C16
14	B	1208	CLA	C6-C7-C8-C10
14	B	1234	CLA	C6-C7-C8-C10
16	G	2001	PQN	C21-C22-C23-C25
16	A	2001	PQN	C21-C22-C23-C25
14	a	1013	CLA	C3-C5-C6-C7
14	A	1013	CLA	C3-C5-C6-C7
14	G	1125	CLA	CBA-CGA-O2A-C1
14	a	1125	CLA	CBA-CGA-O2A-C1
14	A	1125	CLA	CBA-CGA-O2A-C1
14	a	1118	CLA	C6-C7-C8-C10
14	G	1116	CLA	CAA-CBA-CGA-O2A
14	a	1116	CLA	CAA-CBA-CGA-O2A
14	A	1116	CLA	CAA-CBA-CGA-O2A
14	H	1210	CLA	O1A-CGA-O2A-C1
14	G	1013	CLA	C3-C5-C6-C7
14	G	1110	CLA	O1D-CGD-O2D-CED
14	b	1210	CLA	O1A-CGA-O2A-C1
14	B	1210	CLA	O1A-CGA-O2A-C1
18	l	4019	BCR	C9-C10-C11-C12
18	R	4018	BCR	C14-C15-C16-C17
14	G	1118	CLA	C6-C7-C8-C10
14	A	1118	CLA	C6-C7-C8-C10
14	a	1110	CLA	O1D-CGD-O2D-CED
14	a	1109	CLA	C3-C5-C6-C7
14	A	1109	CLA	C3-C5-C6-C7
14	H	1023	CLA	C10-C11-C12-C13
14	b	1023	CLA	C10-C11-C12-C13
14	B	1023	CLA	C10-C11-C12-C13
14	A	1110	CLA	O1D-CGD-O2D-CED
14	A	1127	CLA	C13-C15-C16-C17
14	G	1127	CLA	C13-C15-C16-C17
14	a	1127	CLA	C13-C15-C16-C17
15	G	1121	F6C	C4B-C3B-CAB-CBB
15	a	1121	F6C	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
15	A	1121	F6C	C4B-C3B-CAB-CBB
15	H	1207	F6C	C16-C17-C18-C20
15	b	1207	F6C	C16-C17-C18-C20
15	B	1207	F6C	C16-C17-C18-C20
14	G	1109	CLA	C3-C5-C6-C7
14	G	1132	CLA	C2-C3-C5-C6
14	a	1132	CLA	C2-C3-C5-C6
14	A	1132	CLA	C2-C3-C5-C6
14	H	1203	CLA	C3-C5-C6-C7
14	b	1203	CLA	C3-C5-C6-C7
14	B	1203	CLA	C3-C5-C6-C7
14	G	1109	CLA	C11-C10-C8-C9
14	G	1140	CLA	C14-C13-C15-C16
14	H	1208	CLA	C6-C7-C8-C9
14	H	1211	CLA	C11-C12-C13-C14
14	H	1223	CLA	C11-C10-C8-C9
14	a	1109	CLA	C11-C10-C8-C9
14	a	1140	CLA	C14-C13-C15-C16
14	b	1208	CLA	C6-C7-C8-C9
14	b	1211	CLA	C11-C12-C13-C14
14	b	1223	CLA	C11-C10-C8-C9
14	A	1109	CLA	C11-C10-C8-C9
14	A	1140	CLA	C14-C13-C15-C16
14	B	1208	CLA	C6-C7-C8-C9
14	B	1211	CLA	C11-C12-C13-C14
14	B	1223	CLA	C11-C10-C8-C9
20	L	5007	LMG	O10-C28-O8-C9
19	b	5004	LHG	C34-C35-C36-C37
14	U	1502	CLA	C10-C11-C12-C13
14	l	1502	CLA	C10-C11-C12-C13
14	L	1502	CLA	C10-C11-C12-C13
19	H	5004	LHG	C34-C35-C36-C37
19	B	5004	LHG	C34-C35-C36-C37
15	H	1238	F6C	C15-C16-C17-C18
20	U	5007	LMG	O10-C28-O8-C9
20	l	5007	LMG	O10-C28-O8-C9
14	G	1119	CLA	C2-C1-O2A-CGA
14	U	1502	CLA	C2-C1-O2A-CGA
14	a	1119	CLA	C2-C1-O2A-CGA
14	l	1502	CLA	C2-C1-O2A-CGA
14	A	1119	CLA	C2-C1-O2A-CGA
14	L	1502	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
15	b	1238	F6C	C15-C16-C17-C18
15	B	1238	F6C	C15-C16-C17-C18
14	H	1210	CLA	C2A-CAA-CBA-CGA
14	b	1210	CLA	C2A-CAA-CBA-CGA
14	B	1210	CLA	C2A-CAA-CBA-CGA
14	G	1129	CLA	CBA-CGA-O2A-C1
14	a	1129	CLA	CBA-CGA-O2A-C1
14	A	1129	CLA	CBA-CGA-O2A-C1
14	G	1118	CLA	C6-C7-C8-C9
14	G	1132	CLA	C16-C17-C18-C19
14	G	1132	CLA	C16-C17-C18-C20
14	a	1118	CLA	C6-C7-C8-C9
14	a	1132	CLA	C16-C17-C18-C20
14	A	1118	CLA	C6-C7-C8-C9
14	A	1132	CLA	C16-C17-C18-C19
14	A	1132	CLA	C16-C17-C18-C20
14	B	1204	CLA	O1A-CGA-O2A-C1
14	a	1136	CLA	C15-C16-C17-C18
14	A	1136	CLA	C15-C16-C17-C18
20	R	5006	LMG	C29-C30-C31-C32
20	i	5006	LMG	C29-C30-C31-C32
20	I	5006	LMG	C29-C30-C31-C32
14	a	1132	CLA	C16-C17-C18-C19
14	H	1204	CLA	O1A-CGA-O2A-C1
14	b	1204	CLA	O1A-CGA-O2A-C1
14	G	1103	CLA	CBD-CGD-O2D-CED
14	G	1110	CLA	C4B-C3B-CAB-CBB
14	G	1129	CLA	C1A-C2A-CAA-CBA
14	G	1136	CLA	C4B-C3B-CAB-CBB
14	H	1202	CLA	C1A-C2A-CAA-CBA
14	H	1216	CLA	C4B-C3B-CAB-CBB
14	a	1110	CLA	C4B-C3B-CAB-CBB
14	a	1129	CLA	C1A-C2A-CAA-CBA
14	a	1136	CLA	C4B-C3B-CAB-CBB
14	b	1202	CLA	C1A-C2A-CAA-CBA
14	b	1216	CLA	C4B-C3B-CAB-CBB
14	A	1101	CLA	C4B-C3B-CAB-CBB
14	A	1110	CLA	C4B-C3B-CAB-CBB
14	A	1129	CLA	C1A-C2A-CAA-CBA
14	A	1136	CLA	C4B-C3B-CAB-CBB
14	B	1202	CLA	C1A-C2A-CAA-CBA
14	B	1216	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	H	1215	CLA	C4-C3-C5-C6
14	U	1501	CLA	C4-C3-C5-C6
14	b	1215	CLA	C4-C3-C5-C6
14	l	1501	CLA	C4-C3-C5-C6
14	B	1215	CLA	C4-C3-C5-C6
14	L	1501	CLA	C4-C3-C5-C6
14	G	1136	CLA	C15-C16-C17-C18
14	A	1103	CLA	CBD-CGD-O2D-CED
19	G	5001	LHG	O6-C4-C5-C6
19	H	5004	LHG	O6-C4-C5-C6
19	a	5001	LHG	O6-C4-C5-C6
19	b	5004	LHG	O6-C4-C5-C6
19	A	5001	LHG	O6-C4-C5-C6
19	B	5004	LHG	O6-C4-C5-C6
19	a	5001	LHG	C31-C32-C33-C34
14	a	1103	CLA	CBD-CGD-O2D-CED
19	G	5001	LHG	C31-C32-C33-C34
19	A	5001	LHG	C31-C32-C33-C34
13	G	1011	CL0	C12-C13-C15-C16
13	a	1011	CL0	C12-C13-C15-C16
13	A	1011	CL0	C12-C13-C15-C16
14	G	1115	CLA	C11-C12-C13-C15
14	G	1126	CLA	C6-C7-C8-C10
14	G	1128	CLA	C11-C10-C8-C7
14	G	1135	CLA	C6-C7-C8-C10
14	H	1223	CLA	C6-C7-C8-C10
14	H	1239	CLA	C11-C12-C13-C15
14	a	1115	CLA	C11-C12-C13-C15
14	a	1126	CLA	C6-C7-C8-C10
14	a	1128	CLA	C11-C10-C8-C7
14	a	1135	CLA	C6-C7-C8-C10
14	b	1223	CLA	C6-C7-C8-C10
14	b	1239	CLA	C11-C12-C13-C15
14	A	1115	CLA	C11-C12-C13-C15
14	A	1126	CLA	C6-C7-C8-C10
14	A	1128	CLA	C11-C10-C8-C7
14	A	1135	CLA	C6-C7-C8-C10
14	B	1223	CLA	C6-C7-C8-C10
14	B	1239	CLA	C11-C12-C13-C15
16	H	2002	PQN	C21-C22-C23-C25
16	b	2002	PQN	C21-C22-C23-C25
16	B	2002	PQN	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
14	b	1023	CLA	C16-C17-C18-C20
20	a	5005	LMG	C36-C37-C38-C39
14	G	1125	CLA	O1A-CGA-O2A-C1
14	a	1125	CLA	O1A-CGA-O2A-C1
14	A	1125	CLA	O1A-CGA-O2A-C1
20	A	5005	LMG	C36-C37-C38-C39
20	G	5005	LMG	C36-C37-C38-C39
14	H	1204	CLA	C4-C3-C5-C6
14	B	1204	CLA	C4-C3-C5-C6
14	H	1023	CLA	C16-C17-C18-C20
14	B	1023	CLA	C16-C17-C18-C20
14	b	1215	CLA	C2-C3-C5-C6
18	i	4018	BCR	C14-C15-C16-C17
18	I	4018	BCR	C14-C15-C16-C17
14	G	1112	CLA	C3-C5-C6-C7
14	a	1112	CLA	C3-C5-C6-C7
14	A	1112	CLA	C3-C5-C6-C7
13	G	1011	CL0	C14-C13-C15-C16
13	a	1011	CL0	C14-C13-C15-C16
13	A	1011	CL0	C14-C13-C15-C16
14	H	1022	CLA	C6-C7-C8-C9
14	H	1211	CLA	C14-C13-C15-C16
14	b	1022	CLA	C6-C7-C8-C9
14	b	1211	CLA	C14-C13-C15-C16
14	B	1022	CLA	C6-C7-C8-C9
14	B	1211	CLA	C14-C13-C15-C16
18	H	4016	BCR	C9-C10-C11-C12
18	U	4019	BCR	C9-C10-C11-C12
18	U	4022	BCR	C9-C10-C11-C12
18	V	4021	BCR	C9-C10-C11-C12
18	b	4016	BCR	C9-C10-C11-C12
18	m	4021	BCR	C9-C10-C11-C12
18	B	4016	BCR	C9-C10-C11-C12
18	L	4019	BCR	C9-C10-C11-C12
18	M	4021	BCR	C9-C10-C11-C12
14	U	1503	CLA	C16-C17-C18-C20
14	l	1503	CLA	C16-C17-C18-C20
13	G	1011	CL0	O1A-CGA-O2A-C1
13	a	1011	CL0	O1A-CGA-O2A-C1
13	A	1011	CL0	O1A-CGA-O2A-C1
14	H	1023	CLA	O1A-CGA-O2A-C1
14	b	1023	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	1023	CLA	O1A-CGA-O2A-C1
14	L	1503	CLA	C16-C17-C18-C20
14	b	1204	CLA	C4-C3-C5-C6
14	H	1215	CLA	C2-C3-C5-C6
14	B	1215	CLA	C2-C3-C5-C6
14	G	1111	CLA	CAD-CBD-CGD-O2D
14	G	1113	CLA	CAD-CBD-CGD-O2D
14	G	1123	CLA	CAD-CBD-CGD-O2D
14	H	1022	CLA	CAD-CBD-CGD-O2D
14	H	1223	CLA	CAD-CBD-CGD-O2D
14	H	1234	CLA	CAD-CBD-CGD-O2D
14	a	1111	CLA	CAD-CBD-CGD-O2D
14	a	1113	CLA	CAD-CBD-CGD-O2D
14	a	1123	CLA	CAD-CBD-CGD-O2D
14	b	1022	CLA	CAD-CBD-CGD-O2D
14	b	1223	CLA	CAD-CBD-CGD-O2D
14	b	1234	CLA	CAD-CBD-CGD-O2D
14	A	1111	CLA	CAD-CBD-CGD-O2D
14	A	1113	CLA	CAD-CBD-CGD-O2D
14	A	1123	CLA	CAD-CBD-CGD-O2D
14	B	1022	CLA	CAD-CBD-CGD-O2D
14	B	1223	CLA	CAD-CBD-CGD-O2D
14	B	1234	CLA	CAD-CBD-CGD-O2D
14	G	1129	CLA	O1A-CGA-O2A-C1
14	a	1129	CLA	O1A-CGA-O2A-C1
14	A	1129	CLA	O1A-CGA-O2A-C1
21	G	6002	LMT	C5'-C4'-O1B-C1B
14	a	1103	CLA	O1D-CGD-O2D-CED
14	G	1115	CLA	C16-C17-C18-C19
14	a	1115	CLA	C16-C17-C18-C19
14	A	1115	CLA	C16-C17-C18-C19
21	a	6002	LMT	C5'-C4'-O1B-C1B
21	A	6002	LMT	C5'-C4'-O1B-C1B
14	G	1120	CLA	C2A-CAA-CBA-CGA
14	a	1120	CLA	C2A-CAA-CBA-CGA
14	A	1120	CLA	C2A-CAA-CBA-CGA
14	G	1123	CLA	O1A-CGA-O2A-C1
14	a	1123	CLA	O1A-CGA-O2A-C1
14	A	1123	CLA	O1A-CGA-O2A-C1
14	A	1103	CLA	O1D-CGD-O2D-CED
19	G	5001	LHG	C24-C25-C26-C27
19	A	5001	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
19	a	5001	LHG	C24-C25-C26-C27
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	1113	CLA	CAD-CBD-CGD-O1D
14	G	1117	CLA	CHA-CBD-CGD-O1D
14	G	1117	CLA	CHA-CBD-CGD-O2D
14	G	1122	CLA	CHA-CBD-CGD-O1D
14	G	1122	CLA	CHA-CBD-CGD-O2D
14	G	1123	CLA	CAD-CBD-CGD-O1D
14	G	1135	CLA	CHA-CBD-CGD-O1D
14	H	1022	CLA	CAD-CBD-CGD-O1D
14	H	1203	CLA	CHA-CBD-CGD-O1D
14	H	1203	CLA	CHA-CBD-CGD-O2D
14	H	1223	CLA	CAD-CBD-CGD-O1D
14	H	1234	CLA	CAD-CBD-CGD-O1D
14	a	1111	CLA	CAD-CBD-CGD-O1D
14	a	1112	CLA	CHA-CBD-CGD-O1D
14	a	1112	CLA	CHA-CBD-CGD-O2D
14	a	1113	CLA	CAD-CBD-CGD-O1D
14	a	1117	CLA	CHA-CBD-CGD-O1D
14	a	1117	CLA	CHA-CBD-CGD-O2D
14	a	1122	CLA	CHA-CBD-CGD-O1D
14	a	1122	CLA	CHA-CBD-CGD-O2D
14	a	1123	CLA	CAD-CBD-CGD-O1D
14	a	1135	CLA	CHA-CBD-CGD-O1D
14	b	1022	CLA	CAD-CBD-CGD-O1D
14	b	1203	CLA	CHA-CBD-CGD-O1D
14	b	1203	CLA	CHA-CBD-CGD-O2D
14	b	1223	CLA	CAD-CBD-CGD-O1D
14	b	1234	CLA	CAD-CBD-CGD-O1D
14	A	1111	CLA	CAD-CBD-CGD-O1D
14	A	1112	CLA	CHA-CBD-CGD-O1D
14	A	1112	CLA	CHA-CBD-CGD-O2D
14	A	1113	CLA	CAD-CBD-CGD-O1D
14	A	1117	CLA	CHA-CBD-CGD-O1D
14	A	1117	CLA	CHA-CBD-CGD-O2D
14	A	1122	CLA	CHA-CBD-CGD-O1D
14	A	1122	CLA	CHA-CBD-CGD-O2D
14	A	1123	CLA	CAD-CBD-CGD-O1D
14	A	1135	CLA	CHA-CBD-CGD-O1D
14	B	1022	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	B	1203	CLA	CHA-CBD-CGD-O1D
14	B	1203	CLA	CHA-CBD-CGD-O2D
14	B	1223	CLA	CAD-CBD-CGD-O1D
14	B	1234	CLA	CAD-CBD-CGD-O1D
18	R	4020	BCR	C9-C10-C11-C12
18	l	4022	BCR	C9-C10-C11-C12
18	I	4020	BCR	C9-C10-C11-C12
18	L	4022	BCR	C9-C10-C11-C12
19	G	5001	LHG	C3-O3-P-O5
19	G	5001	LHG	C4-O6-P-O5
19	H	5004	LHG	C3-O3-P-O6
19	H	5004	LHG	C4-O6-P-O5
19	a	5001	LHG	C3-O3-P-O5
19	a	5001	LHG	C4-O6-P-O5
19	b	5004	LHG	C3-O3-P-O6
19	b	5004	LHG	C4-O6-P-O5
19	A	5001	LHG	C3-O3-P-O5
19	A	5001	LHG	C4-O6-P-O5
19	B	5004	LHG	C3-O3-P-O6
19	B	5004	LHG	C4-O6-P-O5
14	G	1125	CLA	C4-C3-C5-C6
14	a	1125	CLA	C4-C3-C5-C6
14	A	1125	CLA	C4-C3-C5-C6
14	G	1103	CLA	O1D-CGD-O2D-CED
14	G	1012	CLA	C2B-C3B-CAB-CBB
14	G	1101	CLA	C2B-C3B-CAB-CBB
14	G	1110	CLA	C2B-C3B-CAB-CBB
14	G	1116	CLA	C2B-C3B-CAB-CBB
14	G	1129	CLA	C2B-C3B-CAB-CBB
14	G	1132	CLA	C2B-C3B-CAB-CBB
14	H	1204	CLA	C2B-C3B-CAB-CBB
14	a	1012	CLA	C2B-C3B-CAB-CBB
14	a	1101	CLA	C2B-C3B-CAB-CBB
14	a	1110	CLA	C2B-C3B-CAB-CBB
14	a	1116	CLA	C2B-C3B-CAB-CBB
14	a	1129	CLA	C2B-C3B-CAB-CBB
14	a	1132	CLA	C2B-C3B-CAB-CBB
14	b	1204	CLA	C2B-C3B-CAB-CBB
14	A	1012	CLA	C2B-C3B-CAB-CBB
14	A	1101	CLA	C2B-C3B-CAB-CBB
14	A	1110	CLA	C2B-C3B-CAB-CBB
14	A	1116	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	A	1129	CLA	C2B-C3B-CAB-CBB
14	A	1132	CLA	C2B-C3B-CAB-CBB
14	B	1204	CLA	C2B-C3B-CAB-CBB
18	H	4017	BCR	C23-C24-C25-C26
18	U	4019	BCR	C23-C24-C25-C26
18	b	4017	BCR	C23-C24-C25-C26
18	l	4019	BCR	C23-C24-C25-C26
18	B	4017	BCR	C23-C24-C25-C26
18	L	4019	BCR	C23-C24-C25-C26
14	G	1133	CLA	C3-C5-C6-C7
14	a	1133	CLA	C3-C5-C6-C7
14	A	1133	CLA	C3-C5-C6-C7
14	H	1203	CLA	C5-C6-C7-C8
14	b	1203	CLA	C5-C6-C7-C8
14	H	1228	CLA	C6-C7-C8-C9
14	b	1228	CLA	C6-C7-C8-C9
14	B	1228	CLA	C6-C7-C8-C9
14	H	1216	CLA	O1A-CGA-O2A-C1
14	B	1216	CLA	O1A-CGA-O2A-C1
14	B	1203	CLA	C5-C6-C7-C8
18	G	4003	BCR	C18-C19-C20-C21
18	H	4006	BCR	C18-C19-C20-C21
18	H	4013	BCR	C18-C19-C20-C21
18	R	4020	BCR	C18-C19-C20-C21
18	a	4003	BCR	C18-C19-C20-C21
18	b	4006	BCR	C18-C19-C20-C21
18	b	4013	BCR	C18-C19-C20-C21
18	i	4020	BCR	C18-C19-C20-C21
18	A	4003	BCR	C18-C19-C20-C21
18	B	4006	BCR	C18-C19-C20-C21
18	B	4013	BCR	C18-C19-C20-C21
18	I	4020	BCR	C18-C19-C20-C21
14	G	1125	CLA	CAA-CBA-CGA-O2A
14	H	1220	CLA	CAA-CBA-CGA-O2A
14	b	1220	CLA	CAA-CBA-CGA-O2A
14	A	1125	CLA	CAA-CBA-CGA-O2A
14	B	1220	CLA	CAA-CBA-CGA-O2A
18	i	4020	BCR	C9-C10-C11-C12
14	U	1503	CLA	C16-C17-C18-C19
14	l	1503	CLA	C16-C17-C18-C19
14	b	1216	CLA	O1A-CGA-O2A-C1
14	a	1125	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	H	1203	CLA	C14-C13-C15-C16
14	H	1214	CLA	C6-C7-C8-C9
14	H	1216	CLA	C6-C7-C8-C9
14	b	1203	CLA	C14-C13-C15-C16
14	b	1214	CLA	C6-C7-C8-C9
14	b	1216	CLA	C6-C7-C8-C9
14	B	1203	CLA	C14-C13-C15-C16
14	B	1214	CLA	C6-C7-C8-C9
14	B	1216	CLA	C6-C7-C8-C9
14	H	1211	CLA	C12-C13-C15-C16
14	b	1211	CLA	C12-C13-C15-C16
14	B	1211	CLA	C12-C13-C15-C16
19	G	5001	LHG	O6-C4-C5-O7
19	a	5001	LHG	O6-C4-C5-O7
19	A	5001	LHG	O6-C4-C5-O7
14	A	1130	CLA	C6-C7-C8-C10
14	L	1503	CLA	C16-C17-C18-C19
20	G	5005	LMG	C2-C1-O1-C7
20	a	5005	LMG	C2-C1-O1-C7
20	A	5005	LMG	C2-C1-O1-C7
14	H	1235	CLA	C2-C3-C5-C6
14	b	1235	CLA	C2-C3-C5-C6
14	B	1235	CLA	C2-C3-C5-C6
14	G	1130	CLA	C6-C7-C8-C10
14	H	1021	CLA	C16-C17-C18-C19
14	H	1228	CLA	C6-C7-C8-C10
14	a	1130	CLA	C6-C7-C8-C10
14	b	1021	CLA	C16-C17-C18-C19
14	B	1021	CLA	C16-C17-C18-C19
14	B	1228	CLA	C6-C7-C8-C10
18	B	4010	BCR	C19-C20-C21-C22
14	H	1021	CLA	C16-C17-C18-C20
14	b	1021	CLA	C16-C17-C18-C20
14	b	1228	CLA	C6-C7-C8-C10
14	B	1021	CLA	C16-C17-C18-C20
14	H	1216	CLA	C15-C16-C17-C18
14	b	1216	CLA	C15-C16-C17-C18
14	B	1216	CLA	C15-C16-C17-C18
14	a	1123	CLA	CBA-CGA-O2A-C1
14	G	1103	CLA	C2-C1-O2A-CGA
14	H	1228	CLA	C2-C1-O2A-CGA
14	a	1103	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
14	b	1228	CLA	C2-C1-O2A-CGA
14	A	1103	CLA	C2-C1-O2A-CGA
14	B	1228	CLA	C2-C1-O2A-CGA
20	U	5007	LMG	C32-C33-C34-C35
20	l	5007	LMG	C32-C33-C34-C35
14	H	1213	CLA	CAA-CBA-CGA-O2A
14	b	1213	CLA	CAA-CBA-CGA-O2A
14	B	1213	CLA	CAA-CBA-CGA-O2A
20	L	5007	LMG	C32-C33-C34-C35
14	b	1210	CLA	C15-C16-C17-C18
14	B	1210	CLA	C15-C16-C17-C18
14	G	1123	CLA	CBA-CGA-O2A-C1
14	b	1204	CLA	CBA-CGA-O2A-C1
14	A	1123	CLA	CBA-CGA-O2A-C1
14	G	1127	CLA	CAA-CBA-CGA-O2A
14	a	1127	CLA	CAA-CBA-CGA-O2A
14	A	1127	CLA	CAA-CBA-CGA-O2A
19	G	5001	LHG	C15-C16-C17-C18
19	a	5001	LHG	C15-C16-C17-C18
19	A	5001	LHG	C15-C16-C17-C18
14	H	1204	CLA	CBA-CGA-O2A-C1
14	B	1204	CLA	CBA-CGA-O2A-C1
14	H	1210	CLA	C15-C16-C17-C18
18	H	4010	BCR	C19-C20-C21-C22
18	R	4020	BCR	C15-C16-C17-C18
18	b	4010	BCR	C19-C20-C21-C22
18	i	4020	BCR	C15-C16-C17-C18
18	I	4020	BCR	C15-C16-C17-C18
14	H	1217	CLA	C4-C3-C5-C6
14	b	1217	CLA	C4-C3-C5-C6
14	B	1217	CLA	C4-C3-C5-C6
14	l	1501	CLA	C2-C3-C5-C6
13	G	1011	CL0	CBA-CGA-O2A-C1
13	a	1011	CL0	CBA-CGA-O2A-C1
13	A	1011	CL0	CBA-CGA-O2A-C1
14	b	1216	CLA	CBA-CGA-O2A-C1
21	G	6001	LMT	C2-C1-O1'-C1'
21	a	6001	LMT	C2-C1-O1'-C1'
21	A	6001	LMT	C2-C1-O1'-C1'
14	G	1106	CLA	C11-C12-C13-C14
14	H	1222	CLA	C16-C17-C18-C20
14	b	1222	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	A	1106	CLA	C11-C12-C13-C14
14	B	1222	CLA	C16-C17-C18-C20
14	G	1115	CLA	C11-C12-C13-C14
14	G	1128	CLA	C11-C10-C8-C9
14	a	1115	CLA	C11-C12-C13-C14
14	a	1128	CLA	C11-C10-C8-C9
14	A	1115	CLA	C11-C12-C13-C14
14	A	1128	CLA	C11-C10-C8-C9
16	G	2001	PQN	C21-C22-C23-C24
16	a	2001	PQN	C21-C22-C23-C24
16	A	2001	PQN	C21-C22-C23-C24
14	H	1216	CLA	CBA-CGA-O2A-C1
14	B	1216	CLA	CBA-CGA-O2A-C1
14	G	1113	CLA	C4B-C3B-CAB-CBB
14	H	1202	CLA	C4B-C3B-CAB-CBB
14	H	1231	CLA	C4B-C3B-CAB-CBB
14	a	1113	CLA	C4B-C3B-CAB-CBB
14	b	1202	CLA	C4B-C3B-CAB-CBB
14	b	1231	CLA	C4B-C3B-CAB-CBB
14	A	1113	CLA	C4B-C3B-CAB-CBB
14	B	1202	CLA	C4B-C3B-CAB-CBB
14	B	1231	CLA	C4B-C3B-CAB-CBB
21	A	6002	LMT	O5'-C5'-C6'-O6'
15	H	1237	F6C	C2A-CAA-CBA-CGA
15	b	1237	F6C	C2A-CAA-CBA-CGA
15	B	1237	F6C	C2A-CAA-CBA-CGA
14	a	1106	CLA	C11-C12-C13-C14
14	G	1125	CLA	C2-C3-C5-C6
14	H	1204	CLA	C2-C3-C5-C6
14	U	1501	CLA	C2-C3-C5-C6
14	a	1125	CLA	C2-C3-C5-C6
14	b	1204	CLA	C2-C3-C5-C6
14	A	1125	CLA	C2-C3-C5-C6
14	B	1204	CLA	C2-C3-C5-C6
14	L	1501	CLA	C2-C3-C5-C6
14	a	1122	CLA	C3-C5-C6-C7
14	A	1122	CLA	C3-C5-C6-C7
21	G	6002	LMT	O5'-C5'-C6'-O6'
21	a	6002	LMT	O5'-C5'-C6'-O6'
14	G	1119	CLA	C11-C10-C8-C7
14	G	1119	CLA	C12-C13-C15-C16
14	H	1021	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
14	a	1119	CLA	C11-C10-C8-C7
14	a	1119	CLA	C12-C13-C15-C16
14	b	1021	CLA	C6-C7-C8-C10
14	A	1119	CLA	C11-C10-C8-C7
14	A	1119	CLA	C12-C13-C15-C16
14	B	1021	CLA	C6-C7-C8-C10
15	H	1207	F6C	C12-C13-C15-C16
15	b	1207	F6C	C12-C13-C15-C16
15	B	1207	F6C	C12-C13-C15-C16
14	G	1127	CLA	C5-C6-C7-C8
14	a	1127	CLA	C5-C6-C7-C8
14	A	1127	CLA	C5-C6-C7-C8
14	G	1122	CLA	C3-C5-C6-C7
20	i	5006	LMG	O9-C10-C11-C12
14	H	1208	CLA	CAA-CBA-CGA-O1A
14	b	1208	CLA	CAA-CBA-CGA-O1A
14	B	1208	CLA	CAA-CBA-CGA-O1A
20	R	5006	LMG	O9-C10-C11-C12
20	I	5006	LMG	O9-C10-C11-C12
20	U	5007	LMG	O1-C7-C8-O7
20	l	5007	LMG	O1-C7-C8-O7
20	L	5007	LMG	O1-C7-C8-O7
14	H	1202	CLA	C3A-C2A-CAA-CBA
14	H	1209	CLA	C3A-C2A-CAA-CBA
14	H	1219	CLA	C3A-C2A-CAA-CBA
14	H	1233	CLA	C3A-C2A-CAA-CBA
14	b	1202	CLA	C3A-C2A-CAA-CBA
14	b	1209	CLA	C3A-C2A-CAA-CBA
14	b	1219	CLA	C3A-C2A-CAA-CBA
14	b	1233	CLA	C3A-C2A-CAA-CBA
14	B	1202	CLA	C3A-C2A-CAA-CBA
14	B	1209	CLA	C3A-C2A-CAA-CBA
14	B	1219	CLA	C3A-C2A-CAA-CBA
14	B	1233	CLA	C3A-C2A-CAA-CBA
14	H	1226	CLA	C15-C16-C17-C18
18	G	4007	BCR	C16-C17-C18-C36
18	G	4011	BCR	C16-C17-C18-C36
18	H	4006	BCR	C11-C10-C9-C34
18	H	4010	BCR	C16-C17-C18-C36
18	H	4016	BCR	C35-C13-C14-C15
18	a	4007	BCR	C16-C17-C18-C36
18	a	4011	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
18	b	4006	BCR	C11-C10-C9-C34
18	b	4010	BCR	C16-C17-C18-C36
18	b	4016	BCR	C35-C13-C14-C15
18	A	4007	BCR	C16-C17-C18-C36
18	A	4011	BCR	C16-C17-C18-C36
18	B	4006	BCR	C11-C10-C9-C34
18	B	4010	BCR	C16-C17-C18-C36
18	B	4016	BCR	C35-C13-C14-C15
14	b	1226	CLA	C15-C16-C17-C18
14	B	1226	CLA	C15-C16-C17-C18
20	R	5006	LMG	C33-C34-C35-C36
20	I	5006	LMG	C33-C34-C35-C36
14	H	1205	CLA	C5-C6-C7-C8
14	b	1205	CLA	C5-C6-C7-C8
14	B	1205	CLA	C5-C6-C7-C8
20	i	5006	LMG	C33-C34-C35-C36
14	H	1228	CLA	C4-C3-C5-C6
14	b	1228	CLA	C4-C3-C5-C6
14	B	1228	CLA	C4-C3-C5-C6
15	H	1238	F6C	C4-C3-C5-C6
15	b	1238	F6C	C4-C3-C5-C6
15	B	1238	F6C	C4-C3-C5-C6
14	G	1104	CLA	C2A-CAA-CBA-CGA
13	G	1011	CL0	C5-C6-C7-C8
13	a	1011	CL0	C5-C6-C7-C8
13	A	1011	CL0	C5-C6-C7-C8
14	G	1115	CLA	C6-C7-C8-C9
14	G	1117	CLA	C11-C10-C8-C9
14	G	1140	CLA	C11-C10-C8-C9
14	H	1021	CLA	C6-C7-C8-C9
14	H	1214	CLA	C14-C13-C15-C16
14	H	1229	CLA	C6-C7-C8-C9
14	H	1239	CLA	C14-C13-C15-C16
14	U	1501	CLA	C11-C12-C13-C14
14	a	1115	CLA	C6-C7-C8-C9
14	a	1117	CLA	C11-C10-C8-C9
14	a	1140	CLA	C11-C10-C8-C9
14	b	1021	CLA	C6-C7-C8-C9
14	b	1214	CLA	C14-C13-C15-C16
14	b	1229	CLA	C6-C7-C8-C9
14	b	1239	CLA	C14-C13-C15-C16
14	l	1501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	1115	CLA	C6-C7-C8-C9
14	A	1117	CLA	C11-C10-C8-C9
14	A	1140	CLA	C11-C10-C8-C9
14	B	1021	CLA	C6-C7-C8-C9
14	B	1214	CLA	C14-C13-C15-C16
14	B	1229	CLA	C6-C7-C8-C9
14	B	1239	CLA	C14-C13-C15-C16
14	L	1501	CLA	C11-C12-C13-C14
16	G	2001	PQN	C24-C23-C25-C26
16	a	2001	PQN	C24-C23-C25-C26
16	A	2001	PQN	C24-C23-C25-C26
14	b	1208	CLA	C13-C15-C16-C17
14	B	1208	CLA	C13-C15-C16-C17
15	H	1238	F6C	C2-C3-C5-C6
15	b	1238	F6C	C2-C3-C5-C6
15	B	1238	F6C	C2-C3-C5-C6
14	a	1104	CLA	C2A-CAA-CBA-CGA
14	A	1104	CLA	C2A-CAA-CBA-CGA
14	H	1208	CLA	C13-C15-C16-C17
14	G	1122	CLA	C1A-C2A-CAA-CBA
14	H	1212	CLA	C1A-C2A-CAA-CBA
14	a	1122	CLA	C1A-C2A-CAA-CBA
14	b	1212	CLA	C1A-C2A-CAA-CBA
14	A	1122	CLA	C1A-C2A-CAA-CBA
14	B	1212	CLA	C1A-C2A-CAA-CBA
18	G	4007	BCR	C16-C17-C18-C19
18	G	4011	BCR	C16-C17-C18-C19
18	H	4006	BCR	C11-C10-C9-C8
18	H	4016	BCR	C12-C13-C14-C15
18	a	4007	BCR	C16-C17-C18-C19
18	a	4011	BCR	C16-C17-C18-C19
18	b	4006	BCR	C11-C10-C9-C8
18	b	4016	BCR	C12-C13-C14-C15
18	A	4007	BCR	C16-C17-C18-C19
18	A	4011	BCR	C16-C17-C18-C19
18	B	4006	BCR	C11-C10-C9-C8
18	B	4016	BCR	C12-C13-C14-C15
14	G	1113	CLA	C2B-C3B-CAB-CBB
14	G	1124	CLA	C2B-C3B-CAB-CBB
14	G	1136	CLA	C2B-C3B-CAB-CBB
14	H	1022	CLA	C2B-C3B-CAB-CBB
14	H	1216	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	H	1224	CLA	C2B-C3B-CAB-CBB
14	H	1231	CLA	C2B-C3B-CAB-CBB
14	a	1113	CLA	C2B-C3B-CAB-CBB
14	a	1124	CLA	C2B-C3B-CAB-CBB
14	a	1136	CLA	C2B-C3B-CAB-CBB
14	b	1022	CLA	C2B-C3B-CAB-CBB
14	b	1216	CLA	C2B-C3B-CAB-CBB
14	b	1224	CLA	C2B-C3B-CAB-CBB
14	b	1231	CLA	C2B-C3B-CAB-CBB
14	A	1113	CLA	C2B-C3B-CAB-CBB
14	A	1124	CLA	C2B-C3B-CAB-CBB
14	A	1136	CLA	C2B-C3B-CAB-CBB
14	B	1022	CLA	C2B-C3B-CAB-CBB
14	B	1216	CLA	C2B-C3B-CAB-CBB
14	B	1224	CLA	C2B-C3B-CAB-CBB
14	B	1231	CLA	C2B-C3B-CAB-CBB
18	G	4001	BCR	C5-C6-C7-C8
18	G	4001	BCR	C23-C24-C25-C26
18	G	4003	BCR	C23-C24-C25-C30
18	H	4010	BCR	C23-C24-C25-C30
18	R	4018	BCR	C1-C6-C7-C8
18	R	4020	BCR	C23-C24-C25-C26
18	V	4021	BCR	C5-C6-C7-C8
18	V	4021	BCR	C23-C24-C25-C26
18	a	4001	BCR	C5-C6-C7-C8
18	a	4001	BCR	C23-C24-C25-C26
18	a	4003	BCR	C23-C24-C25-C30
18	a	4011	BCR	C1-C6-C7-C8
18	b	4010	BCR	C23-C24-C25-C30
18	i	4018	BCR	C1-C6-C7-C8
18	i	4020	BCR	C23-C24-C25-C26
18	m	4021	BCR	C5-C6-C7-C8
18	m	4021	BCR	C23-C24-C25-C26
18	A	4001	BCR	C5-C6-C7-C8
18	A	4001	BCR	C23-C24-C25-C26
18	A	4003	BCR	C23-C24-C25-C30
18	A	4011	BCR	C1-C6-C7-C8
18	B	4010	BCR	C23-C24-C25-C30
18	I	4018	BCR	C1-C6-C7-C8
18	I	4020	BCR	C23-C24-C25-C26
18	M	4021	BCR	C5-C6-C7-C8
18	M	4021	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	G	1121	F6C	CAA-CBA-CGA-O2A
15	a	1121	F6C	CAA-CBA-CGA-O2A
15	A	1121	F6C	CAA-CBA-CGA-O2A
14	G	1104	CLA	C6-C7-C8-C10
14	G	1127	CLA	C11-C10-C8-C7
14	H	1021	CLA	C11-C10-C8-C7
14	H	1211	CLA	C11-C10-C8-C7
14	H	1222	CLA	C6-C7-C8-C10
14	U	1502	CLA	C6-C7-C8-C10
14	a	1104	CLA	C6-C7-C8-C10
14	a	1127	CLA	C11-C10-C8-C7
14	b	1021	CLA	C11-C10-C8-C7
14	b	1211	CLA	C11-C10-C8-C7
14	b	1222	CLA	C6-C7-C8-C10
14	l	1502	CLA	C6-C7-C8-C10
14	A	1104	CLA	C6-C7-C8-C10
14	A	1127	CLA	C11-C10-C8-C7
14	B	1021	CLA	C11-C10-C8-C7
14	B	1211	CLA	C11-C10-C8-C7
14	B	1222	CLA	C6-C7-C8-C10
14	L	1502	CLA	C6-C7-C8-C10
16	G	2001	PQN	C17-C18-C20-C21
16	a	2001	PQN	C17-C18-C20-C21
16	A	2001	PQN	C17-C18-C20-C21
15	G	1121	F6C	CAA-CBA-CGA-O1A
15	a	1121	F6C	CAA-CBA-CGA-O1A
14	G	1117	CLA	C3-C5-C6-C7
14	H	1225	CLA	C3-C5-C6-C7
14	a	1117	CLA	C3-C5-C6-C7
14	A	1117	CLA	C3-C5-C6-C7
15	A	1121	F6C	CAA-CBA-CGA-O1A
18	H	4005	BCR	C36-C18-C19-C20
18	B	4005	BCR	C36-C18-C19-C20
18	B	4006	BCR	C7-C8-C9-C34
14	B	1225	CLA	C3-C5-C6-C7
14	H	1023	CLA	C8-C10-C11-C12
14	b	1023	CLA	C8-C10-C11-C12
14	B	1023	CLA	C8-C10-C11-C12
14	G	1126	CLA	C2-C3-C5-C6
14	H	1228	CLA	C2-C3-C5-C6
14	a	1126	CLA	C2-C3-C5-C6
14	b	1228	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	1126	CLA	C2-C3-C5-C6
14	B	1228	CLA	C2-C3-C5-C6
19	a	5001	LHG	C25-C26-C27-C28
19	G	5001	LHG	C25-C26-C27-C28
19	A	5001	LHG	C25-C26-C27-C28
14	b	1220	CLA	CBA-CGA-O2A-C1
14	B	1220	CLA	CBA-CGA-O2A-C1
14	b	1225	CLA	C3-C5-C6-C7
14	A	1108	CLA	CAA-CBA-CGA-O2A
14	H	1021	CLA	C11-C10-C8-C9
14	b	1021	CLA	C11-C10-C8-C9
14	B	1021	CLA	C11-C10-C8-C9
14	G	1108	CLA	CAA-CBA-CGA-O2A
14	a	1108	CLA	CAA-CBA-CGA-O2A
14	H	1220	CLA	CBA-CGA-O2A-C1
14	G	1012	CLA	C4-C3-C5-C6
14	G	1131	CLA	C4-C3-C5-C6
14	U	1502	CLA	C4-C3-C5-C6
14	a	1012	CLA	C4-C3-C5-C6
14	a	1131	CLA	C4-C3-C5-C6
14	l	1502	CLA	C4-C3-C5-C6
14	A	1012	CLA	C4-C3-C5-C6
14	A	1131	CLA	C4-C3-C5-C6
14	L	1502	CLA	C4-C3-C5-C6
14	H	1220	CLA	O1A-CGA-O2A-C1
14	b	1220	CLA	O1A-CGA-O2A-C1
14	B	1220	CLA	O1A-CGA-O2A-C1
16	H	2002	PQN	C23-C25-C26-C27
16	b	2002	PQN	C23-C25-C26-C27
16	B	2002	PQN	C23-C25-C26-C27
14	b	1221	CLA	C10-C11-C12-C13
20	A	5005	LMG	C14-C15-C16-C17
20	a	5005	LMG	C14-C15-C16-C17
20	G	5005	LMG	C14-C15-C16-C17
14	G	1126	CLA	C4B-C3B-CAB-CBB
14	a	1126	CLA	C4B-C3B-CAB-CBB
14	A	1126	CLA	C4B-C3B-CAB-CBB
14	H	1221	CLA	C10-C11-C12-C13
14	B	1221	CLA	C10-C11-C12-C13
14	H	1236	CLA	CAA-CBA-CGA-O2A
14	b	1236	CLA	CAA-CBA-CGA-O2A
14	B	1236	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	a	5005	LMG	C33-C34-C35-C36
20	A	5005	LMG	C33-C34-C35-C36
20	G	5005	LMG	C33-C34-C35-C36
14	l	1503	CLA	C15-C16-C17-C18
14	L	1503	CLA	C15-C16-C17-C18
14	G	1131	CLA	C2-C3-C5-C6
14	U	1502	CLA	C2-C3-C5-C6
14	a	1131	CLA	C2-C3-C5-C6
14	l	1502	CLA	C2-C3-C5-C6
14	A	1131	CLA	C2-C3-C5-C6
14	L	1502	CLA	C2-C3-C5-C6
14	U	1503	CLA	C15-C16-C17-C18
18	b	4005	BCR	C36-C18-C19-C20
14	G	1123	CLA	C11-C10-C8-C7
14	H	1229	CLA	C6-C7-C8-C10
14	a	1123	CLA	C11-C10-C8-C7
14	b	1229	CLA	C6-C7-C8-C10
14	A	1123	CLA	C11-C10-C8-C7
14	B	1229	CLA	C6-C7-C8-C10
14	G	1108	CLA	CAA-CBA-CGA-O1A
14	a	1108	CLA	CAA-CBA-CGA-O1A
14	A	1108	CLA	CAA-CBA-CGA-O1A
14	H	1202	CLA	CAA-CBA-CGA-O1A
14	B	1202	CLA	CAA-CBA-CGA-O1A
14	G	1135	CLA	C6-C7-C8-C9
14	H	1021	CLA	C11-C12-C13-C14
14	H	1203	CLA	C11-C12-C13-C14
14	H	1239	CLA	C11-C12-C13-C14
14	a	1135	CLA	C6-C7-C8-C9
14	b	1021	CLA	C11-C12-C13-C14
14	b	1203	CLA	C11-C12-C13-C14
14	b	1239	CLA	C11-C12-C13-C14
14	A	1135	CLA	C6-C7-C8-C9
14	B	1021	CLA	C11-C12-C13-C14
14	B	1203	CLA	C11-C12-C13-C14
14	B	1239	CLA	C11-C12-C13-C14
16	H	2002	PQN	C19-C18-C20-C21
16	H	2002	PQN	C21-C22-C23-C24
16	b	2002	PQN	C19-C18-C20-C21
16	b	2002	PQN	C21-C22-C23-C24
16	B	2002	PQN	C19-C18-C20-C21
16	B	2002	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	b	1202	CLA	CAA-CBA-CGA-O1A
14	G	1114	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	1114	CLA	CAA-CBA-CGA-O2A
14	B	1236	CLA	CAA-CBA-CGA-O1A
14	G	1129	CLA	C2A-CAA-CBA-CGA
14	a	1129	CLA	C2A-CAA-CBA-CGA
14	A	1129	CLA	C2A-CAA-CBA-CGA
14	H	1022	CLA	C2-C1-O2A-CGA
14	b	1022	CLA	C2-C1-O2A-CGA
14	B	1022	CLA	C2-C1-O2A-CGA
14	G	1012	CLA	C3A-C2A-CAA-CBA
14	G	1136	CLA	C3A-C2A-CAA-CBA
14	H	1231	CLA	C3A-C2A-CAA-CBA
14	a	1012	CLA	C3A-C2A-CAA-CBA
14	a	1136	CLA	C3A-C2A-CAA-CBA
14	b	1231	CLA	C3A-C2A-CAA-CBA
14	A	1012	CLA	C3A-C2A-CAA-CBA
14	A	1136	CLA	C3A-C2A-CAA-CBA
14	B	1231	CLA	C3A-C2A-CAA-CBA
14	G	1136	CLA	CAA-CBA-CGA-O2A
14	a	1136	CLA	CAA-CBA-CGA-O2A
14	A	1136	CLA	CAA-CBA-CGA-O2A
14	G	1101	CLA	CAA-CBA-CGA-O2A
14	a	1101	CLA	CAA-CBA-CGA-O2A
14	A	1101	CLA	CAA-CBA-CGA-O2A
14	a	1134	CLA	CAA-CBA-CGA-O2A
14	A	1134	CLA	CAA-CBA-CGA-O2A
18	H	4010	BCR	C16-C17-C18-C19
18	b	4010	BCR	C16-C17-C18-C19
18	B	4010	BCR	C16-C17-C18-C19
14	G	1114	CLA	CAA-CBA-CGA-O1A
14	a	1101	CLA	CAA-CBA-CGA-O1A
14	a	1114	CLA	CAA-CBA-CGA-O1A
14	A	1114	CLA	CAA-CBA-CGA-O1A
14	G	1101	CLA	CAA-CBA-CGA-O1A
14	G	1134	CLA	CAA-CBA-CGA-O2A
14	A	1101	CLA	CAA-CBA-CGA-O1A
20	U	5007	LMG	O1-C7-C8-C9
20	l	5007	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	L	5007	LMG	O1-C7-C8-C9
14	H	1021	CLA	CAA-CBA-CGA-O1A
14	b	1021	CLA	CAA-CBA-CGA-O1A
14	B	1021	CLA	CAA-CBA-CGA-O1A
18	G	4001	BCR	C19-C20-C21-C22
18	a	4001	BCR	C19-C20-C21-C22
18	A	4001	BCR	C19-C20-C21-C22
14	H	1222	CLA	C16-C17-C18-C19
14	b	1233	CLA	CAA-CBA-CGA-O1A
14	H	1233	CLA	CAA-CBA-CGA-O1A
14	B	1233	CLA	CAA-CBA-CGA-O1A
14	G	1106	CLA	C6-C7-C8-C9
14	G	1127	CLA	C11-C10-C8-C9
14	H	1223	CLA	C6-C7-C8-C9
14	U	1502	CLA	C11-C10-C8-C9
14	a	1106	CLA	C6-C7-C8-C9
14	a	1127	CLA	C11-C10-C8-C9
14	b	1223	CLA	C6-C7-C8-C9
14	l	1502	CLA	C11-C10-C8-C9
14	A	1106	CLA	C6-C7-C8-C9
14	A	1127	CLA	C11-C10-C8-C9
14	B	1223	CLA	C6-C7-C8-C9
14	L	1502	CLA	C11-C10-C8-C9
14	b	1222	CLA	C16-C17-C18-C19
14	B	1222	CLA	C16-C17-C18-C19
20	a	5005	LMG	C31-C32-C33-C34
20	B	5002	LMG	C21-C22-C23-C24
14	G	1110	CLA	CAA-CBA-CGA-O2A
14	a	1110	CLA	CAA-CBA-CGA-O2A
14	A	1110	CLA	CAA-CBA-CGA-O2A
20	A	5005	LMG	C31-C32-C33-C34
20	H	5002	LMG	C21-C22-C23-C24
14	G	1013	CLA	C11-C10-C8-C7
14	G	1140	CLA	C11-C10-C8-C7
14	a	1013	CLA	C11-C10-C8-C7
14	a	1140	CLA	C11-C10-C8-C7
14	A	1013	CLA	C11-C10-C8-C7
14	A	1140	CLA	C11-C10-C8-C7
16	H	2002	PQN	C17-C18-C20-C21
16	b	2002	PQN	C17-C18-C20-C21
16	B	2002	PQN	C17-C18-C20-C21
20	G	5005	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
20	b	5002	LMG	C21-C22-C23-C24
14	G	1126	CLA	C2B-C3B-CAB-CBB
14	H	1023	CLA	C2B-C3B-CAB-CBB
14	H	1225	CLA	C2B-C3B-CAB-CBB
14	H	1227	CLA	C2B-C3B-CAB-CBB
14	a	1126	CLA	C2B-C3B-CAB-CBB
14	b	1023	CLA	C2B-C3B-CAB-CBB
14	b	1225	CLA	C2B-C3B-CAB-CBB
14	b	1227	CLA	C2B-C3B-CAB-CBB
14	A	1126	CLA	C2B-C3B-CAB-CBB
14	B	1023	CLA	C2B-C3B-CAB-CBB
14	B	1225	CLA	C2B-C3B-CAB-CBB
14	B	1227	CLA	C2B-C3B-CAB-CBB
18	G	4002	BCR	C23-C24-C25-C26
18	G	4002	BCR	C23-C24-C25-C30
18	G	4003	BCR	C23-C24-C25-C26
18	G	4011	BCR	C1-C6-C7-C8
18	G	4011	BCR	C5-C6-C7-C8
18	H	4010	BCR	C23-C24-C25-C26
18	H	4017	BCR	C5-C6-C7-C8
18	R	4018	BCR	C5-C6-C7-C8
18	R	4020	BCR	C5-C6-C7-C8
18	a	4002	BCR	C23-C24-C25-C26
18	a	4002	BCR	C23-C24-C25-C30
18	a	4003	BCR	C23-C24-C25-C26
18	a	4011	BCR	C5-C6-C7-C8
18	b	4010	BCR	C23-C24-C25-C26
18	b	4017	BCR	C5-C6-C7-C8
18	i	4018	BCR	C5-C6-C7-C8
18	i	4020	BCR	C5-C6-C7-C8
18	A	4002	BCR	C23-C24-C25-C26
18	A	4002	BCR	C23-C24-C25-C30
18	A	4003	BCR	C23-C24-C25-C26
18	A	4011	BCR	C5-C6-C7-C8
18	B	4010	BCR	C23-C24-C25-C26
18	B	4017	BCR	C5-C6-C7-C8
18	I	4018	BCR	C5-C6-C7-C8
18	I	4020	BCR	C5-C6-C7-C8
14	H	1221	CLA	C2-C1-O2A-CGA
14	b	1221	CLA	C2-C1-O2A-CGA
14	B	1221	CLA	C2-C1-O2A-CGA
13	G	1011	CL0	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	A	1011	CL0	C15-C16-C17-C18
14	H	1239	CLA	CAA-CBA-CGA-O2A
14	b	1239	CLA	CAA-CBA-CGA-O2A
14	B	1239	CLA	CAA-CBA-CGA-O2A
19	G	5001	LHG	O7-C7-C8-C9
13	a	1011	CL0	C15-C16-C17-C18
14	G	1134	CLA	CAA-CBA-CGA-O1A
14	a	1134	CLA	CAA-CBA-CGA-O1A
14	H	1210	CLA	C13-C15-C16-C17
14	B	1210	CLA	C13-C15-C16-C17
14	H	1226	CLA	C2A-CAA-CBA-CGA
14	b	1226	CLA	C2A-CAA-CBA-CGA
14	B	1226	CLA	C2A-CAA-CBA-CGA
14	b	1210	CLA	C13-C15-C16-C17
19	a	5001	LHG	O7-C7-C8-C9
14	A	1134	CLA	CAA-CBA-CGA-O1A
19	A	5001	LHG	O7-C7-C8-C9
14	G	1140	CLA	CAA-CBA-CGA-O1A
14	a	1140	CLA	CAA-CBA-CGA-O1A
14	A	1140	CLA	CAA-CBA-CGA-O1A
14	G	1138	CLA	CAA-CBA-CGA-O2A
14	H	1235	CLA	CAA-CBA-CGA-O2A
14	a	1138	CLA	CAA-CBA-CGA-O2A
14	b	1235	CLA	CAA-CBA-CGA-O2A
14	A	1138	CLA	CAA-CBA-CGA-O2A
14	B	1235	CLA	CAA-CBA-CGA-O2A
14	H	1217	CLA	C2-C3-C5-C6
14	b	1217	CLA	C2-C3-C5-C6
14	B	1217	CLA	C2-C3-C5-C6
14	b	1204	CLA	CAA-CBA-CGA-O2A
19	H	5004	LHG	O9-C7-O7-C5
19	b	5004	LHG	O9-C7-O7-C5
19	B	5004	LHG	O9-C7-O7-C5
14	b	1218	CLA	CAA-CBA-CGA-O2A
14	B	1218	CLA	CAA-CBA-CGA-O2A
14	H	1224	CLA	C6-C7-C8-C9
14	b	1224	CLA	C6-C7-C8-C9
14	B	1224	CLA	C6-C7-C8-C9
18	H	4006	BCR	C7-C8-C9-C34
18	b	4006	BCR	C7-C8-C9-C34
14	H	1204	CLA	CAA-CBA-CGA-O2A
14	G	1139	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	H	1222	CLA	C1A-C2A-CAA-CBA
14	H	1223	CLA	C1A-C2A-CAA-CBA
14	W	1701	CLA	C1A-C2A-CAA-CBA
14	a	1139	CLA	C4B-C3B-CAB-CBB
14	b	1222	CLA	C1A-C2A-CAA-CBA
14	b	1223	CLA	C1A-C2A-CAA-CBA
14	x	1701	CLA	C1A-C2A-CAA-CBA
14	A	1139	CLA	C4B-C3B-CAB-CBB
14	B	1222	CLA	C1A-C2A-CAA-CBA
14	B	1223	CLA	C1A-C2A-CAA-CBA
14	X	1701	CLA	C1A-C2A-CAA-CBA
14	a	1110	CLA	CAA-CBA-CGA-O1A
14	A	1110	CLA	CAA-CBA-CGA-O1A
14	a	1118	CLA	C4-C3-C5-C6
14	A	1118	CLA	C4-C3-C5-C6
14	G	1126	CLA	CAA-CBA-CGA-O2A
14	a	1126	CLA	CAA-CBA-CGA-O2A
14	A	1126	CLA	CAA-CBA-CGA-O2A
14	B	1204	CLA	CAA-CBA-CGA-O2A
20	l	5007	LMG	O8-C28-C29-C30
14	H	1218	CLA	CAA-CBA-CGA-O2A
18	H	4005	BCR	C17-C18-C19-C20
18	b	4005	BCR	C17-C18-C19-C20
18	m	4021	BCR	C21-C22-C23-C24
18	B	4005	BCR	C17-C18-C19-C20
18	H	4009	BCR	C19-C20-C21-C22
18	b	4009	BCR	C19-C20-C21-C22
18	B	4009	BCR	C19-C20-C21-C22
14	G	1126	CLA	C3-C5-C6-C7
14	A	1126	CLA	C3-C5-C6-C7
14	G	1110	CLA	CAA-CBA-CGA-O1A
20	U	5007	LMG	O8-C28-C29-C30
20	L	5007	LMG	O8-C28-C29-C30
14	H	1215	CLA	C2A-CAA-CBA-CGA
14	b	1215	CLA	C2A-CAA-CBA-CGA
14	B	1215	CLA	C2A-CAA-CBA-CGA
14	a	1126	CLA	C3-C5-C6-C7
14	W	1701	CLA	CAA-CBA-CGA-O2A
14	x	1701	CLA	CAA-CBA-CGA-O2A
14	X	1701	CLA	CAA-CBA-CGA-O2A
19	H	5004	LHG	C8-C7-O7-C5
14	b	1222	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	G	1118	CLA	C4-C3-C5-C6
14	G	1115	CLA	C2-C1-O2A-CGA
14	H	1235	CLA	C2-C1-O2A-CGA
14	a	1115	CLA	C2-C1-O2A-CGA
14	b	1235	CLA	C2-C1-O2A-CGA
14	A	1115	CLA	C2-C1-O2A-CGA
14	B	1235	CLA	C2-C1-O2A-CGA
14	G	1133	CLA	C11-C10-C8-C7
14	H	1213	CLA	C12-C13-C15-C16
14	H	1222	CLA	C11-C12-C13-C15
14	H	1226	CLA	C6-C7-C8-C10
14	U	1501	CLA	C11-C10-C8-C7
14	a	1133	CLA	C11-C10-C8-C7
14	b	1213	CLA	C12-C13-C15-C16
14	b	1222	CLA	C11-C12-C13-C15
14	b	1226	CLA	C6-C7-C8-C10
14	l	1501	CLA	C11-C10-C8-C7
14	A	1133	CLA	C11-C10-C8-C7
14	B	1213	CLA	C12-C13-C15-C16
14	B	1222	CLA	C11-C12-C13-C15
14	B	1226	CLA	C6-C7-C8-C10
14	L	1501	CLA	C11-C10-C8-C7
15	H	1207	F6C	CAA-CBA-CGA-O2A
15	b	1207	F6C	CAA-CBA-CGA-O2A
15	B	1207	F6C	CAA-CBA-CGA-O2A
14	H	1222	CLA	C8-C10-C11-C12
14	B	1222	CLA	C8-C10-C11-C12
14	G	1116	CLA	CAA-CBA-CGA-O1A
14	a	1116	CLA	CAA-CBA-CGA-O1A
14	A	1116	CLA	CAA-CBA-CGA-O1A
14	U	1501	CLA	C2A-CAA-CBA-CGA
14	l	1501	CLA	C2A-CAA-CBA-CGA
14	L	1501	CLA	C2A-CAA-CBA-CGA
14	H	1233	CLA	CAA-CBA-CGA-O2A
14	B	1233	CLA	CAA-CBA-CGA-O2A
15	b	1230	F6C	CAA-CBA-CGA-O2A
14	b	1233	CLA	CAA-CBA-CGA-O2A
15	H	1230	F6C	CAA-CBA-CGA-O2A
15	B	1230	F6C	CAA-CBA-CGA-O2A
14	H	1022	CLA	C3A-C2A-CAA-CBA
14	H	1228	CLA	C3A-C2A-CAA-CBA
14	b	1022	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
14	b	1228	CLA	C3A-C2A-CAA-CBA
14	B	1022	CLA	C3A-C2A-CAA-CBA
14	B	1228	CLA	C3A-C2A-CAA-CBA
21	a	6001	LMT	C4B-C5B-C6B-O6B
14	G	1126	CLA	CAA-CBA-CGA-O1A
14	a	1126	CLA	CAA-CBA-CGA-O1A
14	A	1126	CLA	CAA-CBA-CGA-O1A
19	b	5004	LHG	C8-C7-O7-C5
14	G	1013	CLA	C2A-CAA-CBA-CGA
14	a	1013	CLA	C2A-CAA-CBA-CGA
14	A	1013	CLA	C2A-CAA-CBA-CGA
14	H	1218	CLA	CAA-CBA-CGA-O1A
14	B	1218	CLA	CAA-CBA-CGA-O1A
21	A	6001	LMT	C4B-C5B-C6B-O6B
14	H	1211	CLA	C11-C10-C8-C9
14	H	1222	CLA	C11-C12-C13-C14
14	b	1211	CLA	C11-C10-C8-C9
14	b	1222	CLA	C11-C12-C13-C14
14	B	1211	CLA	C11-C10-C8-C9
14	B	1222	CLA	C11-C12-C13-C14
14	W	1701	CLA	CAA-CBA-CGA-O1A
14	B	1235	CLA	CAA-CBA-CGA-O1A
14	X	1701	CLA	CAA-CBA-CGA-O1A
20	l	5007	LMG	C28-C29-C30-C31
21	G	6001	LMT	C4B-C5B-C6B-O6B
14	b	1218	CLA	CAA-CBA-CGA-O1A
15	H	1238	F6C	C5-C6-C7-C8
15	b	1238	F6C	C5-C6-C7-C8
15	B	1238	F6C	C5-C6-C7-C8
14	H	1235	CLA	CAA-CBA-CGA-O1A
14	b	1235	CLA	CAA-CBA-CGA-O1A
19	H	5004	LHG	O7-C7-C8-C9
19	b	5004	LHG	O7-C7-C8-C9
19	B	5004	LHG	O7-C7-C8-C9
20	U	5007	LMG	C28-C29-C30-C31
20	L	5007	LMG	C28-C29-C30-C31
14	x	1701	CLA	CAA-CBA-CGA-O1A
20	U	5007	LMG	O10-C28-C29-C30
14	a	1116	CLA	C3-C5-C6-C7
14	G	1105	CLA	CAA-CBA-CGA-O2A
14	G	1113	CLA	CAA-CBA-CGA-O2A
14	a	1105	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	a	1113	CLA	CAA-CBA-CGA-O2A
14	A	1105	CLA	CAA-CBA-CGA-O2A
14	A	1113	CLA	CAA-CBA-CGA-O2A
18	V	4021	BCR	C21-C22-C23-C24
18	M	4021	BCR	C21-C22-C23-C24
19	B	5004	LHG	C8-C7-O7-C5
14	a	1138	CLA	CAA-CBA-CGA-O1A
14	A	1138	CLA	CAA-CBA-CGA-O1A
19	G	5001	LHG	O9-C7-C8-C9
19	a	5001	LHG	O9-C7-C8-C9
19	A	5001	LHG	O9-C7-C8-C9
14	a	1114	CLA	C2C-C3C-CAC-CBC
14	G	1138	CLA	CAA-CBA-CGA-O1A
20	l	5007	LMG	O10-C28-C29-C30
20	L	5007	LMG	O10-C28-C29-C30
13	a	1011	CL0	CAA-CBA-CGA-O2A
13	A	1011	CL0	CAA-CBA-CGA-O2A
14	b	1239	CLA	CAA-CBA-CGA-O1A
14	B	1239	CLA	CAA-CBA-CGA-O1A
14	H	1205	CLA	C13-C15-C16-C17
14	b	1205	CLA	C13-C15-C16-C17
14	B	1205	CLA	C13-C15-C16-C17
14	G	1114	CLA	C2C-C3C-CAC-CBC
14	A	1114	CLA	C2C-C3C-CAC-CBC
14	G	1116	CLA	C3-C5-C6-C7
14	A	1116	CLA	C3-C5-C6-C7
14	H	1239	CLA	CAA-CBA-CGA-O1A
14	A	1103	CLA	O1A-CGA-O2A-C1
20	H	5002	LMG	C29-C30-C31-C32
13	G	1011	CL0	CAA-CBA-CGA-O2A
20	U	5007	LMG	O7-C10-C11-C12
20	l	5007	LMG	O7-C10-C11-C12
20	L	5007	LMG	O7-C10-C11-C12
14	a	1103	CLA	O1A-CGA-O2A-C1
20	B	5002	LMG	C29-C30-C31-C32
14	H	1234	CLA	C2-C1-O2A-CGA
14	b	1234	CLA	C2-C1-O2A-CGA
14	B	1234	CLA	C2-C1-O2A-CGA
20	b	5002	LMG	C29-C30-C31-C32
14	G	1103	CLA	C3-C5-C6-C7
14	a	1103	CLA	C3-C5-C6-C7
21	G	6001	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
19	B	5004	LHG	O9-C7-C8-C9
14	U	1503	CLA	C5-C6-C7-C8
21	a	6002	LMT	C3'-C4'-O1B-C1B
14	G	1103	CLA	O1A-CGA-O2A-C1
14	H	1221	CLA	CAA-CBA-CGA-O2A
20	b	5002	LMG	C11-C12-C13-C14
14	L	1503	CLA	C5-C6-C7-C8
14	A	1103	CLA	C3-C5-C6-C7
20	B	5002	LMG	C11-C12-C13-C14
14	l	1503	CLA	C5-C6-C7-C8
20	H	5002	LMG	C11-C12-C13-C14
14	H	1211	CLA	CAA-CBA-CGA-O2A
14	a	1122	CLA	CAA-CBA-CGA-O2A
14	b	1211	CLA	CAA-CBA-CGA-O2A
14	A	1122	CLA	CAA-CBA-CGA-O2A
14	B	1211	CLA	CAA-CBA-CGA-O2A
20	b	5002	LMG	O7-C10-C11-C12
20	B	5002	LMG	O7-C10-C11-C12
14	H	1204	CLA	CAA-CBA-CGA-O1A
14	b	1204	CLA	CAA-CBA-CGA-O1A
19	H	5004	LHG	O9-C7-C8-C9
19	b	5004	LHG	O9-C7-C8-C9
20	L	5007	LMG	O9-C10-C11-C12
21	a	6001	LMT	O5B-C1B-O1B-C4'
21	A	6002	LMT	C3'-C4'-O1B-C1B

There are no ring outliers.

325 monomers are involved in 1089 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1230	F6C	1	0
14	b	1220	CLA	3	0
14	A	1113	CLA	1	0
14	G	1013	CLA	6	0
14	b	1226	CLA	1	0
14	G	1118	CLA	1	0
16	A	2001	PQN	11	0
14	A	1136	CLA	5	0
21	A	6001	LMT	1	0
16	B	2002	PQN	6	0
18	A	4008	BCR	5	0
14	b	1224	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1217	CLA	2	0
14	a	1132	CLA	6	0
14	G	1132	CLA	5	0
19	B	5004	LHG	1	0
15	B	1207	F6C	1	0
19	A	5001	LHG	3	0
14	a	1133	CLA	1	0
14	a	1134	CLA	2	0
14	b	1235	CLA	2	0
14	a	1124	CLA	6	0
14	H	1225	CLA	5	0
14	L	1503	CLA	6	0
15	B	1238	F6C	1	0
14	H	1219	CLA	4	0
14	G	1138	CLA	5	0
18	H	4014	BCR	2	0
14	a	1111	CLA	6	0
14	A	1115	CLA	5	0
14	b	1222	CLA	9	0
18	R	4020	BCR	5	0
14	G	1113	CLA	2	0
18	L	4019	BCR	3	0
14	a	1128	CLA	2	0
14	B	1217	CLA	2	0
14	b	1215	CLA	3	0
14	H	1221	CLA	9	0
14	H	1213	CLA	5	0
14	H	1021	CLA	7	0
18	H	4009	BCR	7	0
18	I	4018	BCR	2	0
14	a	1126	CLA	5	0
14	W	1701	CLA	5	0
18	b	4013	BCR	2	0
14	G	1124	CLA	5	0
14	B	1221	CLA	9	0
14	a	1102	CLA	2	0
14	a	1107	CLA	2	0
14	G	1120	CLA	2	0
14	H	1216	CLA	7	0
14	a	1122	CLA	2	0
14	b	1203	CLA	5	0
14	b	1232	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	1239	CLA	2	0
19	G	5001	LHG	2	0
20	H	5002	LMG	4	0
18	H	4017	BCR	4	0
14	B	1205	CLA	11	0
14	a	1106	CLA	4	0
14	H	1214	CLA	3	0
14	H	1226	CLA	2	0
14	b	1023	CLA	9	0
18	a	4007	BCR	1	0
13	a	1011	CL0	4	0
14	A	1117	CLA	4	0
14	a	1112	CLA	3	0
15	b	1230	F6C	1	0
14	a	1129	CLA	1	0
14	G	1102	CLA	1	0
14	G	1115	CLA	5	0
14	A	1013	CLA	4	0
14	a	1117	CLA	3	0
14	a	1139	CLA	1	0
14	G	1111	CLA	6	0
14	H	1223	CLA	4	0
14	G	1135	CLA	3	0
14	B	1208	CLA	3	0
14	G	1123	CLA	2	0
18	H	4016	BCR	3	0
14	H	1022	CLA	6	0
14	H	1231	CLA	4	0
14	x	1701	CLA	3	0
14	H	1220	CLA	3	0
18	i	4020	BCR	5	0
20	U	5007	LMG	3	0
14	B	1212	CLA	3	0
14	A	1128	CLA	2	0
14	a	1109	CLA	3	0
18	H	4013	BCR	3	0
14	b	1204	CLA	4	0
14	G	1129	CLA	1	0
19	H	5004	LHG	3	0
14	H	1224	CLA	8	0
14	G	1107	CLA	2	0
14	H	1202	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	1238	F6C	1	0
14	b	1201	CLA	6	0
14	G	1106	CLA	2	0
14	a	1127	CLA	3	0
14	H	1210	CLA	12	0
18	a	4003	BCR	2	0
14	H	1205	CLA	12	0
18	m	4021	BCR	5	0
14	b	1217	CLA	2	0
14	b	1022	CLA	6	0
14	G	1122	CLA	2	0
18	a	4011	BCR	6	0
14	a	1110	CLA	1	0
18	V	4021	BCR	4	0
14	H	1222	CLA	10	0
14	a	1119	CLA	5	0
14	B	1225	CLA	6	0
14	H	1232	CLA	1	0
14	H	1215	CLA	4	0
14	A	1122	CLA	1	0
18	B	4010	BCR	9	0
18	G	4008	BCR	5	0
18	H	4006	BCR	4	0
20	A	5005	LMG	5	0
14	H	1203	CLA	5	0
14	H	1234	CLA	10	0
14	B	1236	CLA	6	0
14	B	1229	CLA	4	0
14	A	1133	CLA	1	0
14	G	1119	CLA	6	0
14	A	1114	CLA	1	0
14	A	1102	CLA	2	0
14	G	1134	CLA	2	0
18	B	4017	BCR	3	0
13	A	1011	CL0	4	0
14	A	1111	CLA	5	0
14	B	1216	CLA	9	0
14	b	1208	CLA	4	0
14	G	1012	CLA	3	0
14	b	1234	CLA	9	0
14	H	1236	CLA	6	0
14	G	1103	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1213	CLA	5	0
14	b	1212	CLA	4	0
14	H	1201	CLA	2	0
14	b	1214	CLA	3	0
14	U	1502	CLA	2	0
14	G	1133	CLA	1	0
14	G	1104	CLA	3	0
18	a	4001	BCR	5	0
14	B	1022	CLA	6	0
14	A	1116	CLA	9	0
18	M	4021	BCR	4	0
14	A	1135	CLA	3	0
17	C	3003	SF4	1	0
14	B	1231	CLA	3	0
14	G	1128	CLA	1	0
14	b	1223	CLA	5	0
14	A	1127	CLA	3	0
14	B	1202	CLA	4	0
14	a	1137	CLA	1	0
18	A	4003	BCR	1	0
18	G	4001	BCR	5	0
14	b	1231	CLA	3	0
14	G	1131	CLA	5	0
14	G	1112	CLA	2	0
14	a	1115	CLA	4	0
14	B	1206	CLA	4	0
14	b	1227	CLA	4	0
14	b	1211	CLA	4	0
14	G	1117	CLA	4	0
18	B	4006	BCR	4	0
14	b	1205	CLA	11	0
14	a	1118	CLA	1	0
20	L	5007	LMG	5	0
14	a	1138	CLA	5	0
14	A	1118	CLA	1	0
14	B	1220	CLA	3	0
14	b	1206	CLA	5	0
14	A	1125	CLA	4	0
14	a	1104	CLA	2	0
18	B	4009	BCR	7	0
14	b	1229	CLA	5	0
14	A	1120	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1224	CLA	9	0
14	B	1228	CLA	5	0
16	b	2002	PQN	5	0
18	a	4002	BCR	1	0
20	R	5006	LMG	4	0
18	b	4010	BCR	9	0
14	a	1116	CLA	8	0
14	G	1140	CLA	7	0
14	l	1501	CLA	6	0
14	B	1210	CLA	11	0
18	B	4014	BCR	4	0
18	B	4013	BCR	3	0
14	a	1131	CLA	5	0
14	A	1138	CLA	5	0
18	G	4002	BCR	3	0
14	B	1222	CLA	11	0
18	U	4019	BCR	2	0
14	G	1136	CLA	5	0
18	B	4016	BCR	2	0
14	A	1104	CLA	3	0
18	b	4014	BCR	5	0
14	L	1502	CLA	4	0
17	c	3003	SF4	1	0
14	B	1215	CLA	4	0
14	H	1212	CLA	3	0
14	A	1124	CLA	5	0
14	b	1221	CLA	10	0
18	H	4005	BCR	3	0
18	b	4009	BCR	6	0
14	B	1219	CLA	4	0
18	G	4003	BCR	2	0
14	B	1232	CLA	1	0
14	H	1204	CLA	7	0
14	B	1214	CLA	3	0
14	b	1225	CLA	6	0
14	a	1140	CLA	8	0
14	B	1021	CLA	7	0
18	l	4022	BCR	6	0
14	H	1208	CLA	2	0
18	A	4001	BCR	5	0
14	H	1206	CLA	5	0
14	A	1131	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	4017	BCR	3	0
14	B	1023	CLA	6	0
14	A	1126	CLA	4	0
14	G	1125	CLA	3	0
14	B	1223	CLA	5	0
18	H	4004	BCR	1	0
14	a	1108	CLA	1	0
14	B	1226	CLA	1	0
14	G	1139	CLA	1	0
14	b	1228	CLA	5	0
18	B	4005	BCR	3	0
14	a	1103	CLA	5	0
18	l	4019	BCR	2	0
14	A	1140	CLA	8	0
14	A	1112	CLA	3	0
14	A	1129	CLA	1	0
15	H	1238	F6C	1	0
18	b	4004	BCR	1	0
14	X	1701	CLA	5	0
18	b	4005	BCR	4	0
14	A	1139	CLA	1	0
14	G	1108	CLA	1	0
14	B	1239	CLA	4	0
18	I	4020	BCR	9	0
14	G	1126	CLA	4	0
14	H	1227	CLA	3	0
16	G	2001	PQN	8	0
14	A	1123	CLA	2	0
14	a	1113	CLA	2	0
18	A	4007	BCR	1	0
20	a	5005	LMG	2	0
15	H	1230	F6C	1	0
18	b	4016	BCR	2	0
14	U	1503	CLA	7	0
14	H	1023	CLA	7	0
21	G	6001	LMT	1	0
14	a	1012	CLA	5	0
14	H	1235	CLA	2	0
14	A	1107	CLA	2	0
14	U	1501	CLA	6	0
18	R	4018	BCR	5	0
18	U	4022	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	i	5006	LMG	1	0
18	A	4002	BCR	2	0
14	b	1021	CLA	8	0
14	A	1106	CLA	2	0
20	G	5005	LMG	5	0
18	A	4011	BCR	4	0
14	a	1123	CLA	2	0
14	A	1109	CLA	3	0
14	b	1236	CLA	7	0
14	a	1135	CLA	3	0
18	i	4018	BCR	3	0
14	L	1501	CLA	6	0
14	A	1119	CLA	7	0
18	L	4022	BCR	6	0
14	b	1210	CLA	10	0
14	b	1239	CLA	3	0
14	H	1229	CLA	4	0
14	A	1134	CLA	2	0
14	l	1502	CLA	3	0
14	b	1216	CLA	9	0
14	B	1204	CLA	5	0
14	H	1233	CLA	1	0
14	B	1235	CLA	2	0
14	A	1012	CLA	5	0
18	G	4007	BCR	1	0
13	G	1011	CL0	4	0
16	a	2001	PQN	10	0
14	a	1136	CLA	6	0
14	B	1234	CLA	9	0
14	A	1103	CLA	5	0
14	b	1213	CLA	4	0
14	G	1116	CLA	7	0
14	l	1503	CLA	6	0
14	b	1219	CLA	3	0
14	H	1211	CLA	4	0
14	G	1109	CLA	4	0
18	a	4008	BCR	6	0
16	H	2002	PQN	6	0
14	B	1201	CLA	4	0
20	I	5006	LMG	1	0
14	A	1137	CLA	1	0
14	a	1013	CLA	4	0

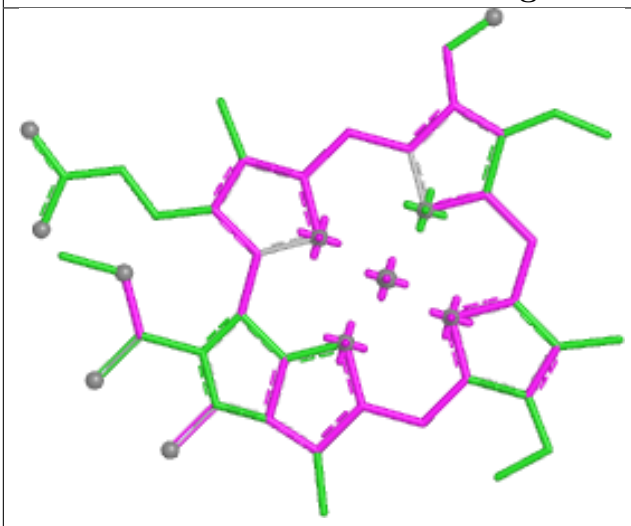
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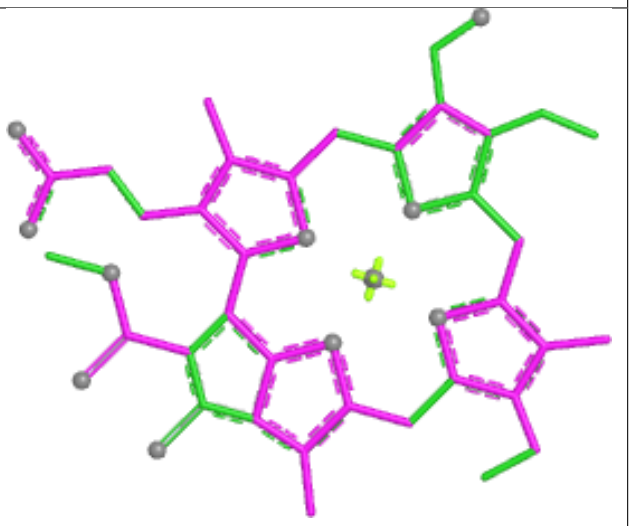
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	1203	CLA	4	0
14	b	1202	CLA	4	0
17	N	3003	SF4	1	0
20	B	5002	LMG	4	0
14	A	1132	CLA	6	0
19	a	5001	LHG	3	0
14	a	1125	CLA	4	0
14	G	1127	CLA	3	0
20	l	5007	LMG	4	0
18	H	4010	BCR	9	0
14	a	1120	CLA	2	0
14	A	1108	CLA	1	0
14	G	1137	CLA	1	0
20	b	5002	LMG	4	0
18	b	4006	BCR	4	0
14	B	1227	CLA	3	0
14	B	1211	CLA	5	0
14	H	1228	CLA	5	0
18	G	4011	BCR	5	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.

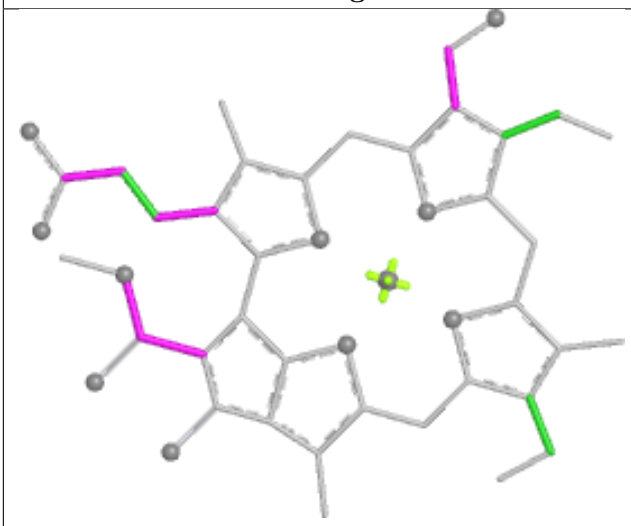
Ligand F6C B 1230



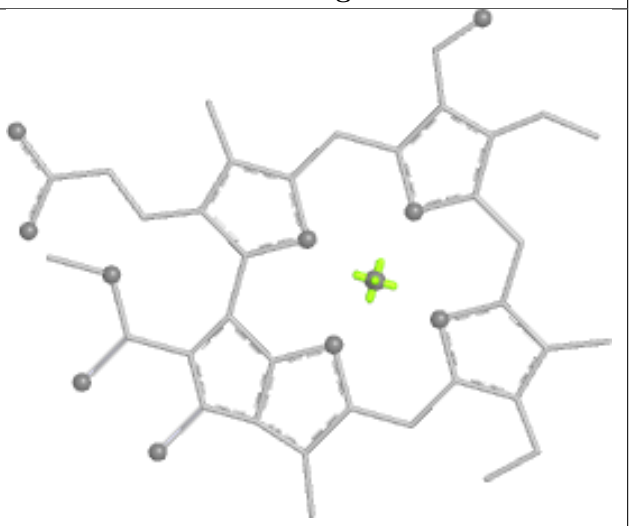
Bond lengths



Bond angles

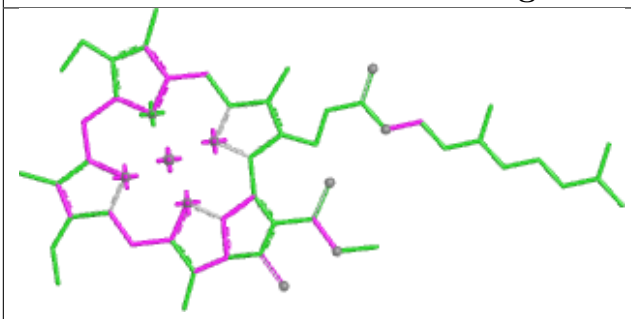


Torsions

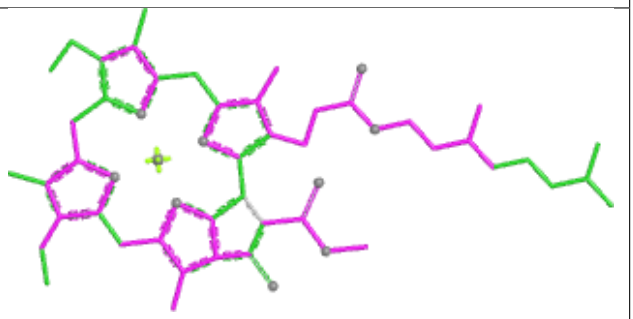


Rings

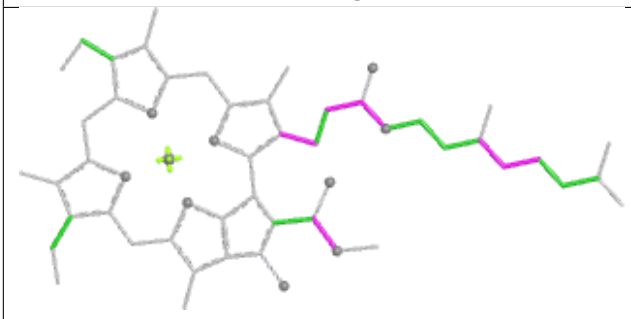
Ligand CLA b 1220



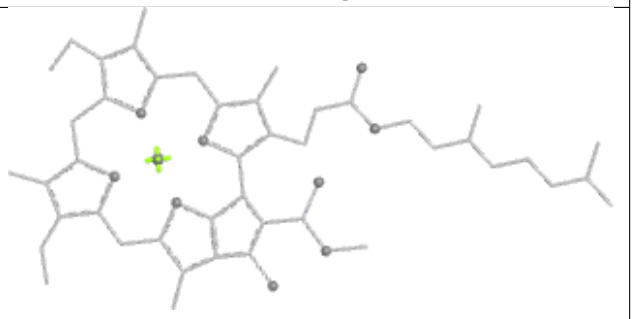
Bond lengths



Bond angles

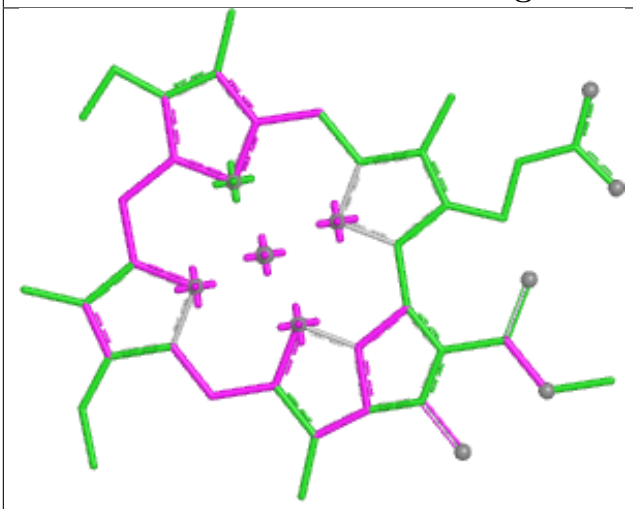


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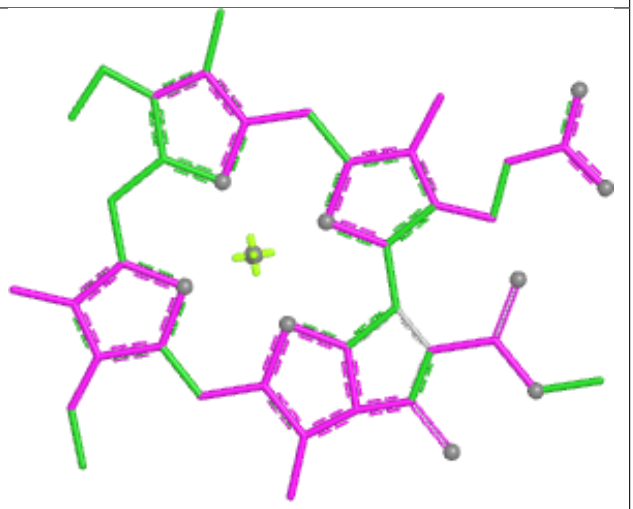


Rings

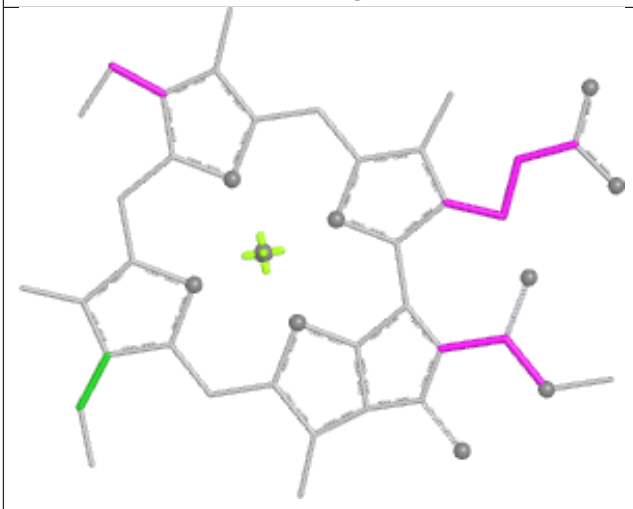
Ligand CLA A 1113



Bond lengths



Bond angles

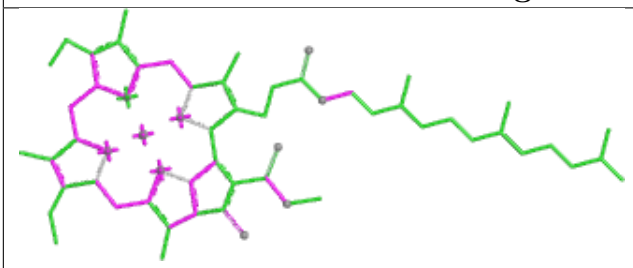


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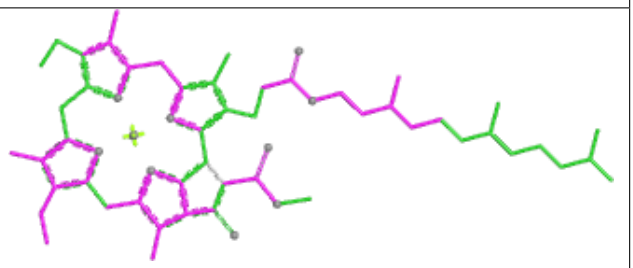


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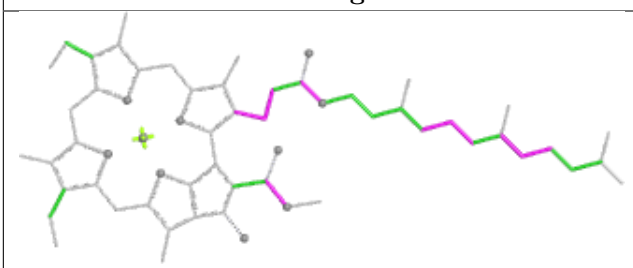
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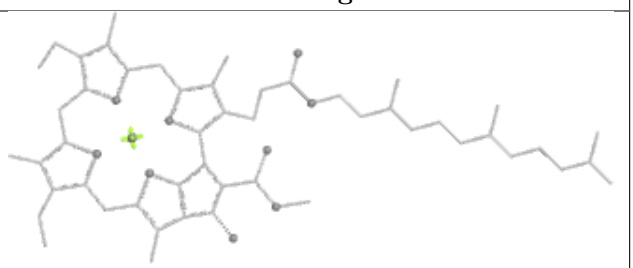
Bond lengths



Bond angles

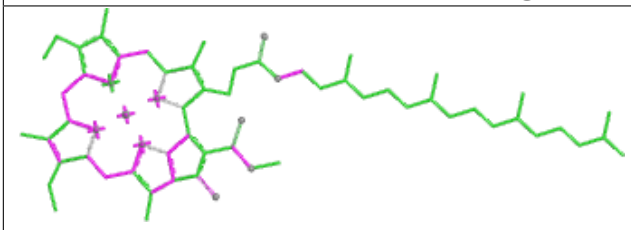


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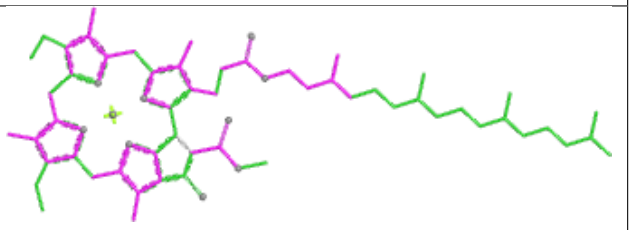


Rings

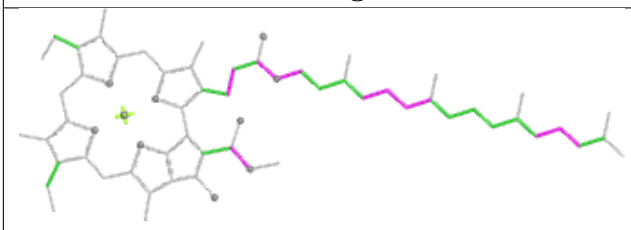
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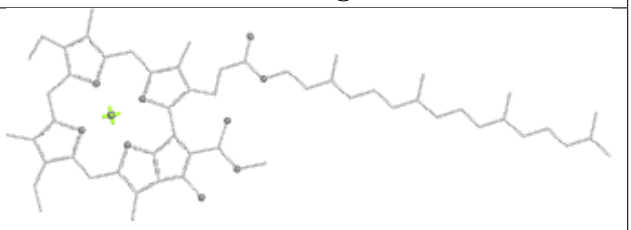
Bond lengths



Bond angles

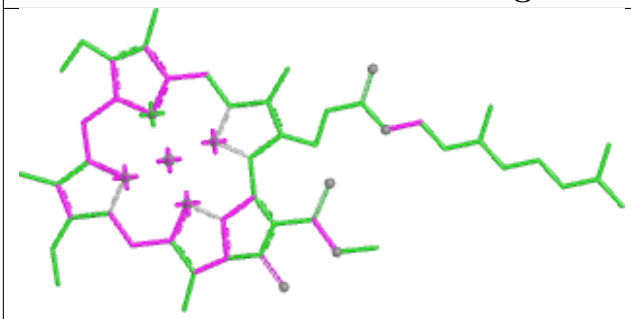


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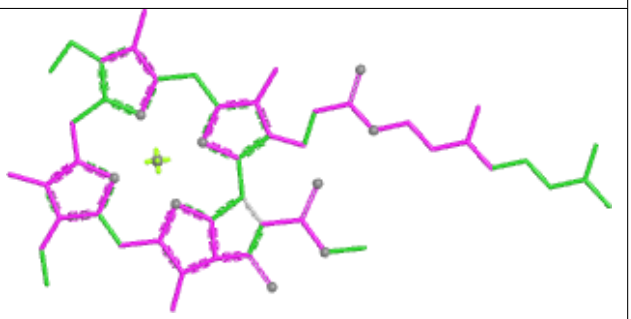


Rings

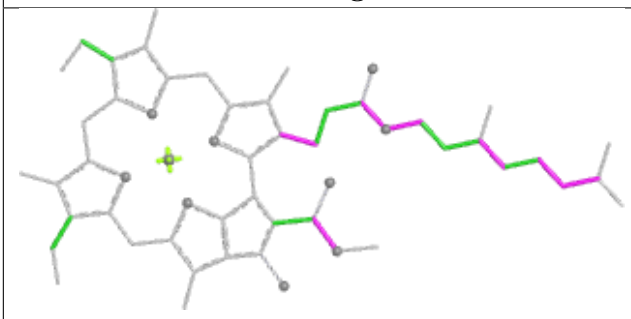
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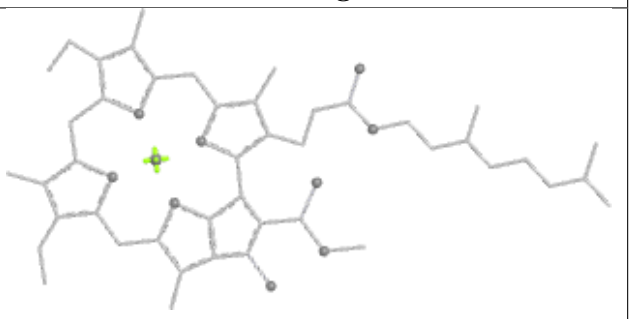
Bond lengths



Bond angles

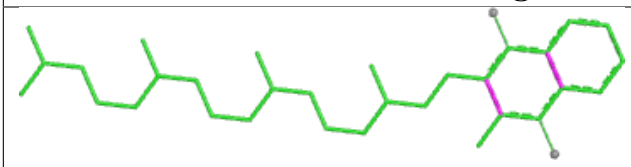


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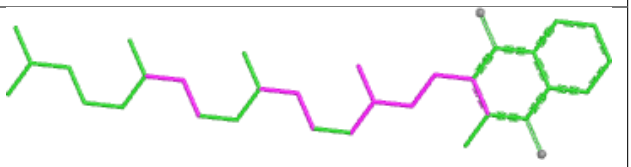


Rings

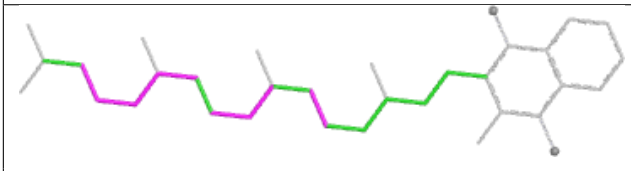
Ligand PQN A 2001



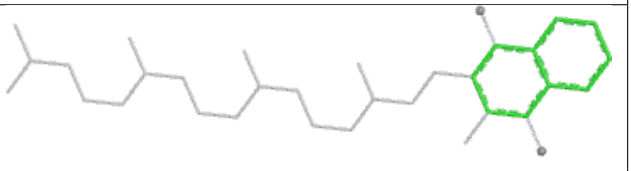
Bond lengths



Bond angles

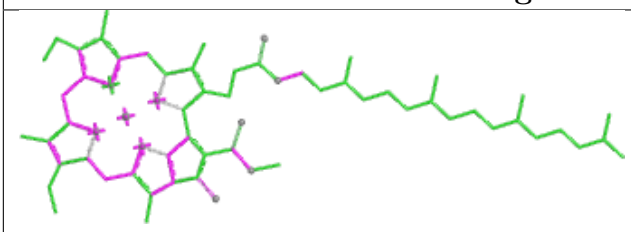


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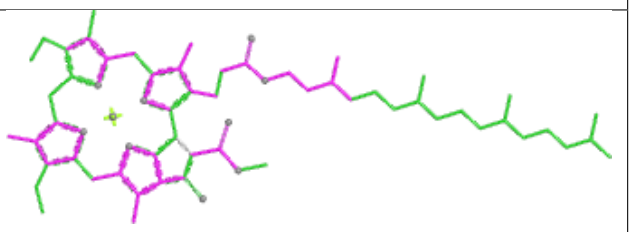


Rings

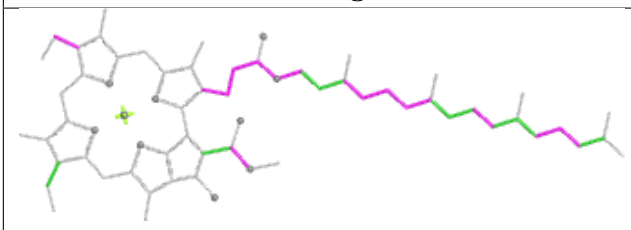
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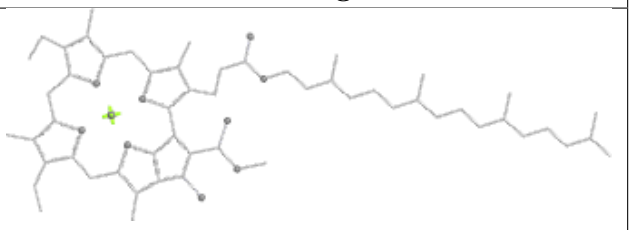
Bond lengths



Bond angles

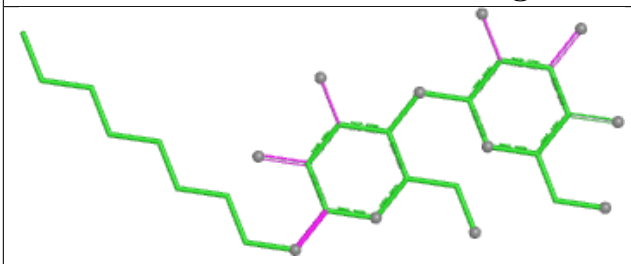


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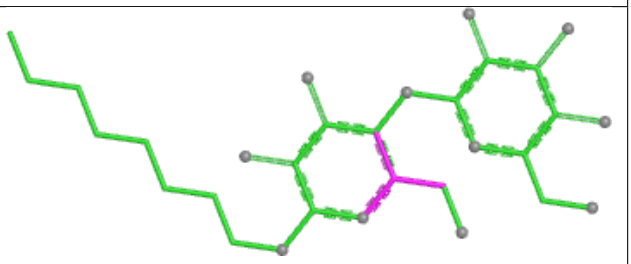


Rings

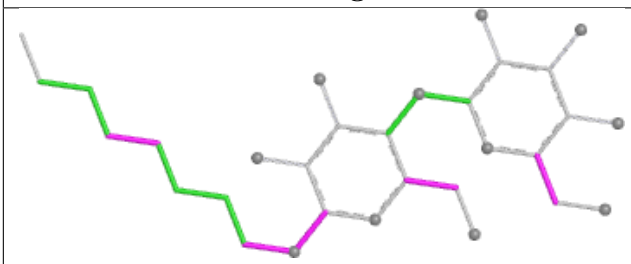
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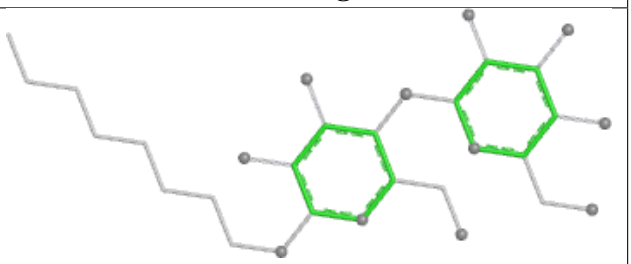
Bond lengths



Bond angles

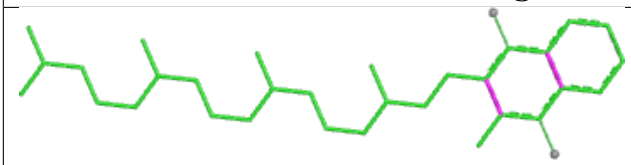


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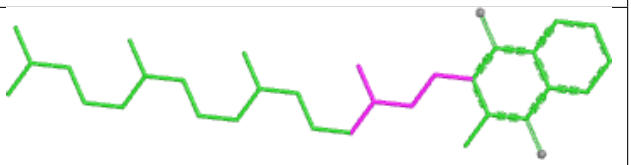


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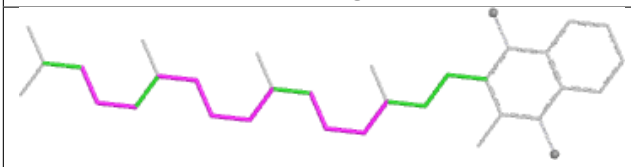
Ligand PQN B 2002



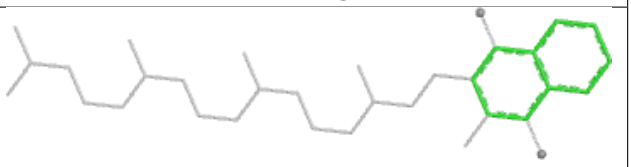
Bond lengths



Bond angles

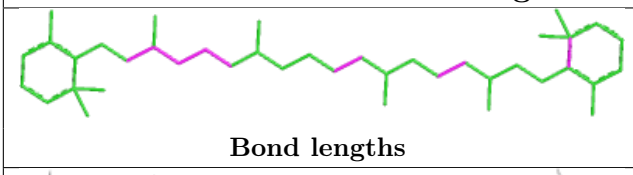


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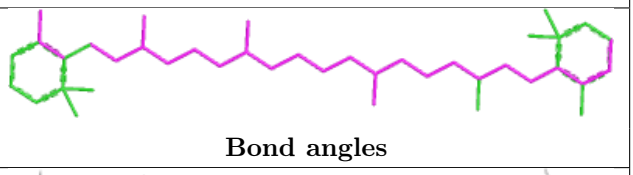


Rings

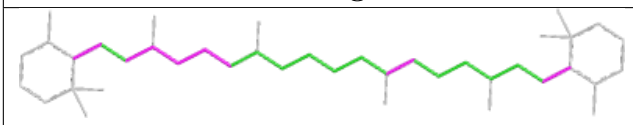
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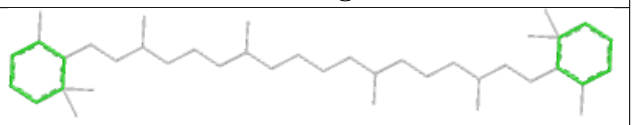
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Bond angles

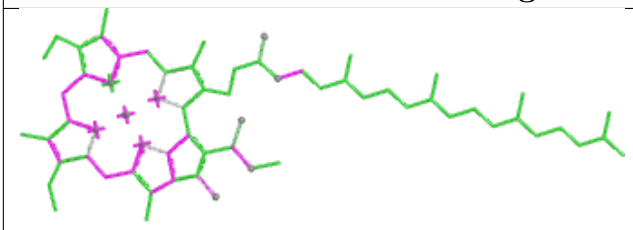


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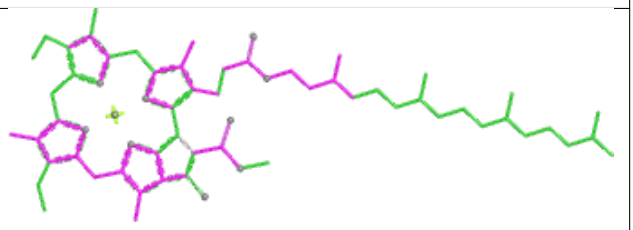


Rings

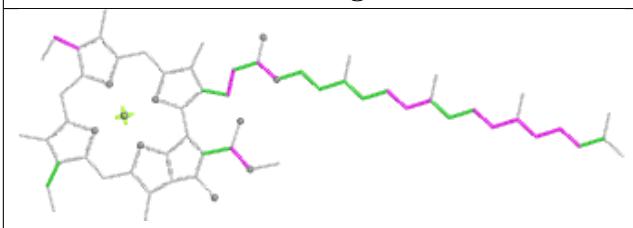
Ligand CLA b 1224



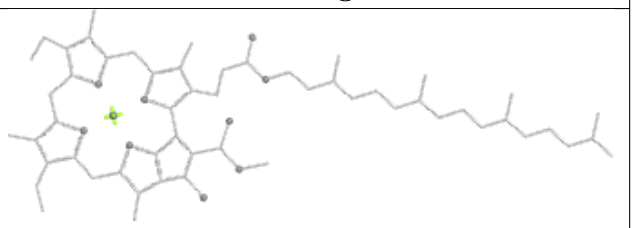
Bond lengths



Bond angles

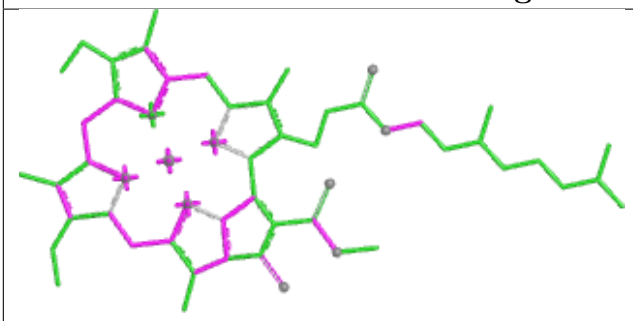


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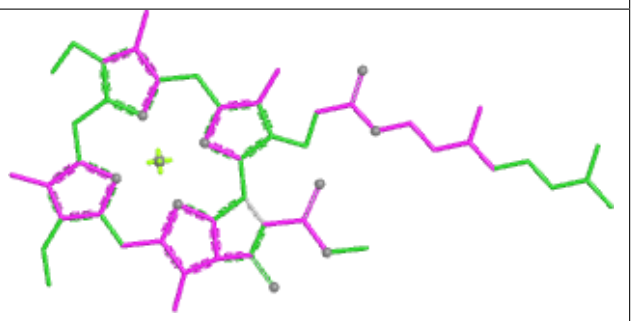


Rings

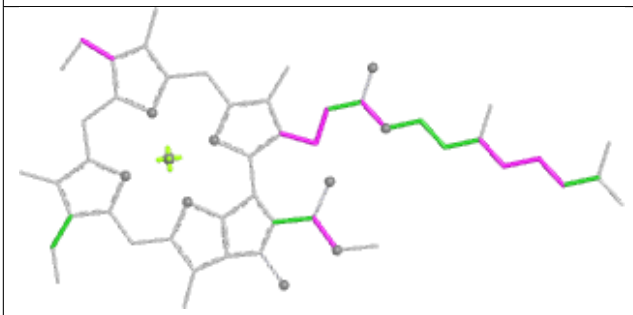
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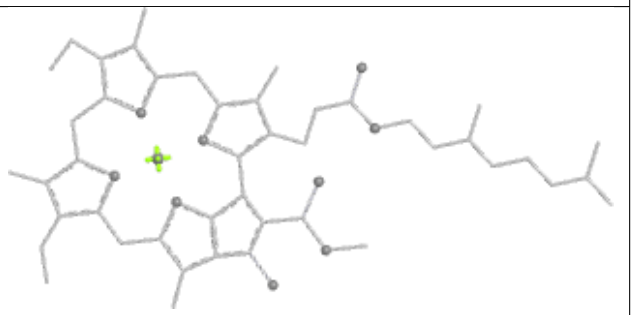
Bond lengths



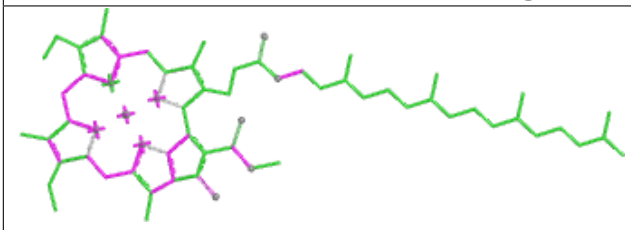
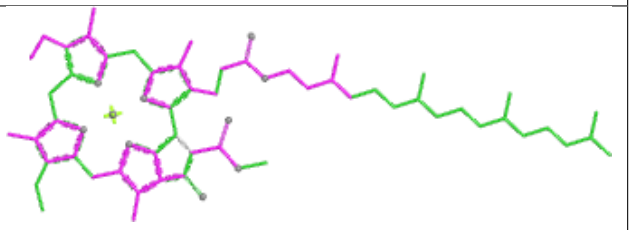
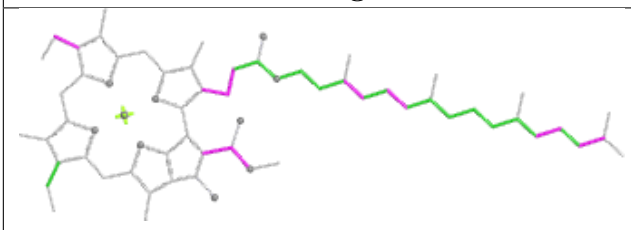
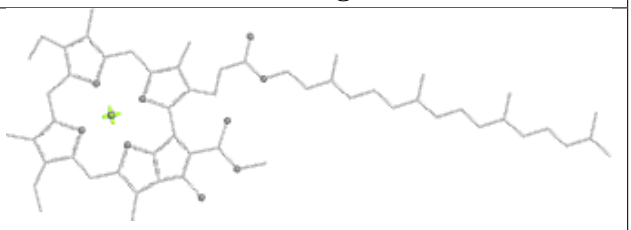
Bond angles

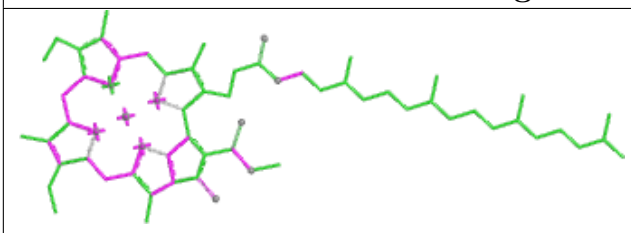
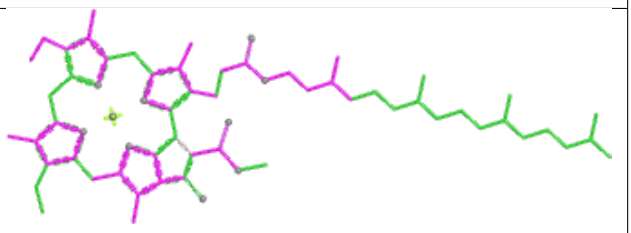
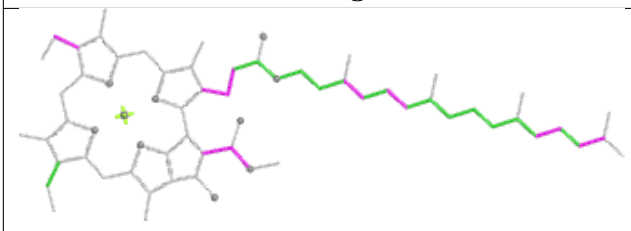
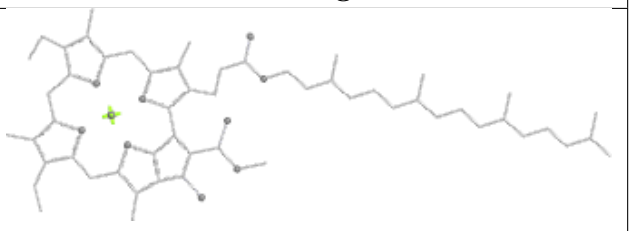


Torsions

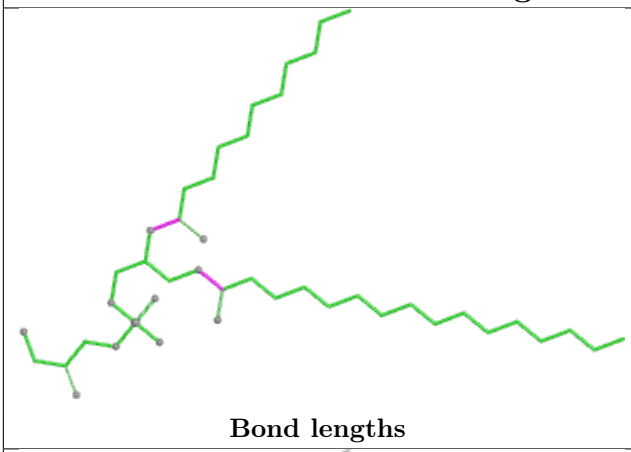


Rings

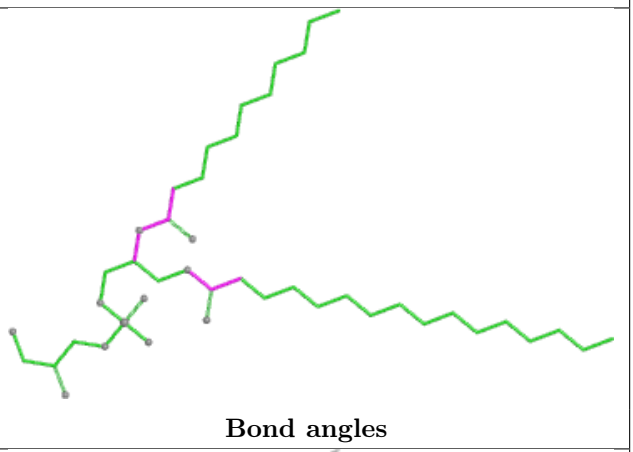
Ligand CLA a 1132	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1132	
	
Bond lengths	Bond angles
	
Torsions	Rings

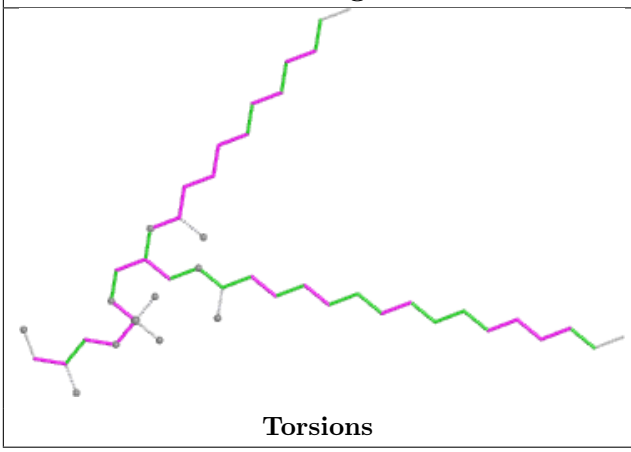
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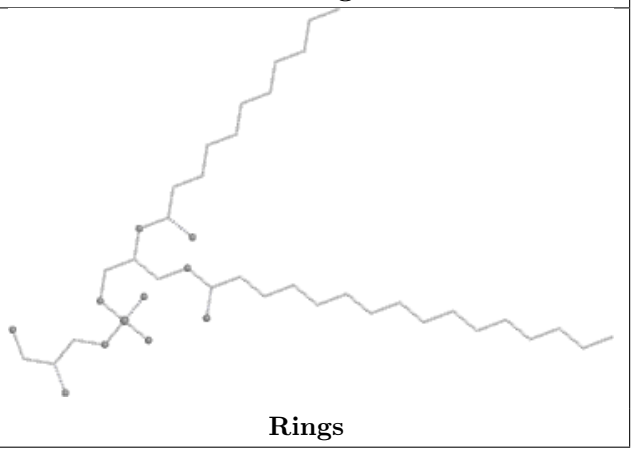
Bond lengths



Bond angles

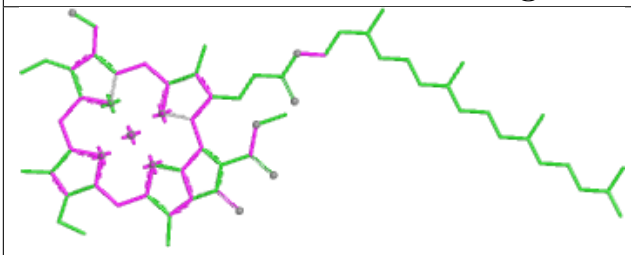


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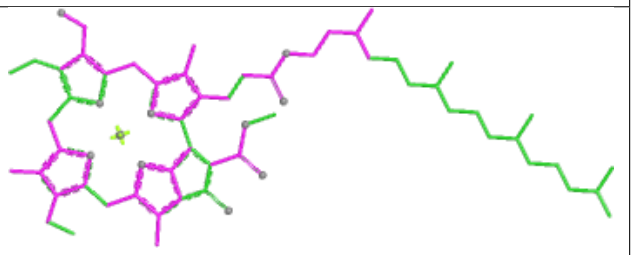


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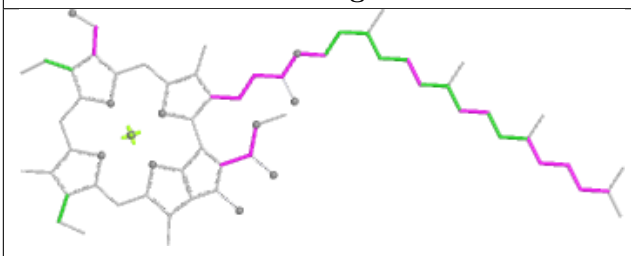
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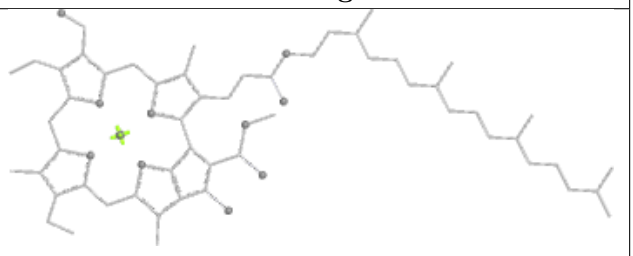
Bond lengths



Bond angles

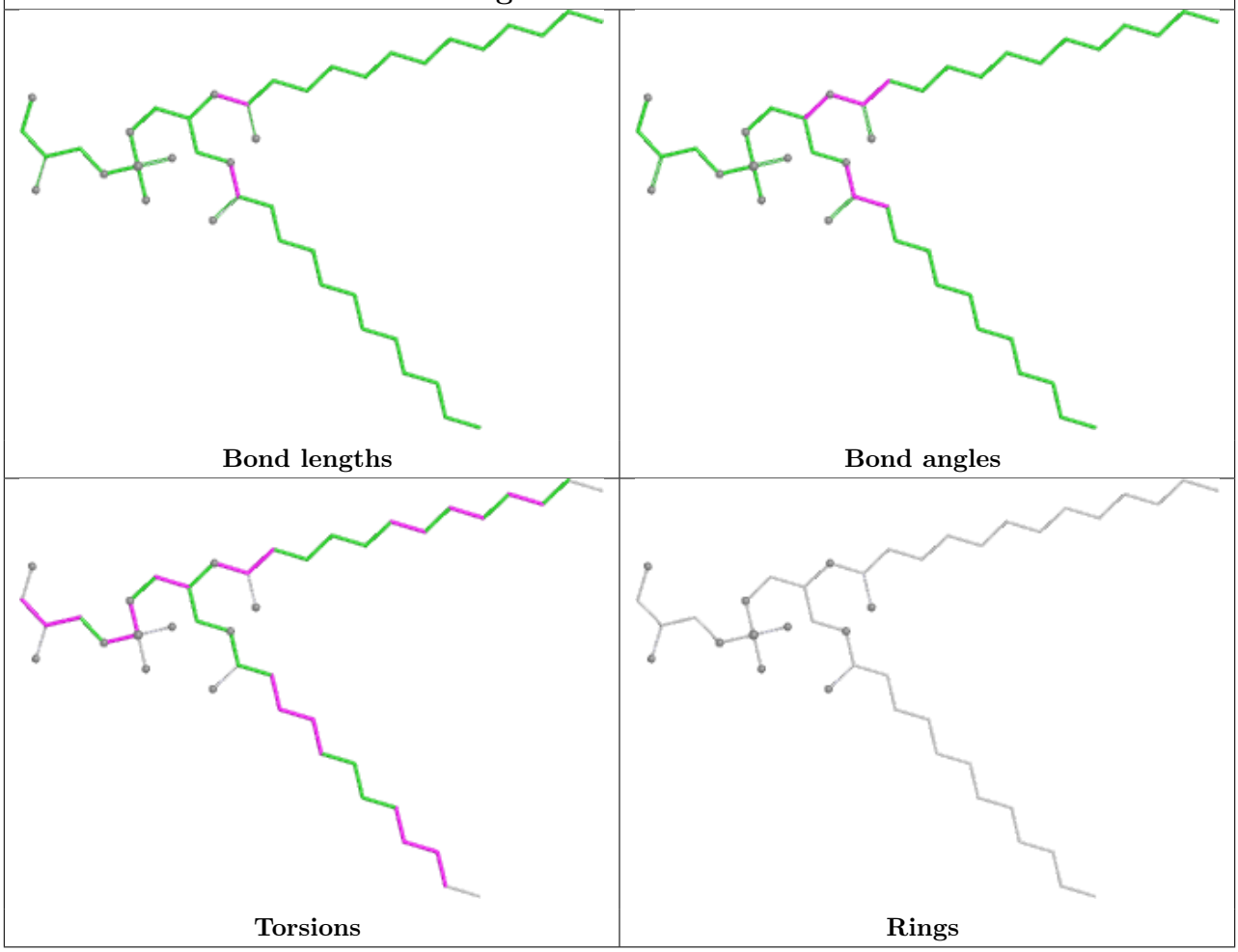


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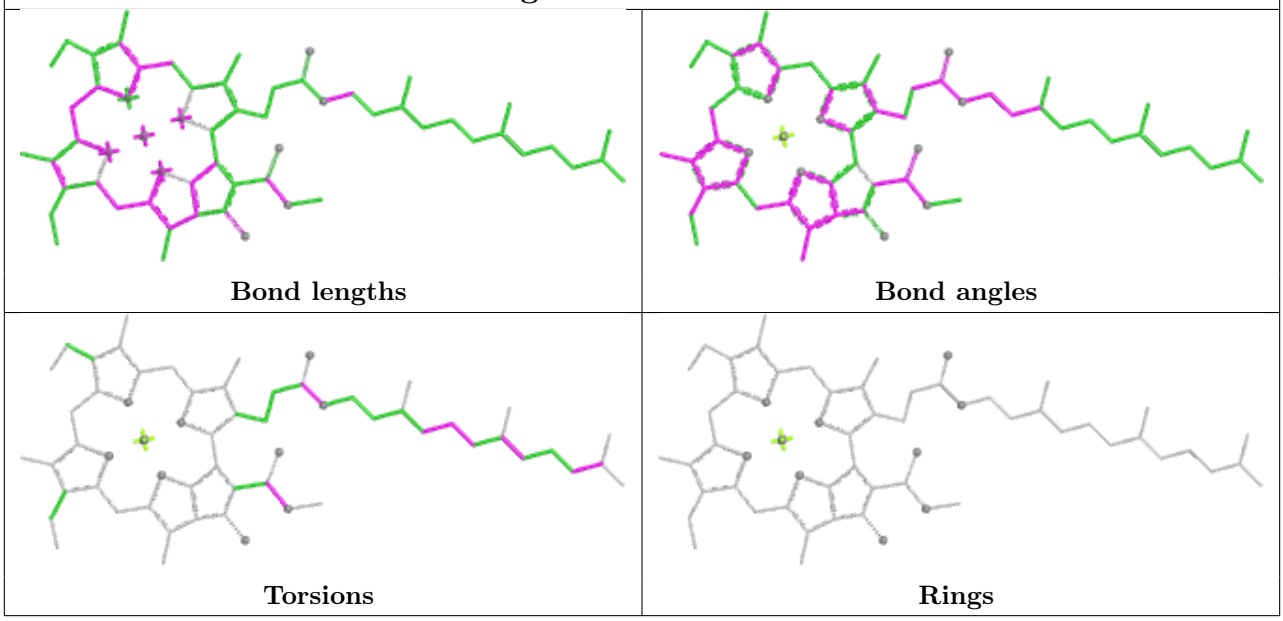


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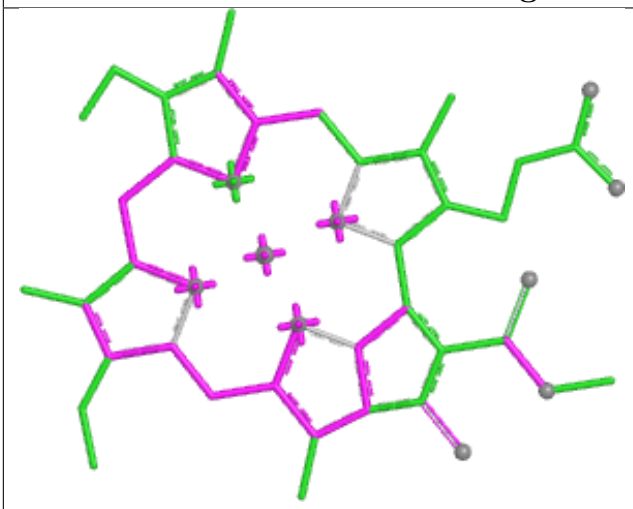
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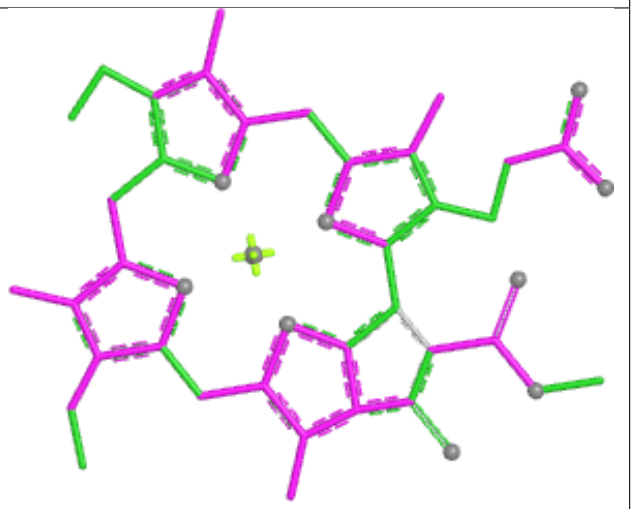
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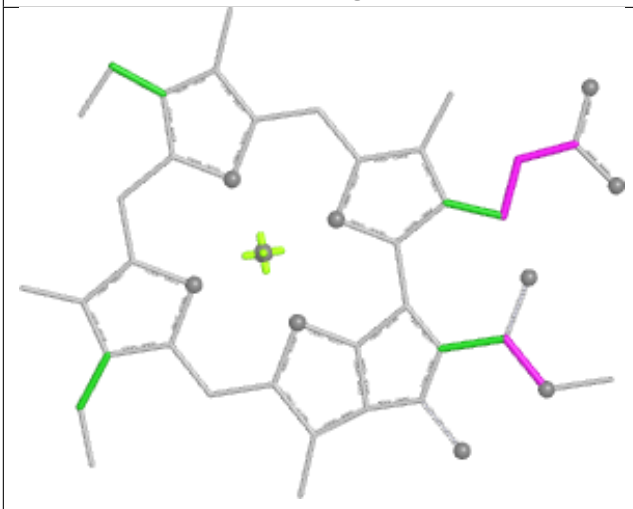
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Bond lengths



Bond angles

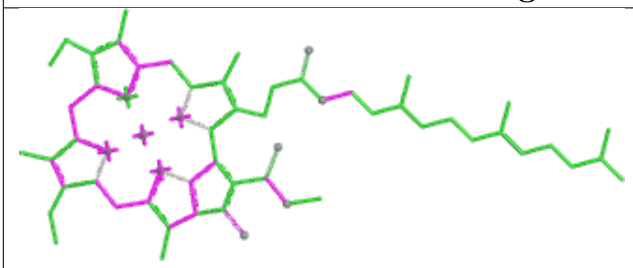


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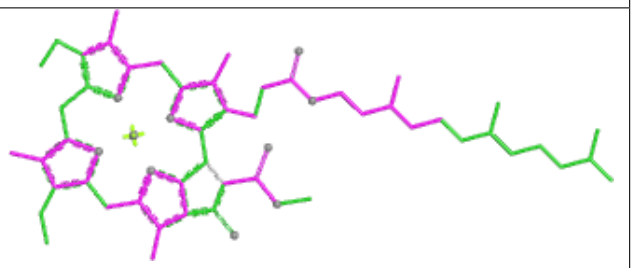


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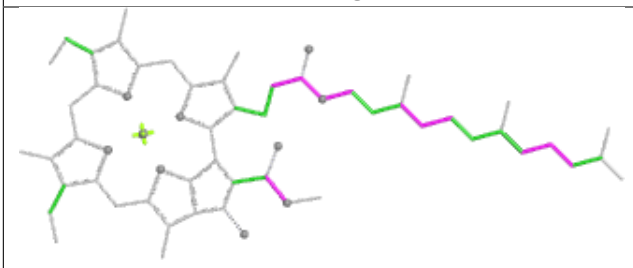
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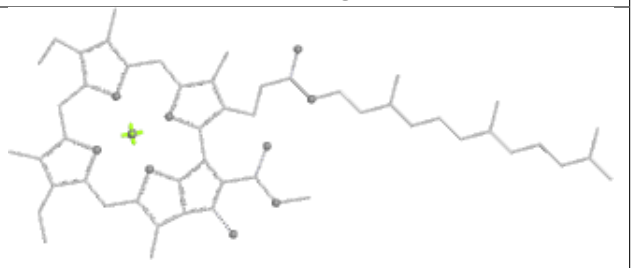
Bond lengths



Bond angles

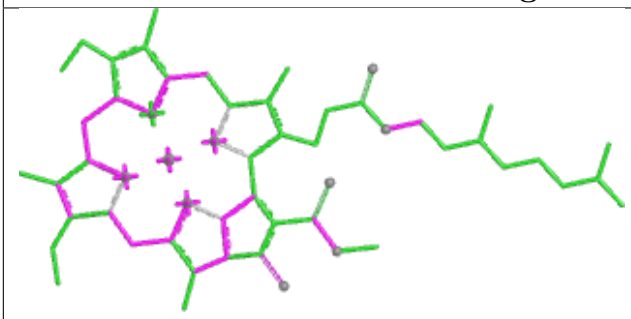


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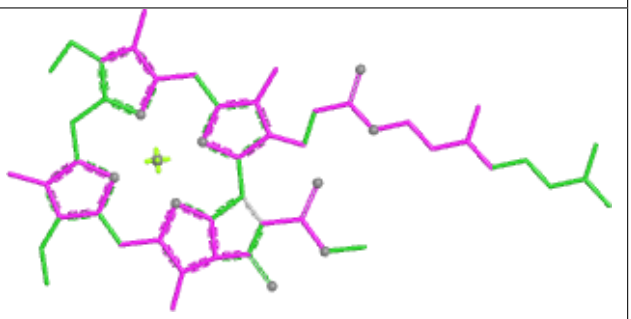


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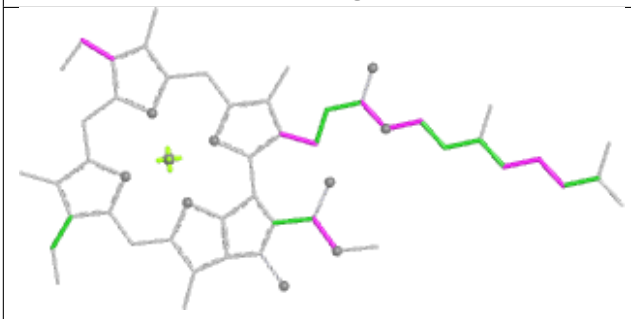
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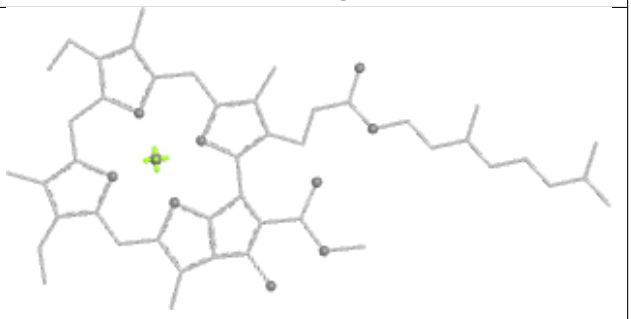
Bond lengths



Bond angles

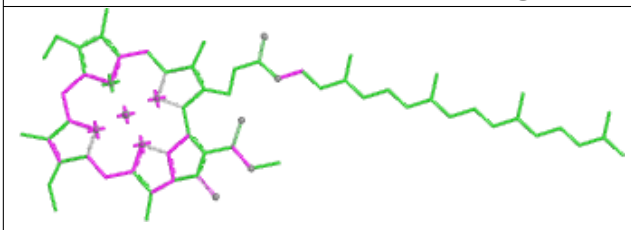


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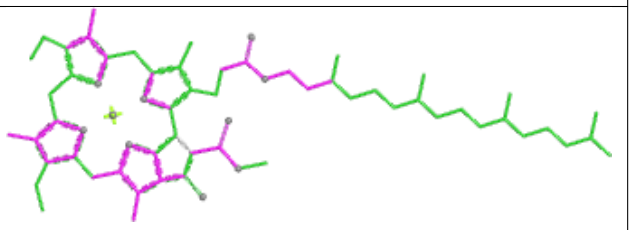


Rings

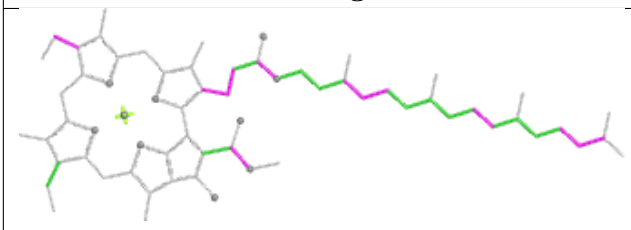
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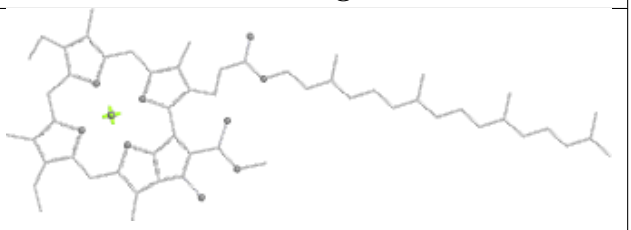
Bond lengths



Bond angles

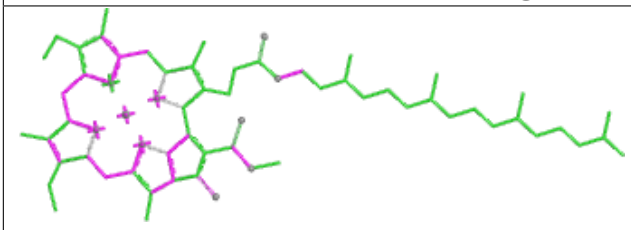


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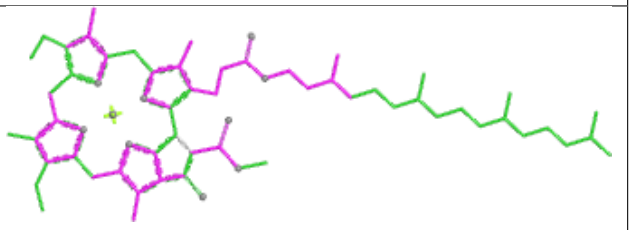


Rings

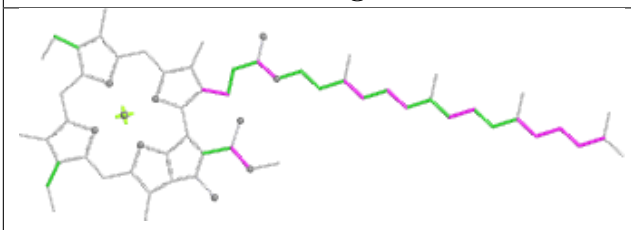
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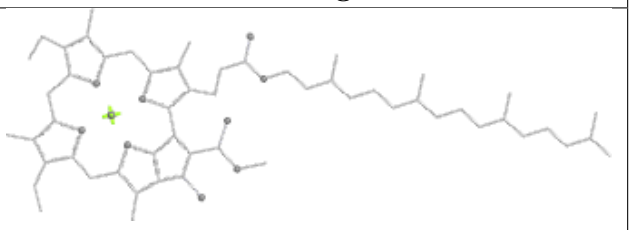
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Bond angles

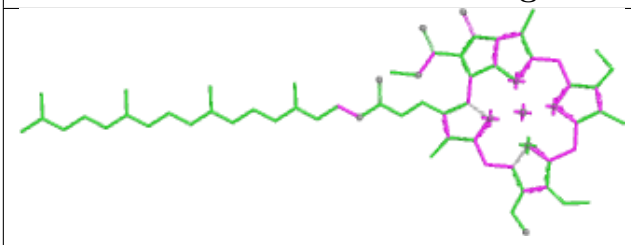


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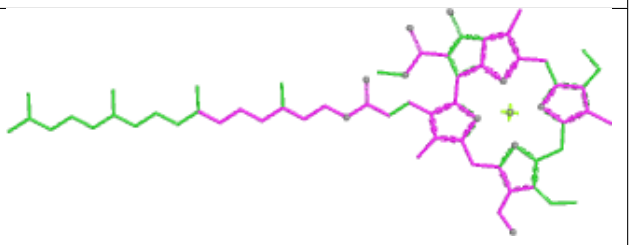


Rings

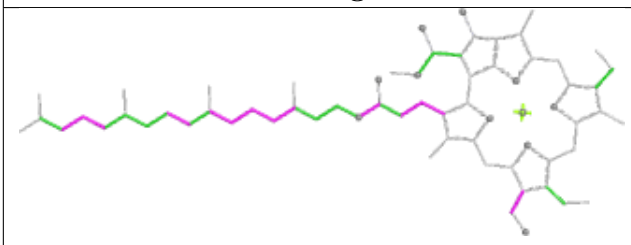
Ligand F6C B 1238



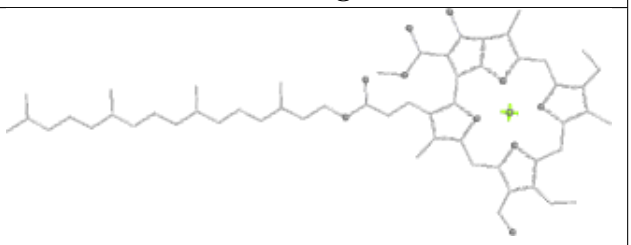
Bond lengths



Bond angles

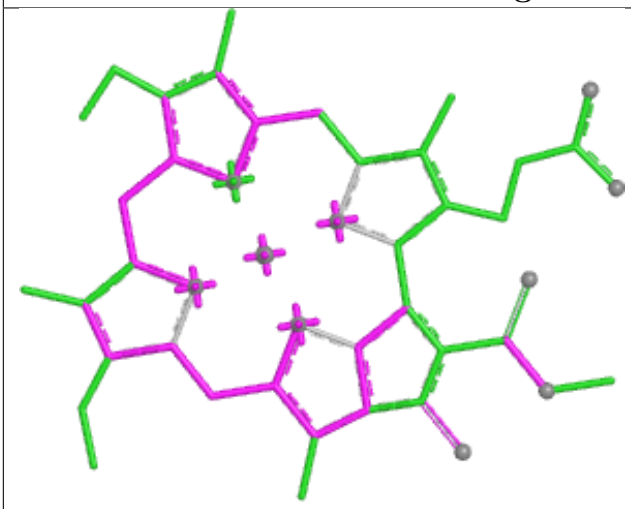


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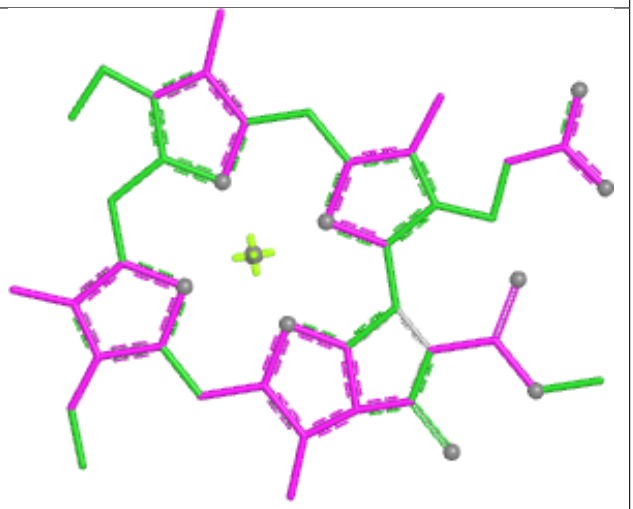


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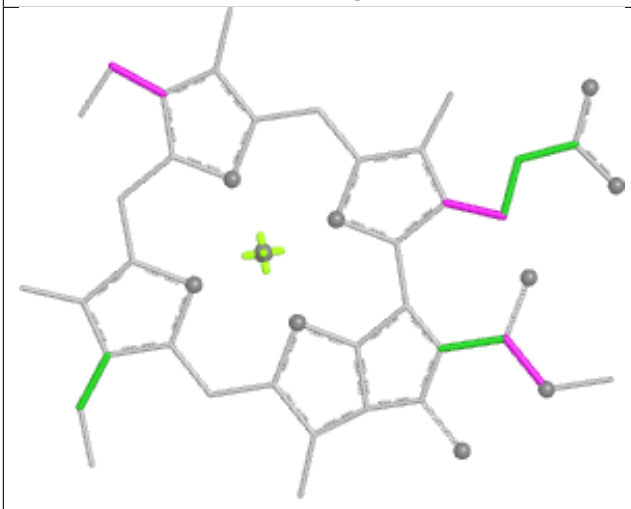
Ligand CLA H 1219



Bond lengths



Bond angles

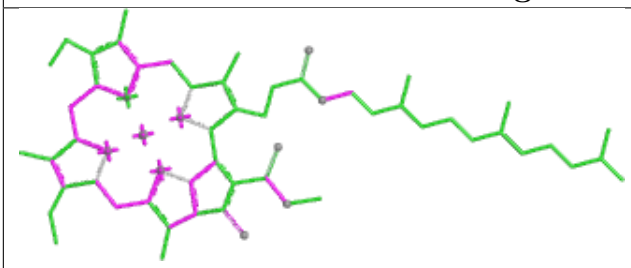


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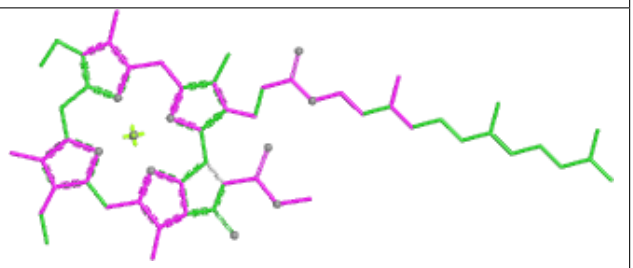


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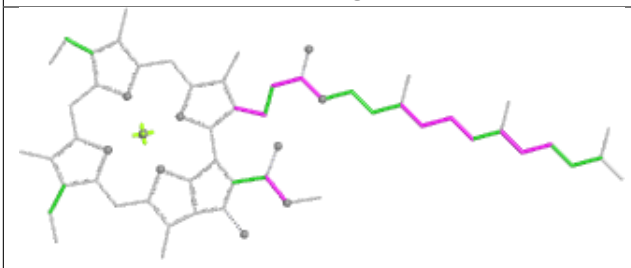
Ligand CLA G 1138



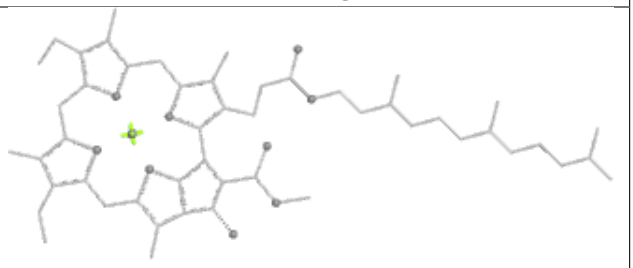
Bond lengths



Bond angles

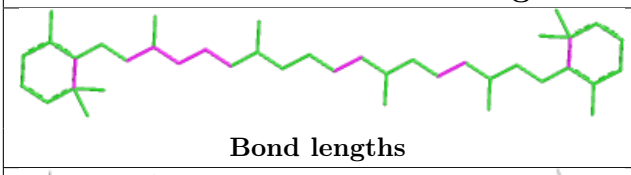


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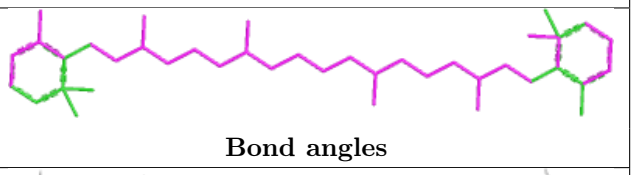


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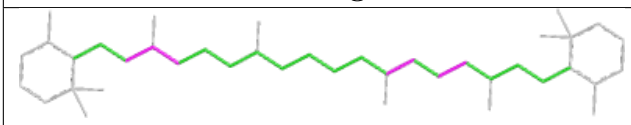
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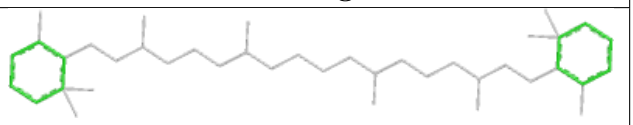
Bond lengths



Bond angles

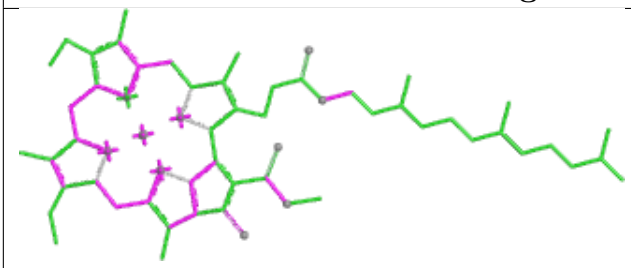


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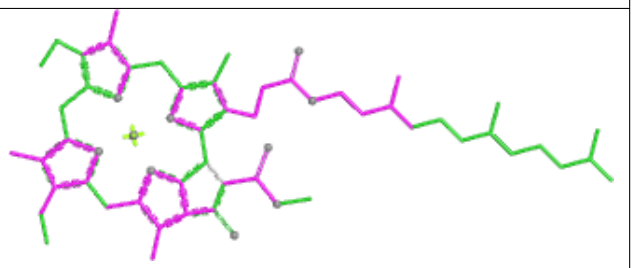


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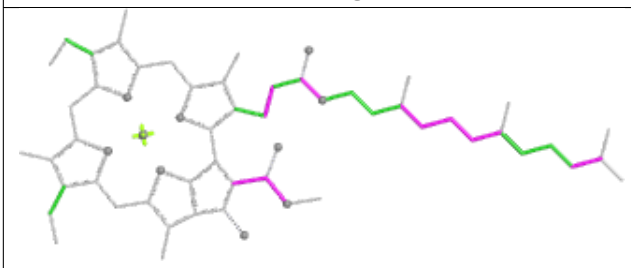
Ligand CLA a 1111



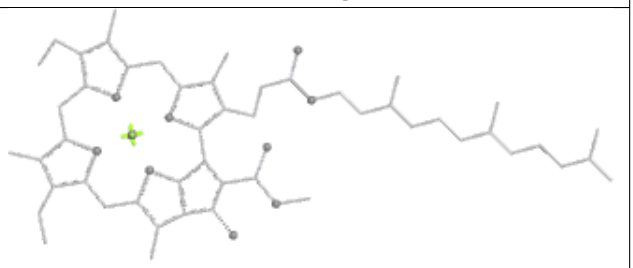
Bond lengths



Bond angles

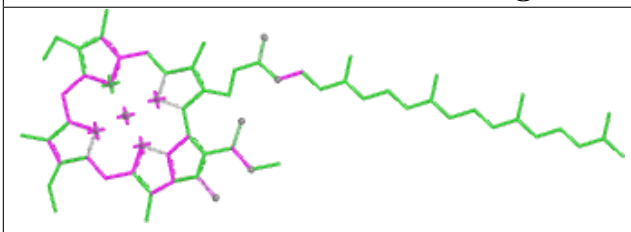


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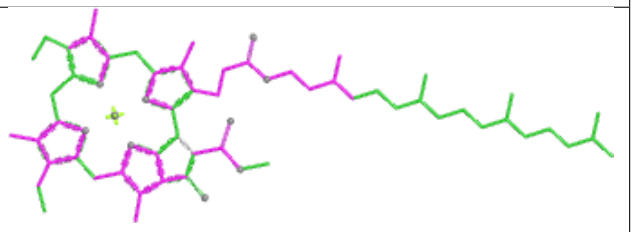


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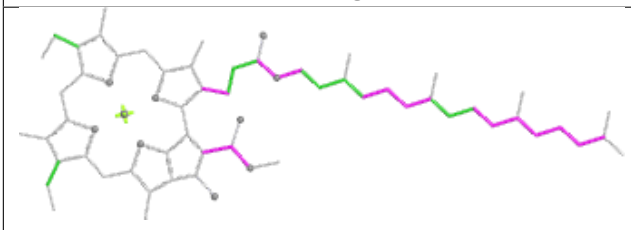
Ligand CLA A 1115



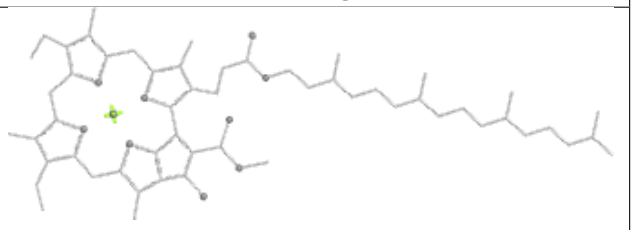
Bond lengths



Bond angles

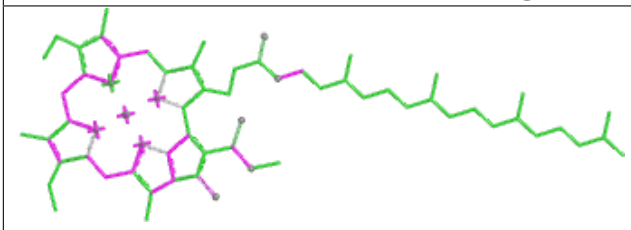


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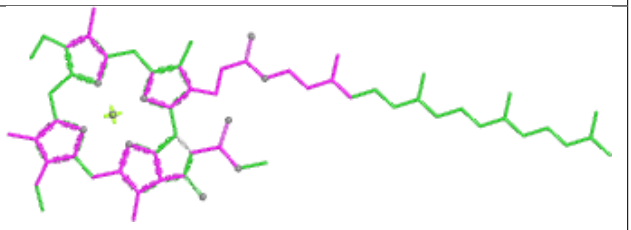


Rings

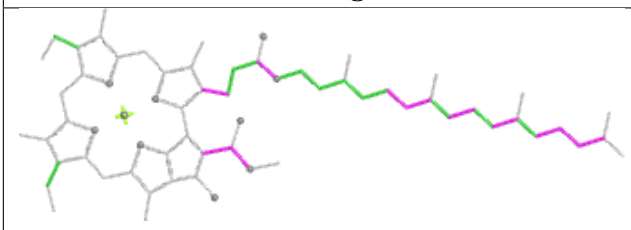
Ligand CLA b 1222



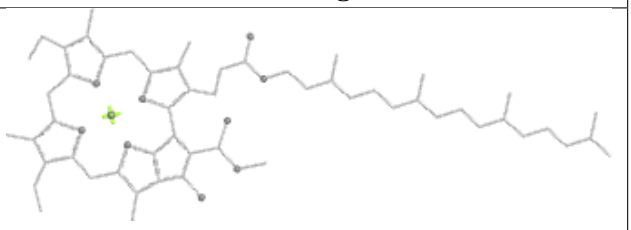
Bond lengths



Bond angles

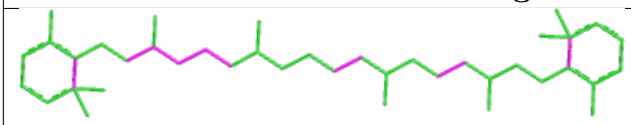


Torsions

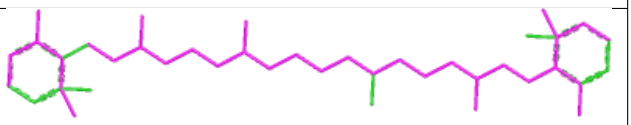


Rings

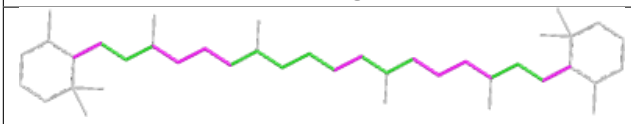
Ligand BCR R 4020



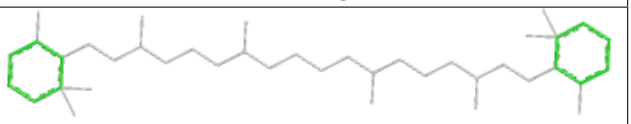
Bond lengths



Bond angles

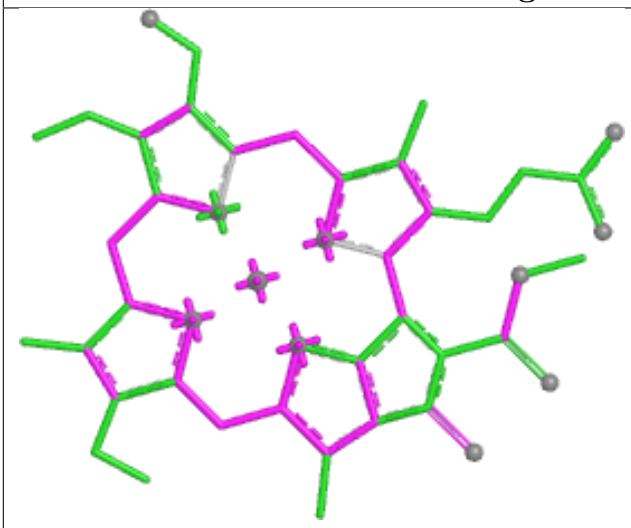


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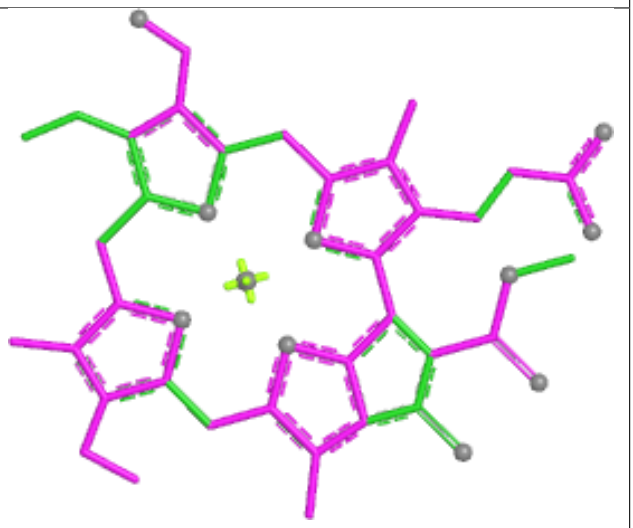


Rings

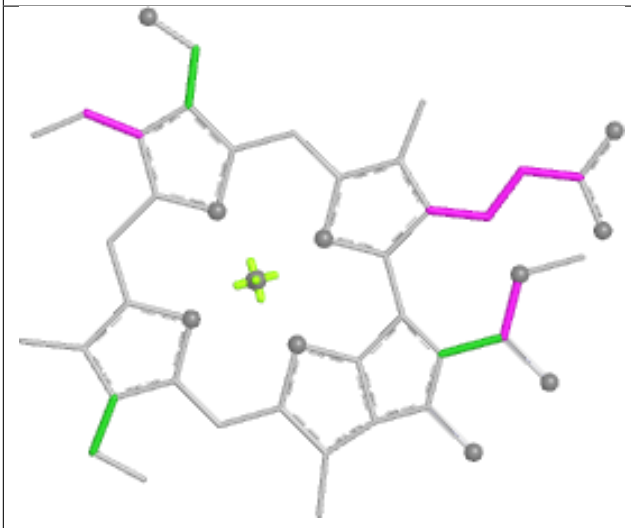
Ligand F6C G 1121



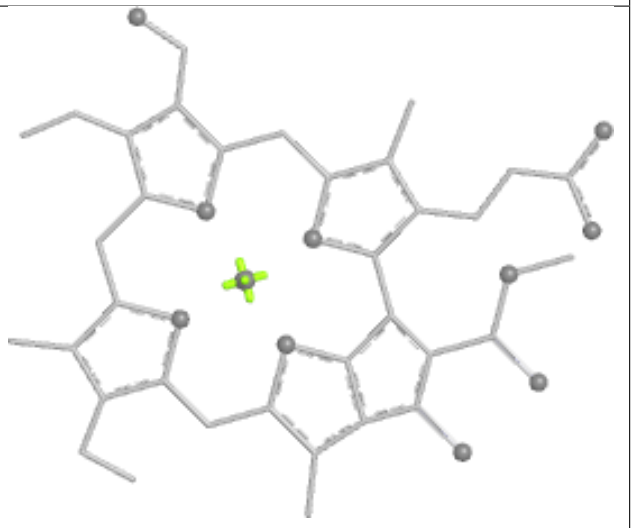
Bond lengths



Bond angles

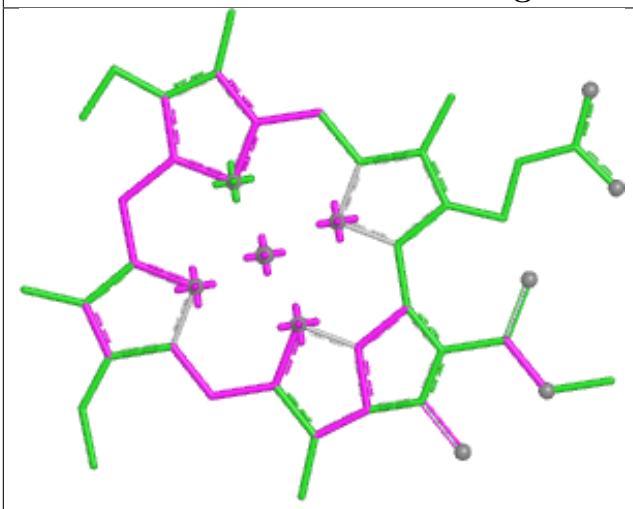


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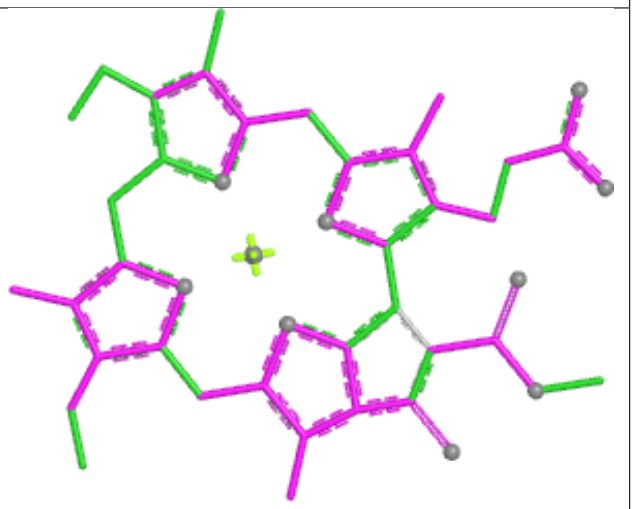


Rings

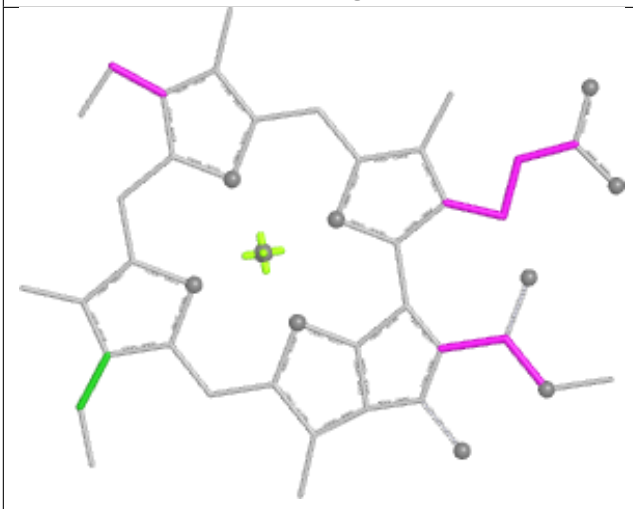
Ligand CLA G 1113



Bond lengths



Bond angles

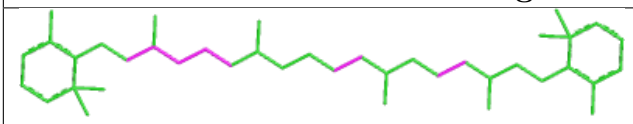


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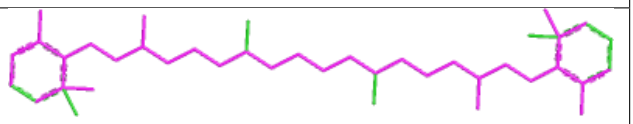


Rings

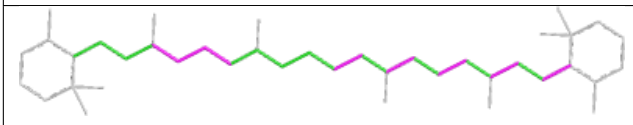
Ligand BCR L 4019



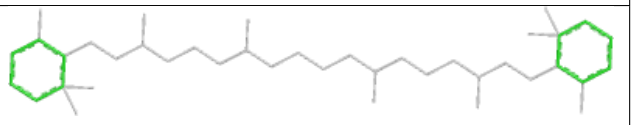
Bond lengths



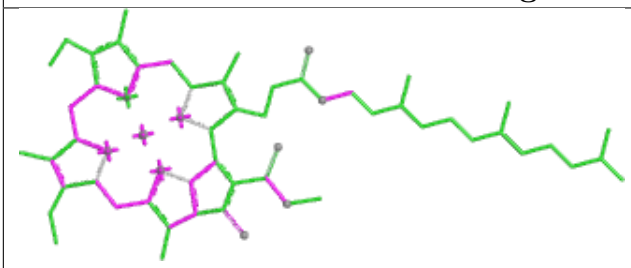
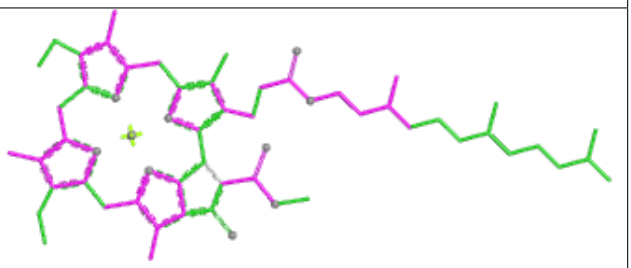
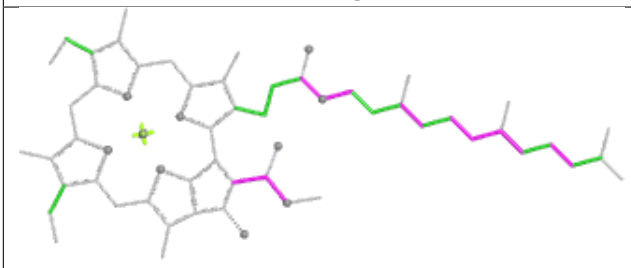
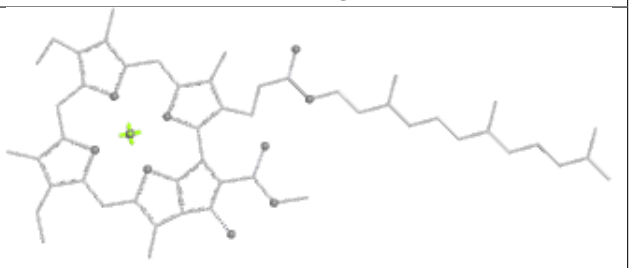
Bond angles

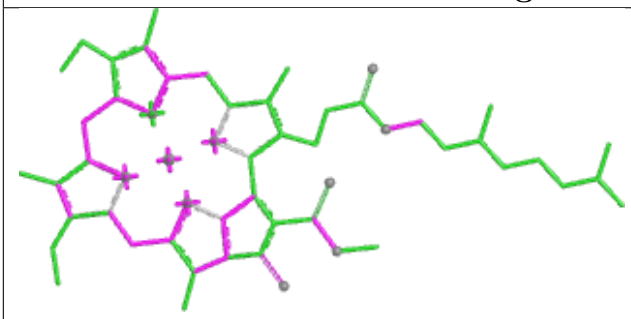
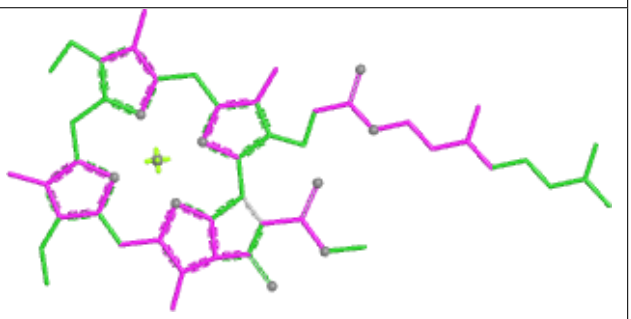
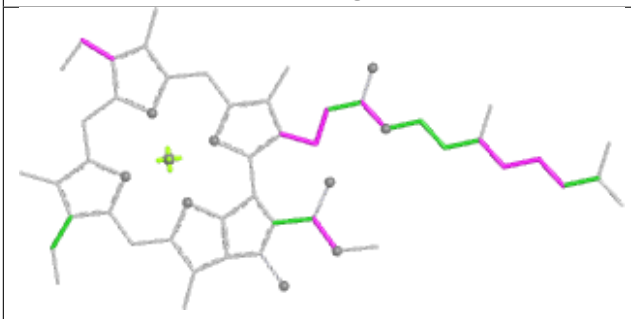
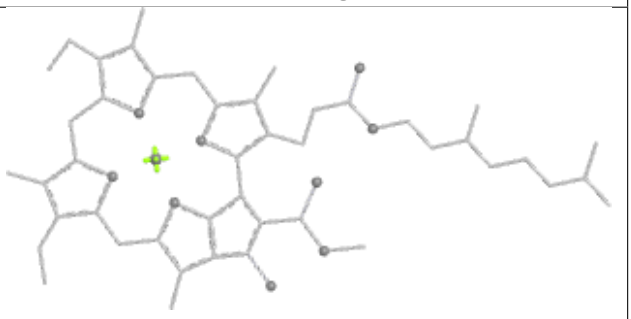


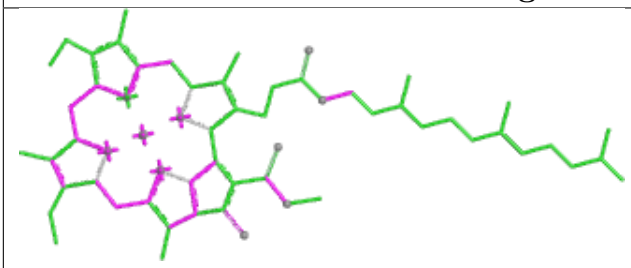
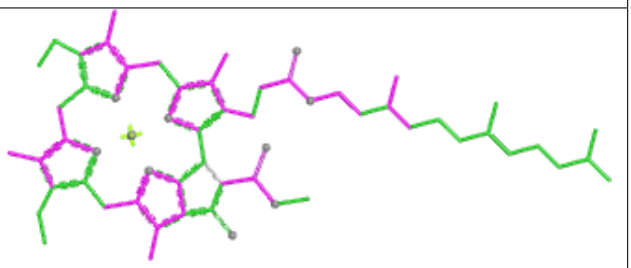
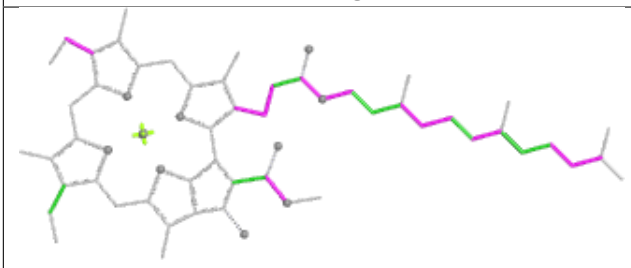
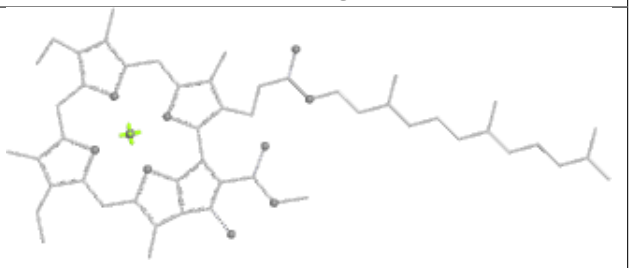
Torsions

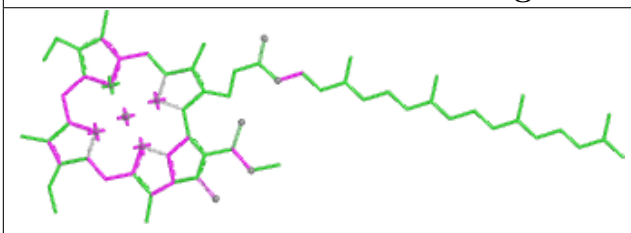
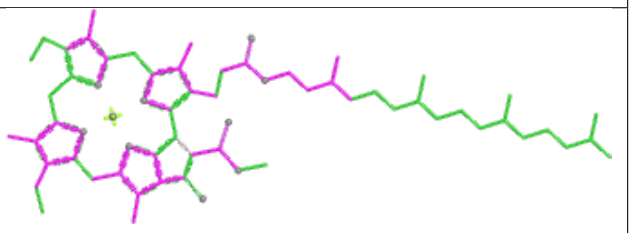
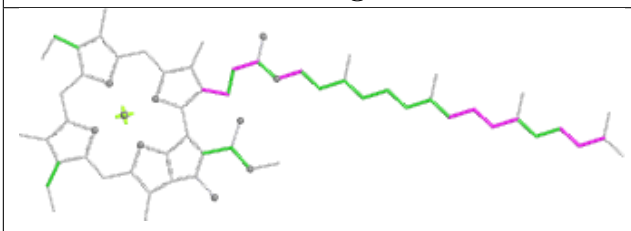
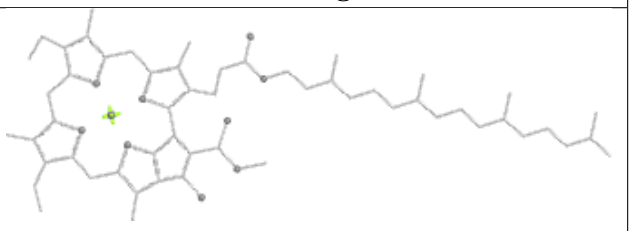


Rings

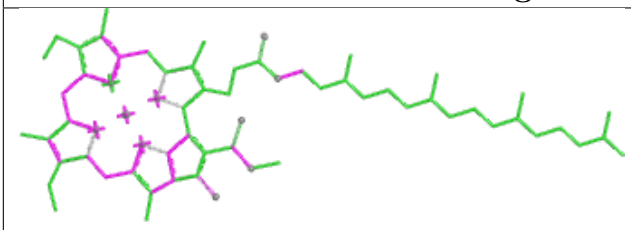
Ligand CLA a 1128	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1217	
	
Bond lengths	Bond angles
	
Torsions	Rings

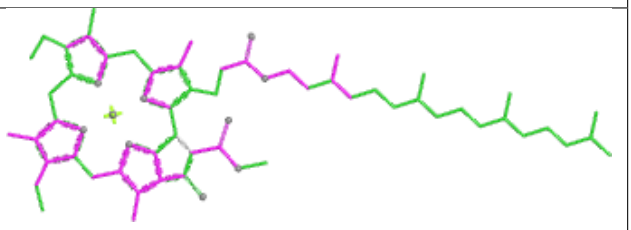
Ligand CLA b 1215	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1221	
	
Bond lengths	Bond angles
	
Torsions	Rings

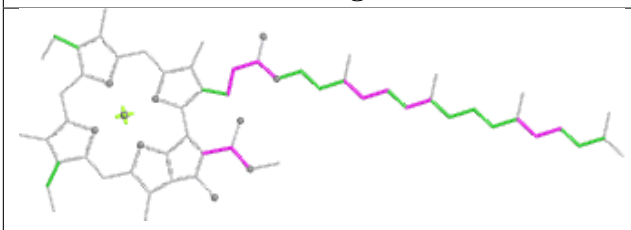
Ligand CLA H 1213



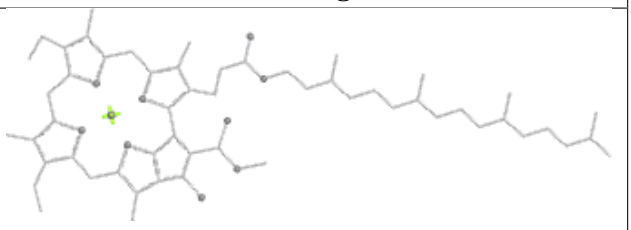
Bond lengths



Bond angles

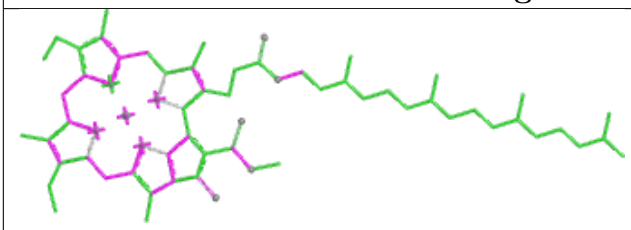


Torsions

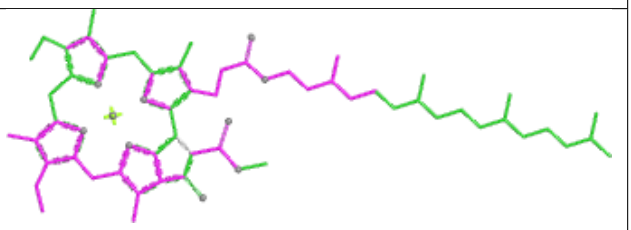


Rings

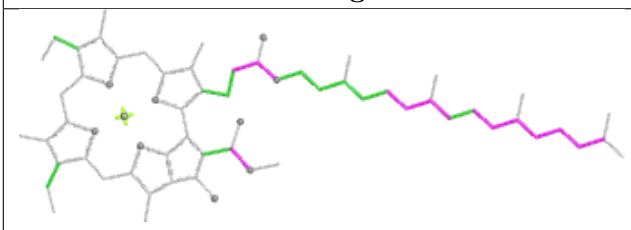
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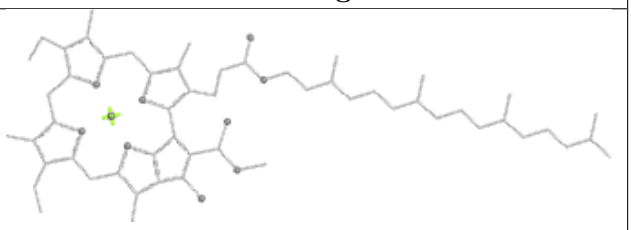
Bond lengths



Bond angles

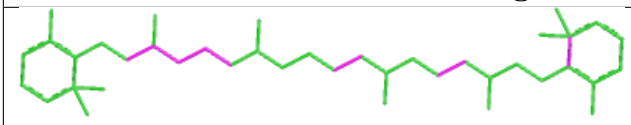


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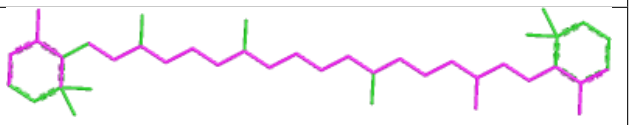


Rings

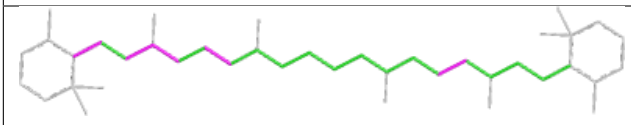
Ligand BCR H 4009



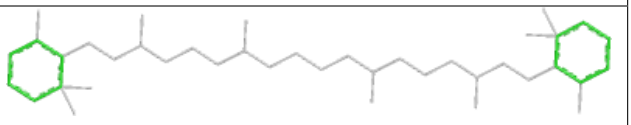
Bond lengths



Bond angles

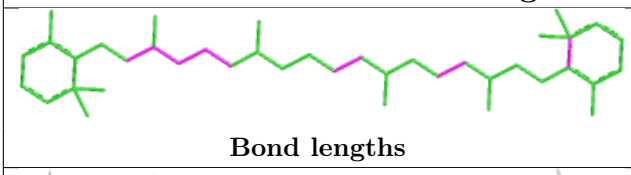


Torsions

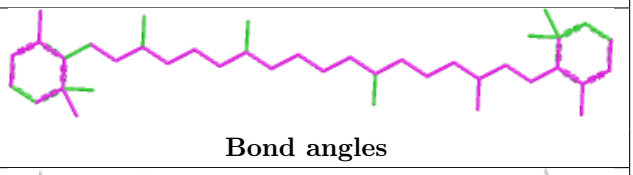


Rings

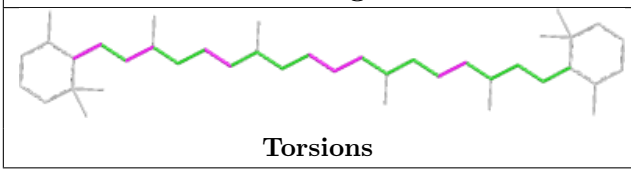
Ligand BCR I 4018



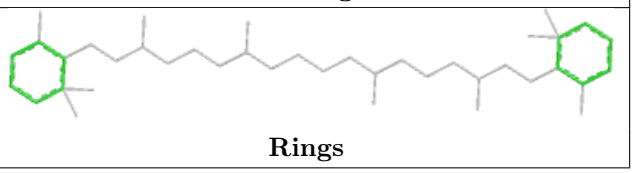
Bond lengths



Bond angles

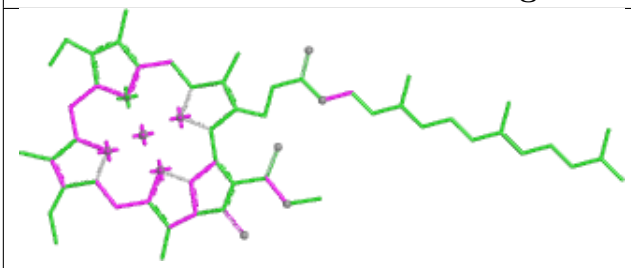


Torsions

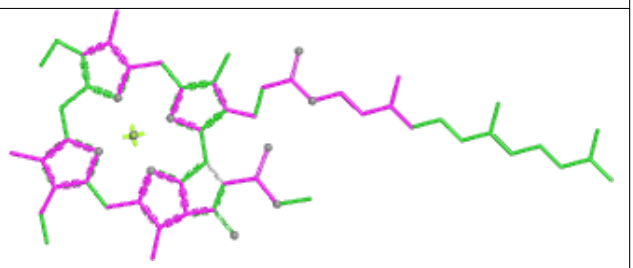


Rings

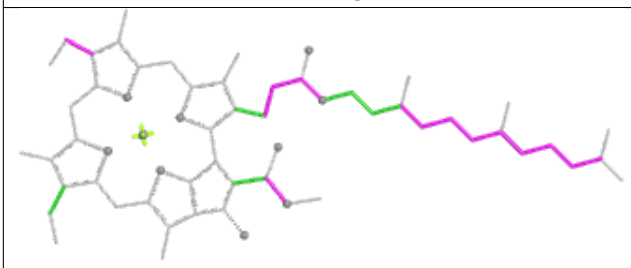
Ligand CLA a 1126



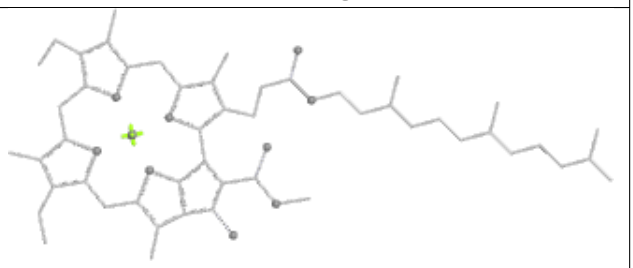
Bond lengths



Bond angles

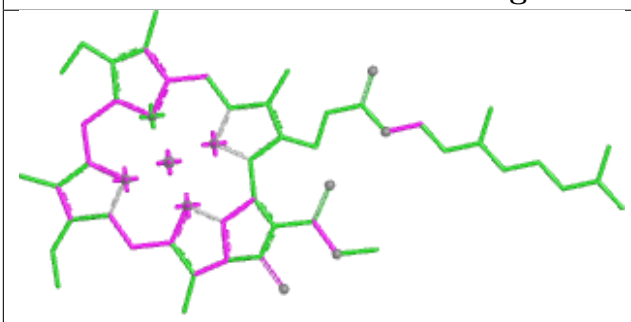


Torsions

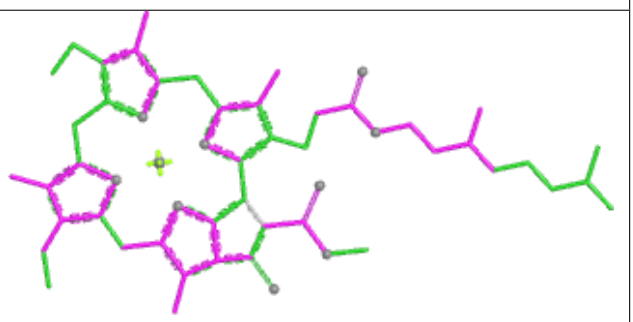


Rings

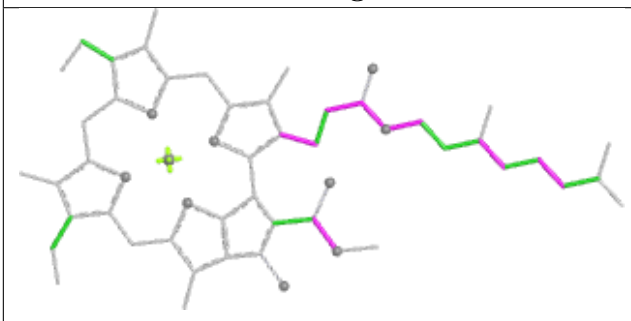
Ligand CLA W 1701



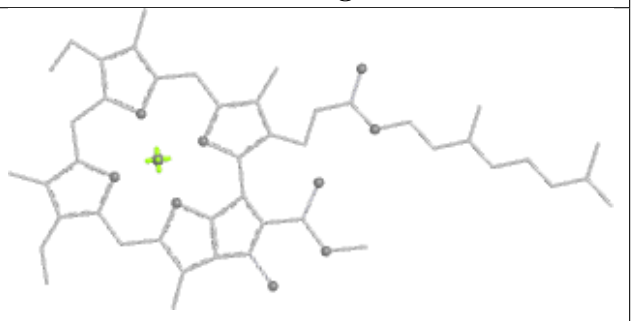
Bond lengths



Bond angles

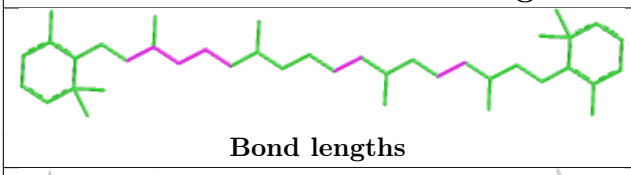


Torsions

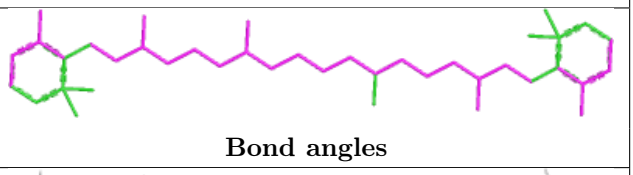


Rings

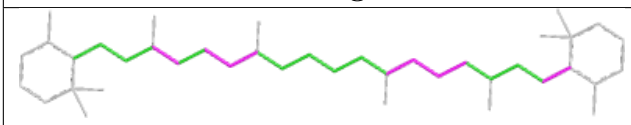
Ligand BCR b 4013



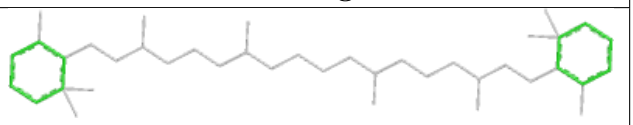
Bond lengths



Bond angles

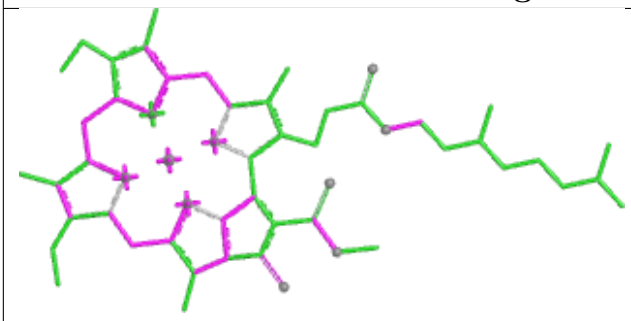


Torsions

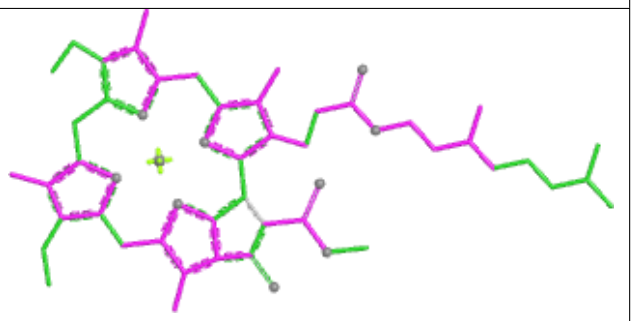


Rings

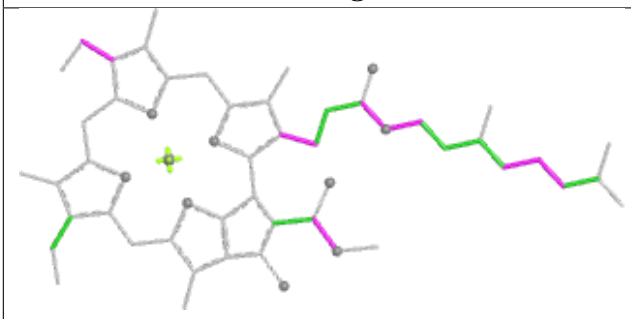
Ligand CLA G 1124



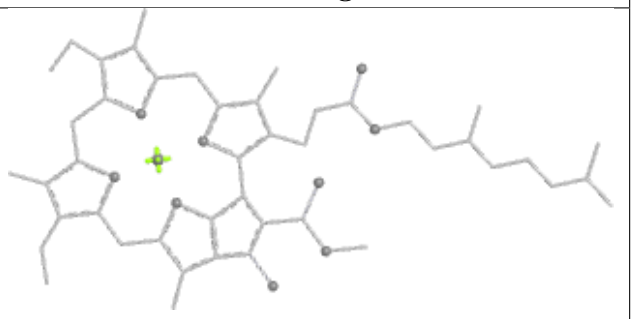
Bond lengths



Bond angles

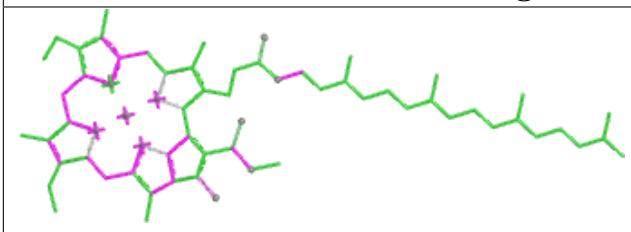


Torsions

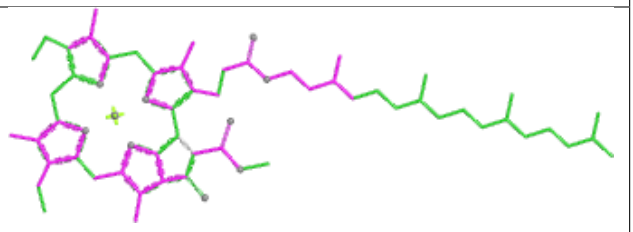


Rings

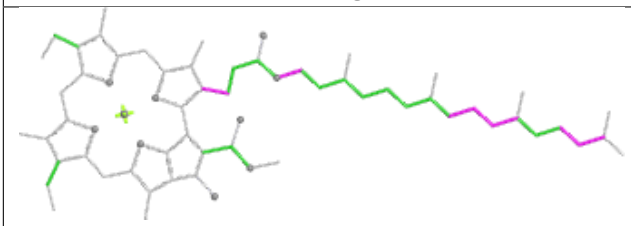
Ligand CLA B 1221



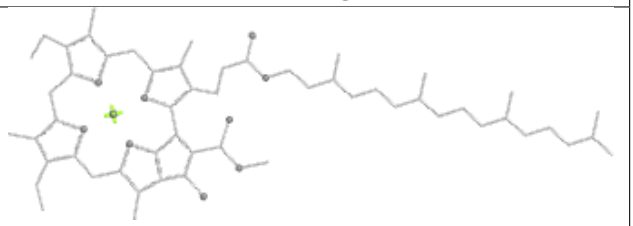
Bond lengths



Bond angles

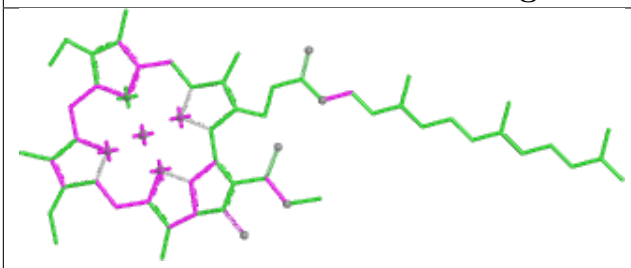


Torsions

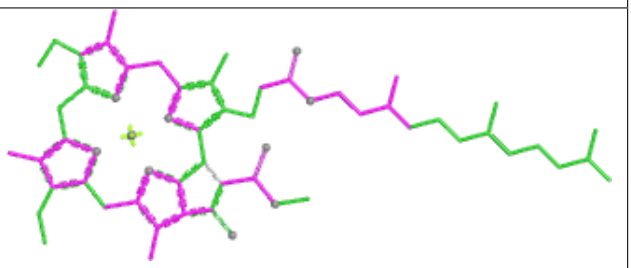


Rings

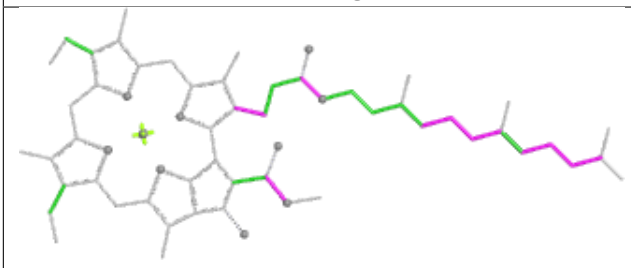
Ligand CLA a 1102



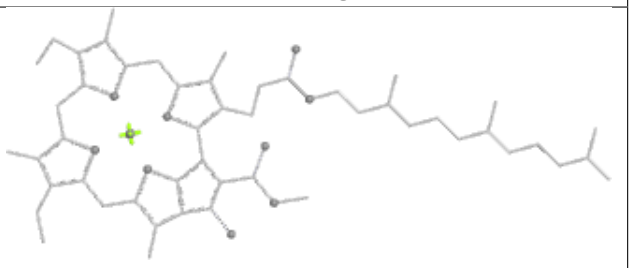
Bond lengths



Bond angles

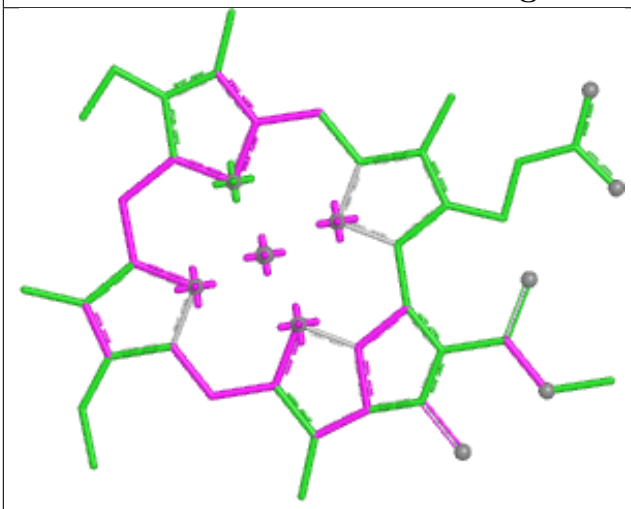


Torsions

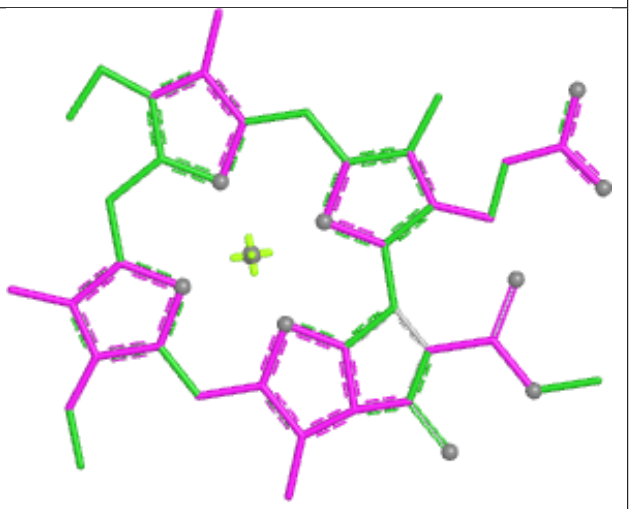


Rings

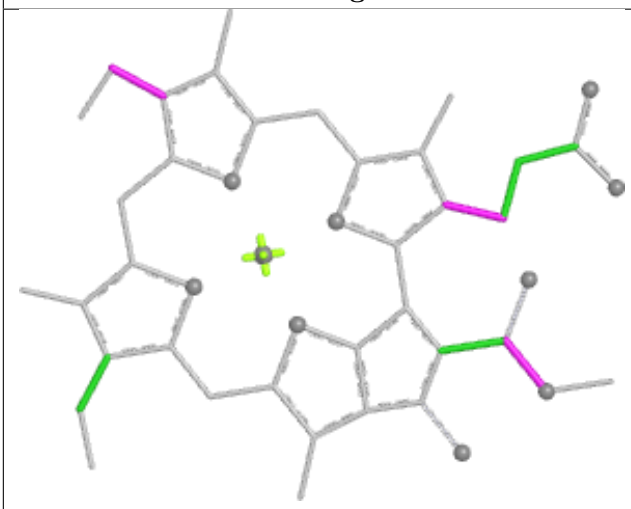
Ligand CLA a 1107



Bond lengths



Bond angles

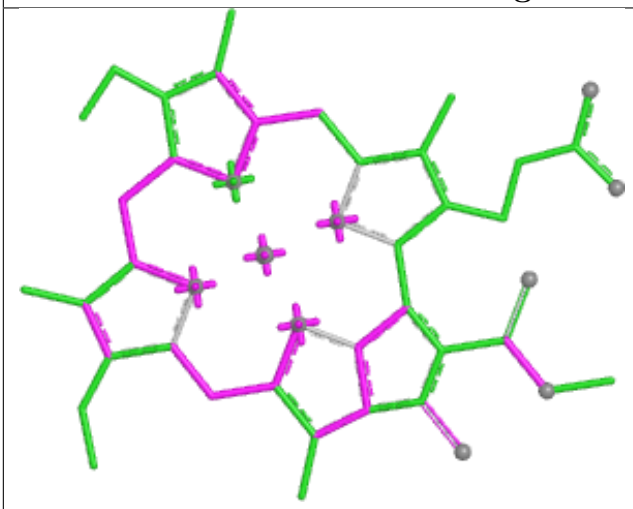


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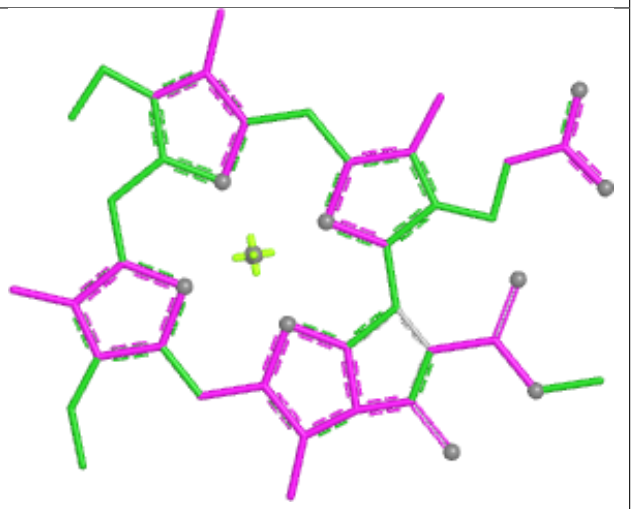


Rings

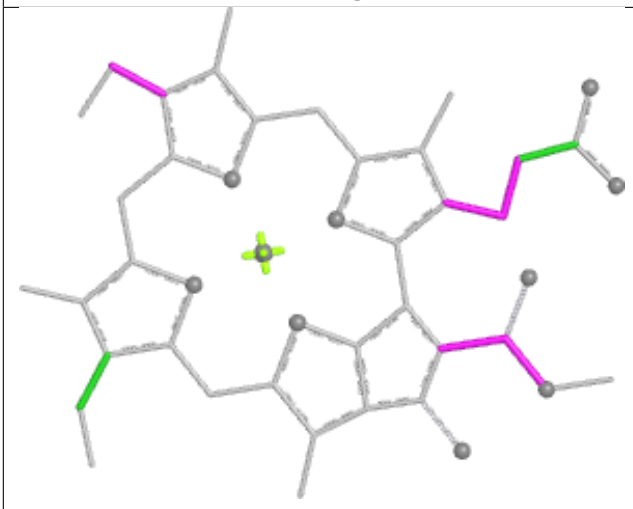
Ligand CLA G 1120



Bond lengths



Bond angles

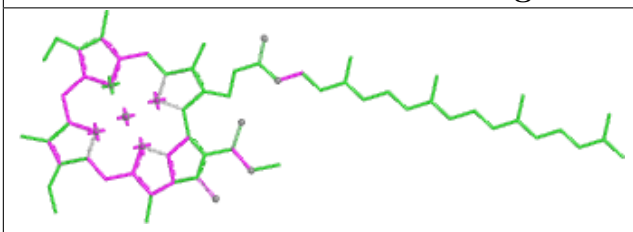


Torsions

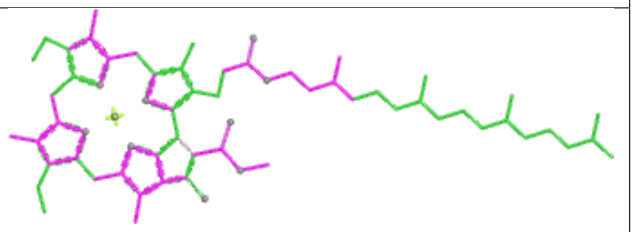


Rings

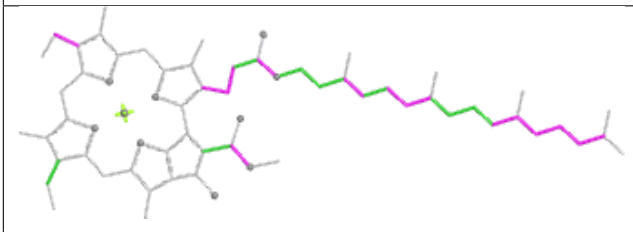
Ligand CLA H 1216



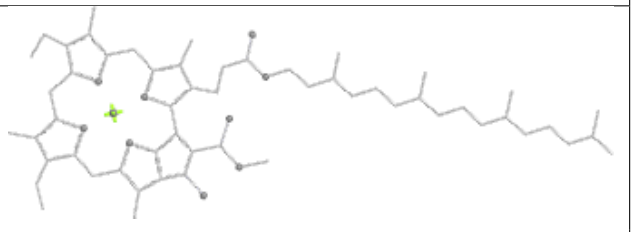
Bond lengths



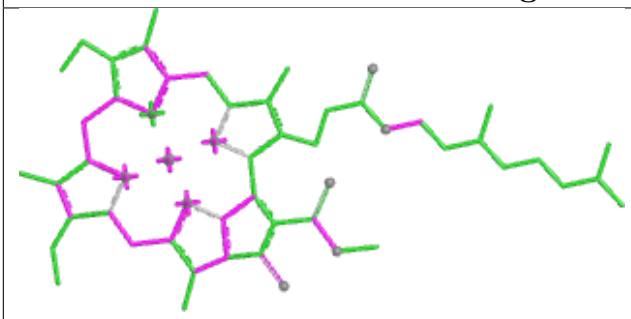
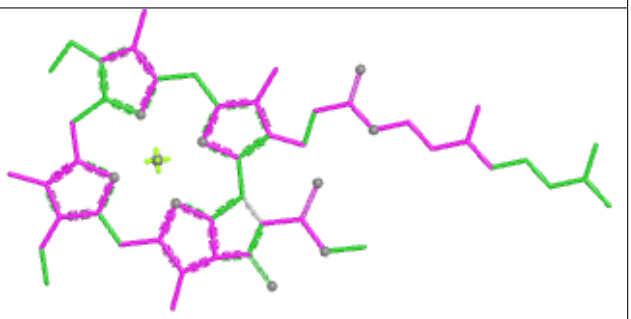
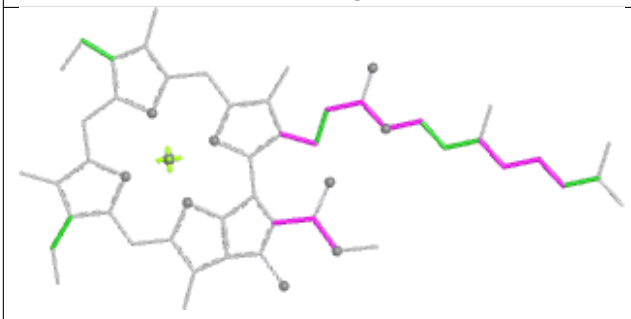
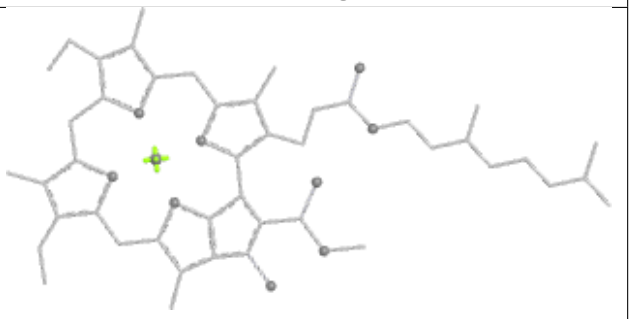
Bond angles

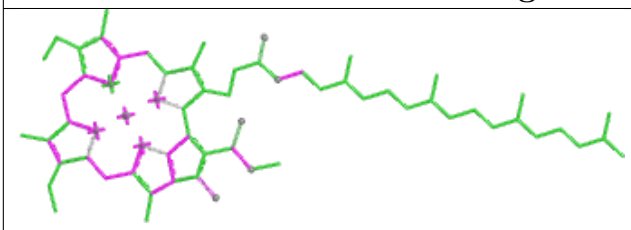
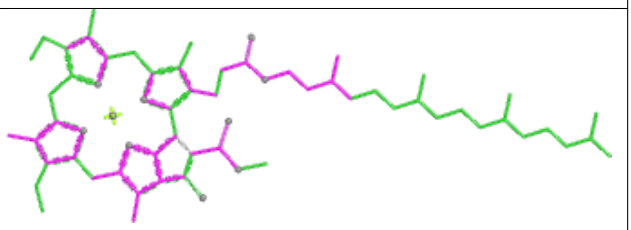
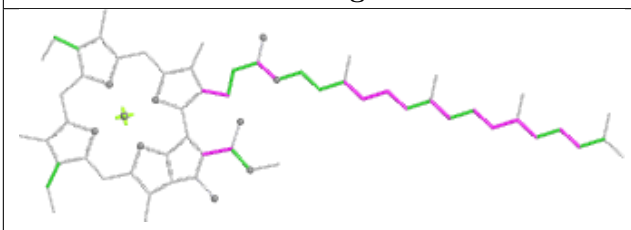
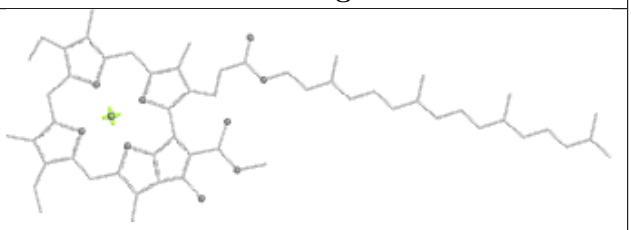


Torsions

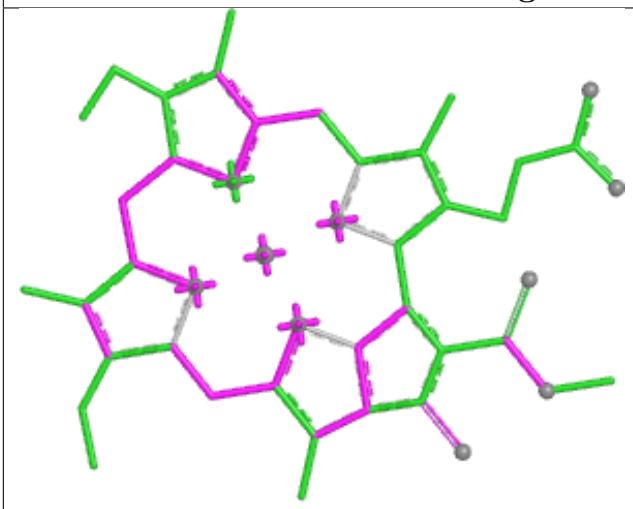


Rings

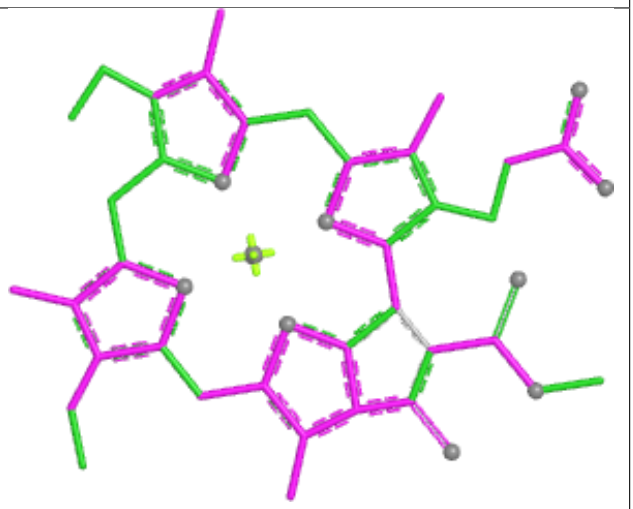
Ligand CLA a 1122	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 1203	
 Bond lengths	 Bond angles
 Torsions	 Rings

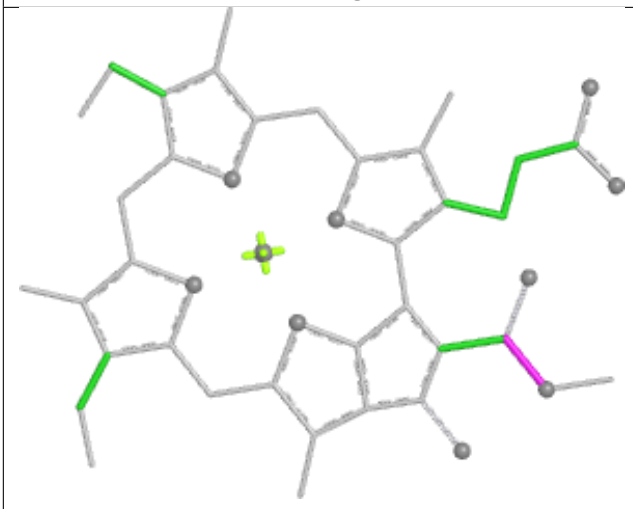
Ligand CLA b 1232



Bond lengths



Bond angles

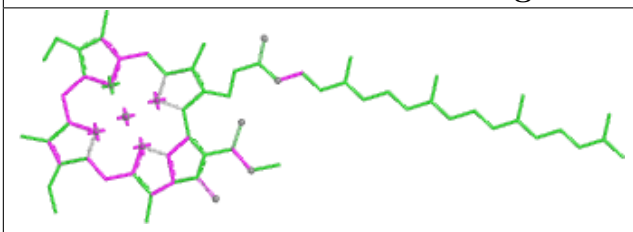


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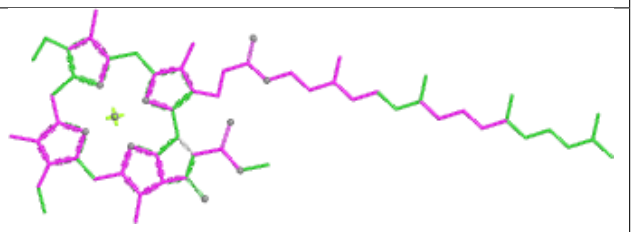


Rings

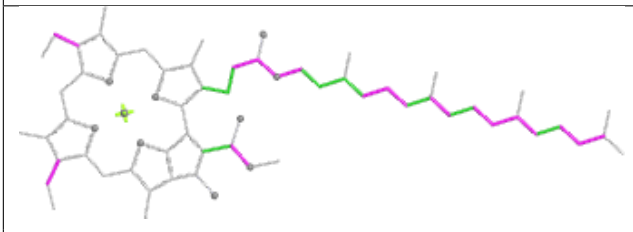
Ligand CLA H 1239



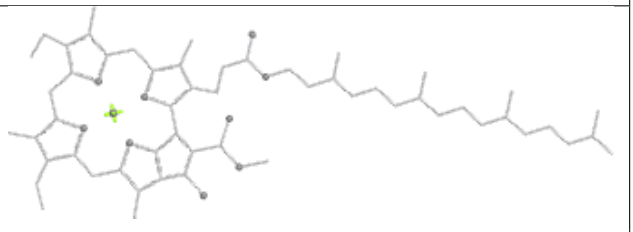
Bond lengths



Bond angles

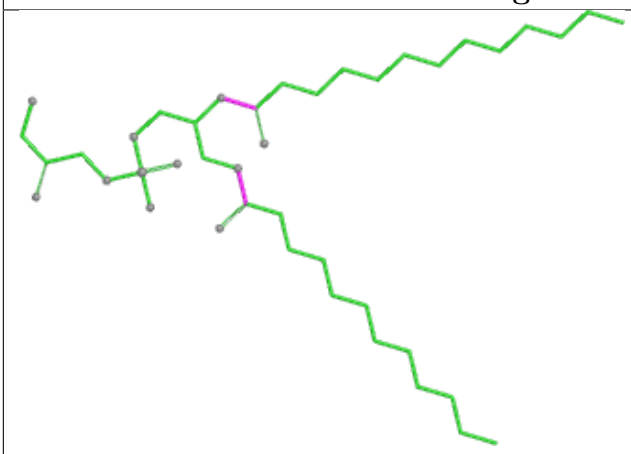


Torsions

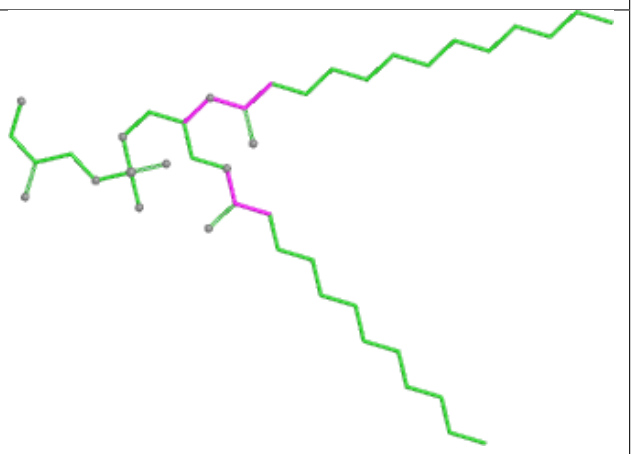


Rings

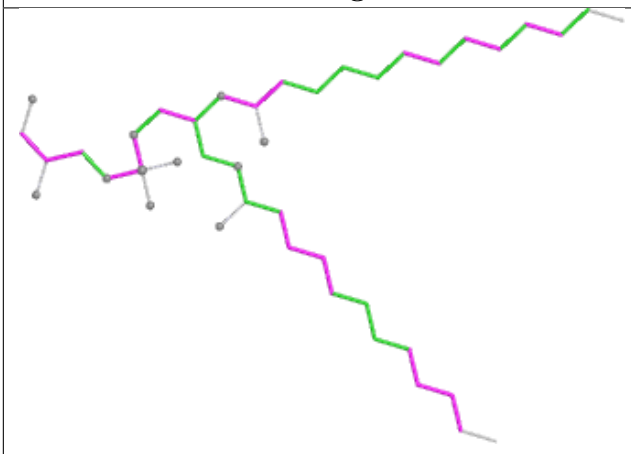
Ligand LHG G 5001



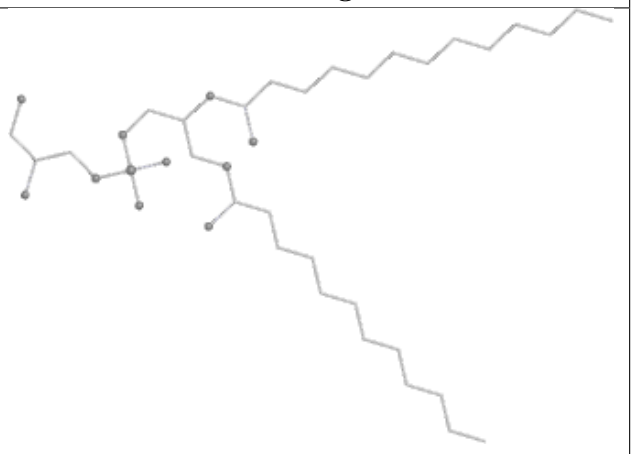
Bond lengths



Bond angles

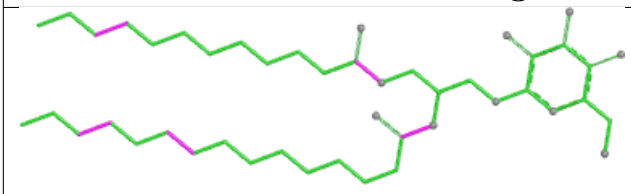


Torsions

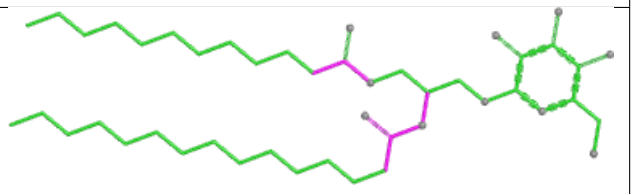


Rings

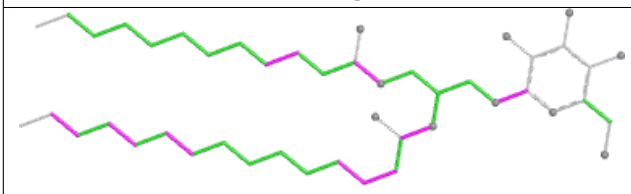
Ligand LMG H 5002



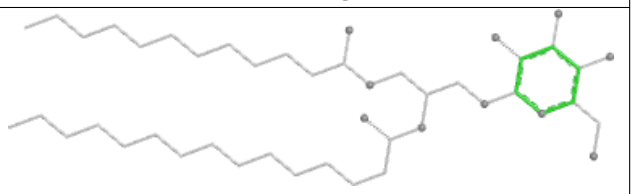
Bond lengths



Bond angles

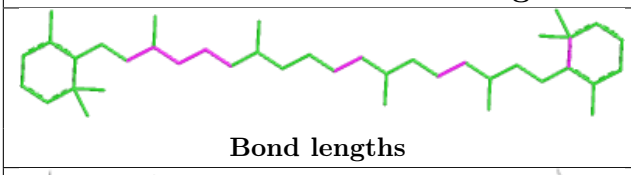


Torsions

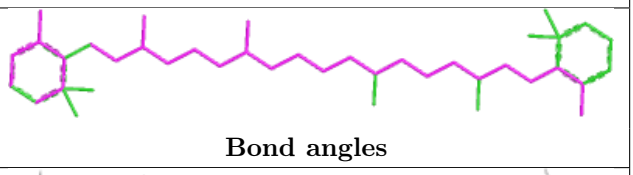


Rings

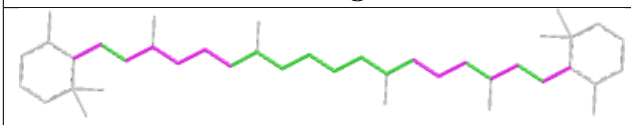
Ligand BCR H 4017



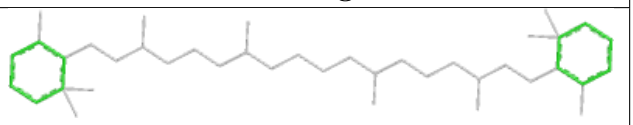
Bond lengths



Bond angles

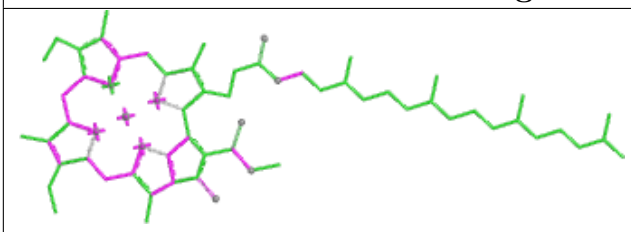


Torsions

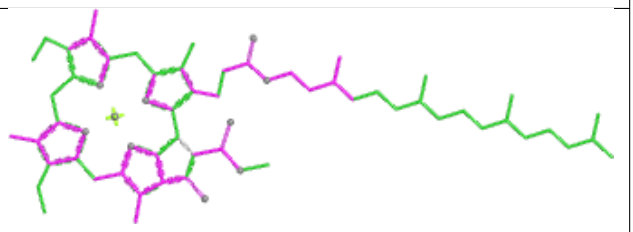


Rings

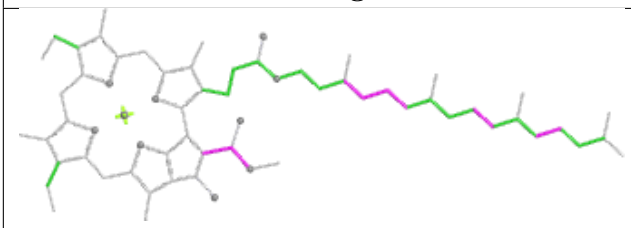
Ligand CLA B 1205



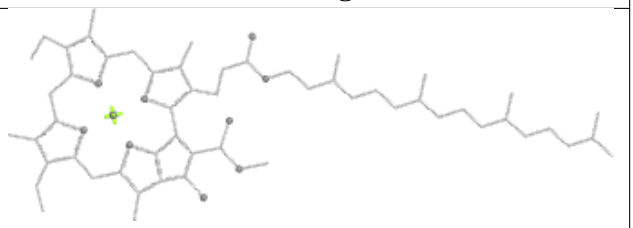
Bond lengths



Bond angles

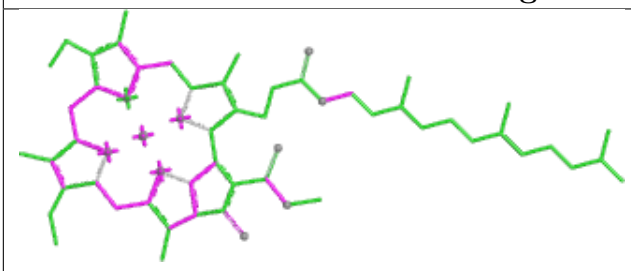


Torsions

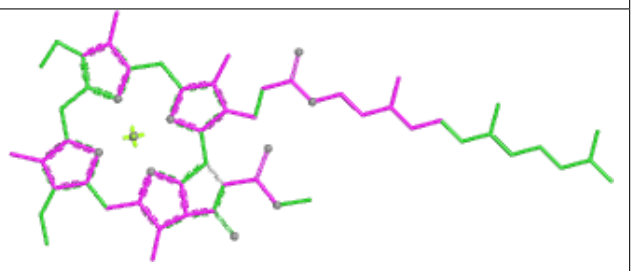


Rings

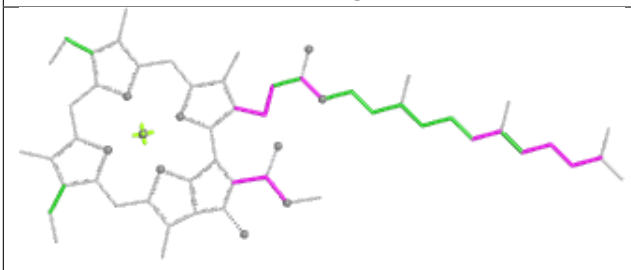
Ligand CLA a 1106



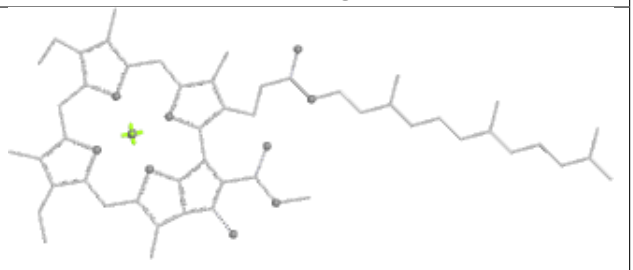
Bond lengths



Bond angles

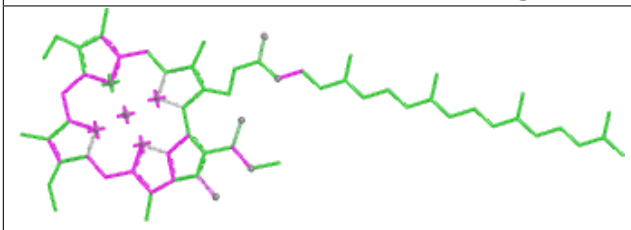


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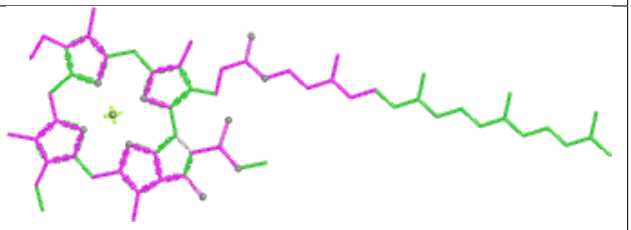


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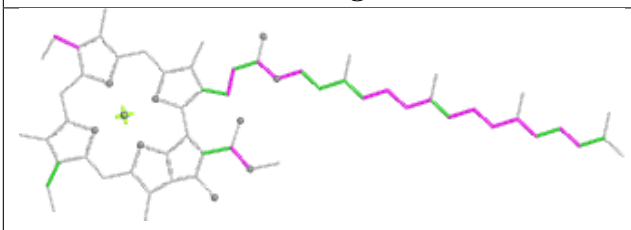
Ligand CLA H 1214



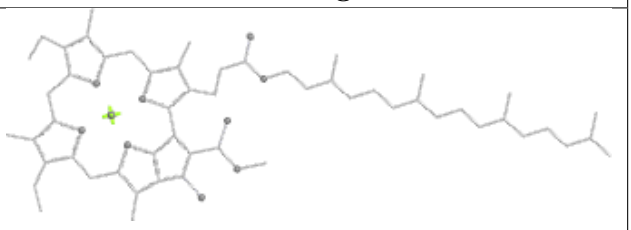
Bond lengths



Bond angles

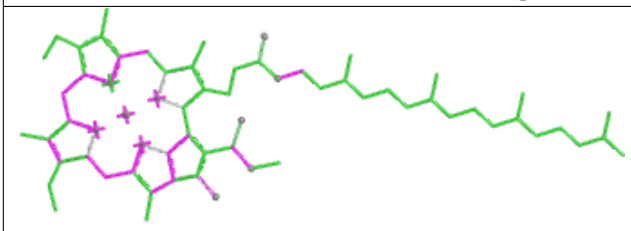


Torsions

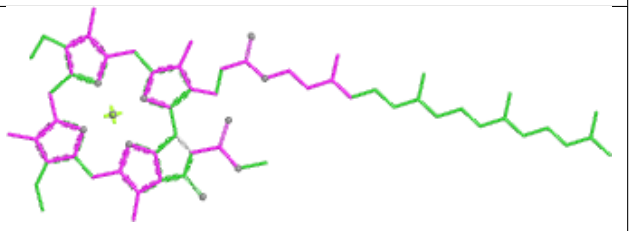


Rings

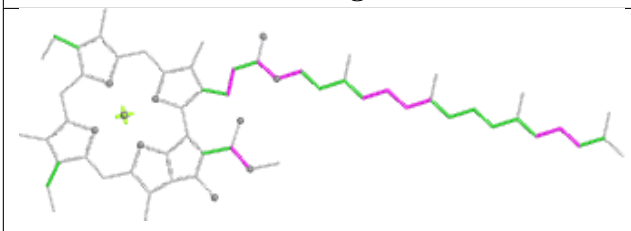
Ligand CLA H 1226



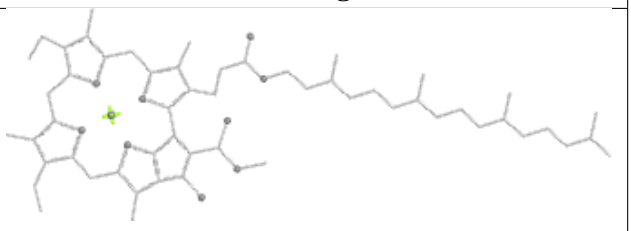
Bond lengths



Bond angles

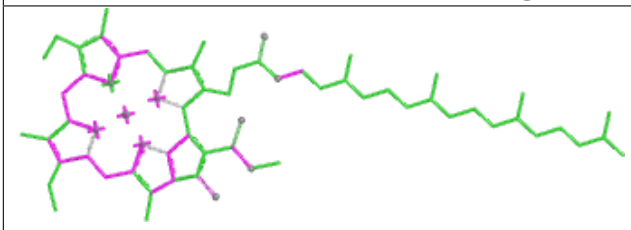


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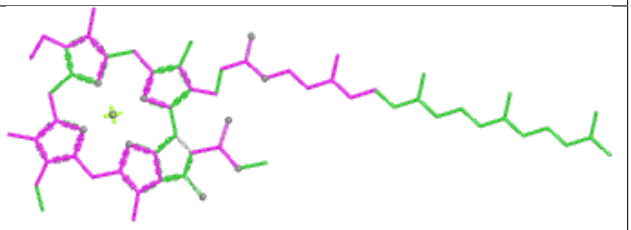


Rings

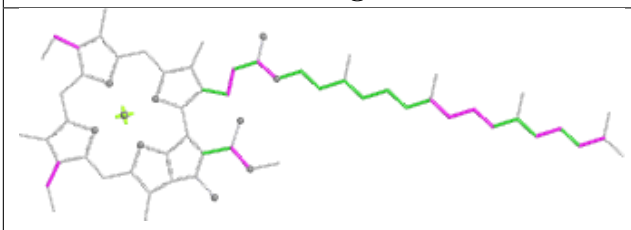
Ligand CLA b 1023



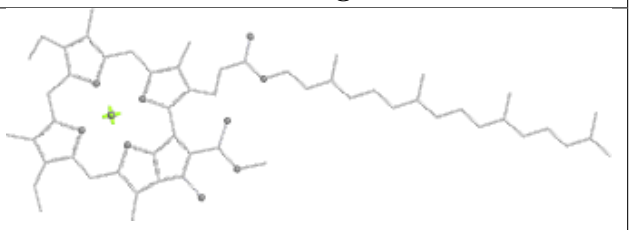
Bond lengths



Bond angles

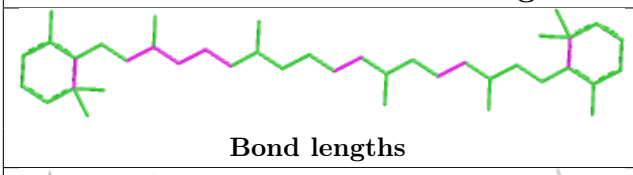


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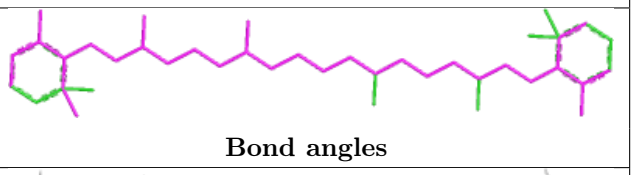


Rings

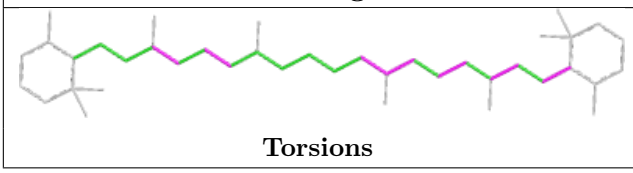
Ligand BCR a 4007



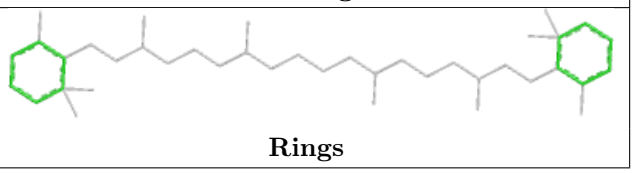
Bond lengths



Bond angles

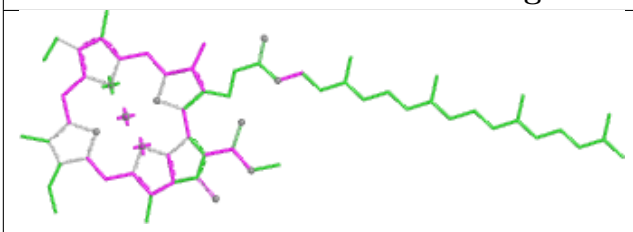


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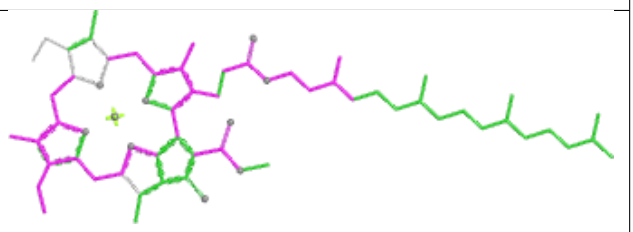


Rings

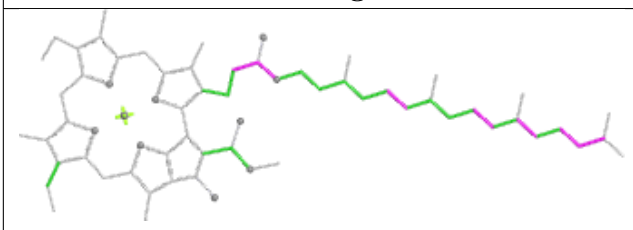
Ligand CL0 a 1011



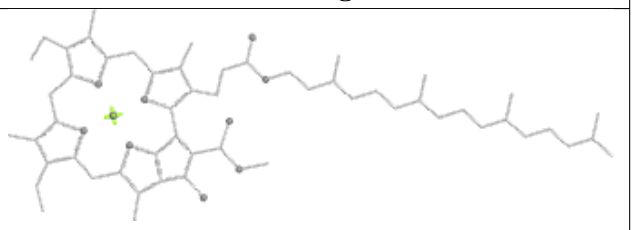
Bond lengths



Bond angles

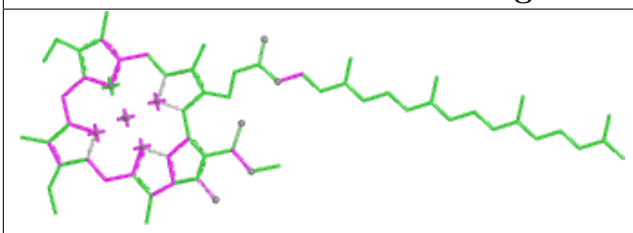


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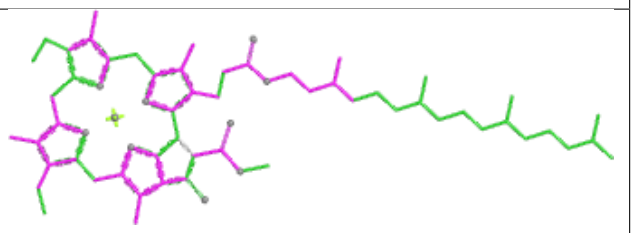


Rings

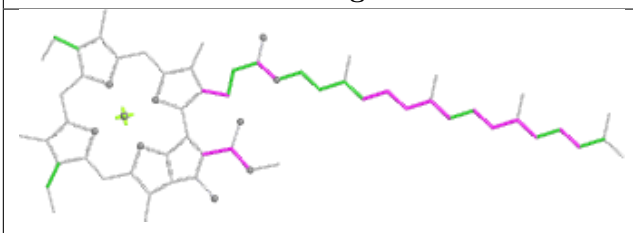
Ligand CLA A 1117



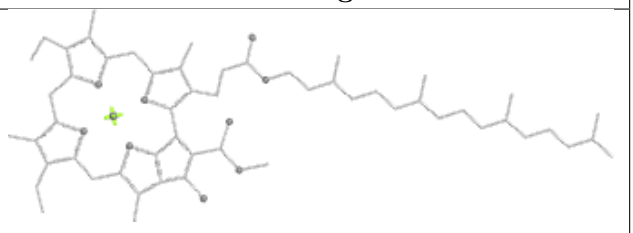
Bond lengths



Bond angles

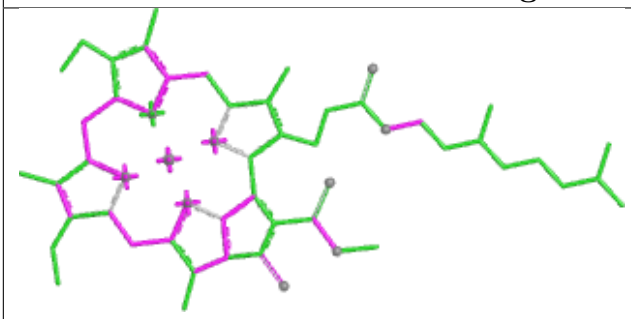


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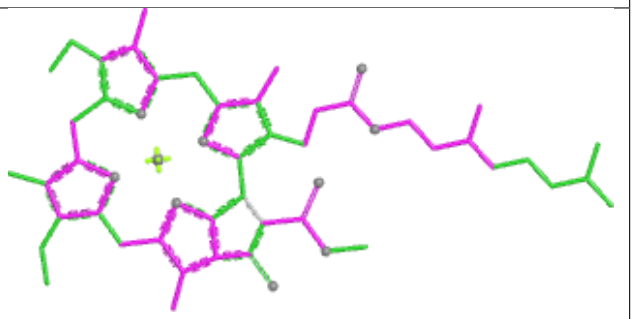


Rings

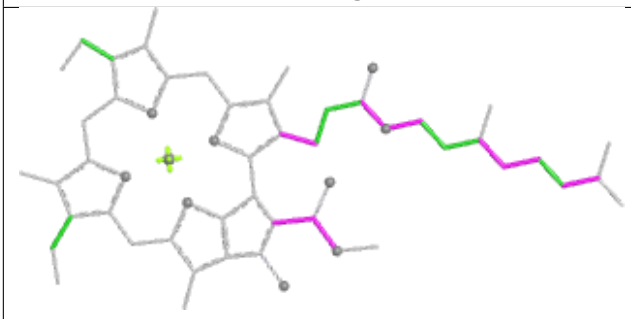
Ligand CLA a 1112



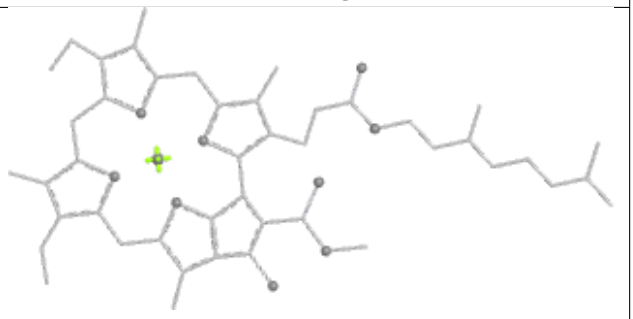
Bond lengths



Bond angles

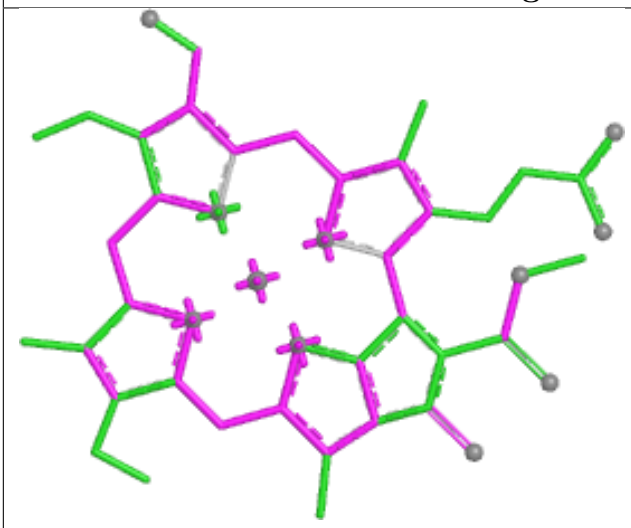


Torsions

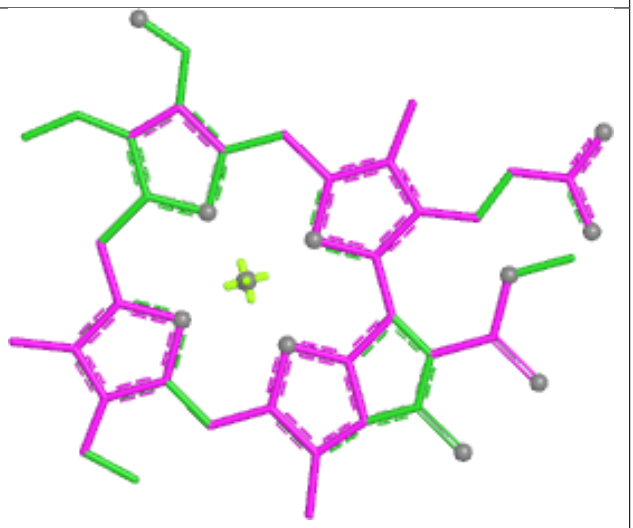


Rings

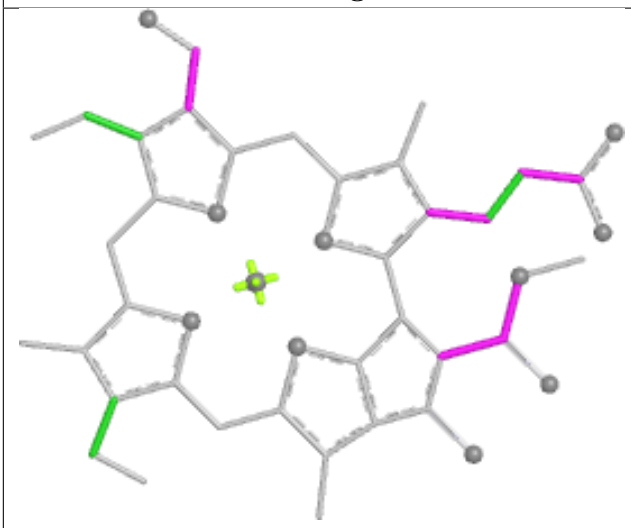
Ligand F6C b 1230



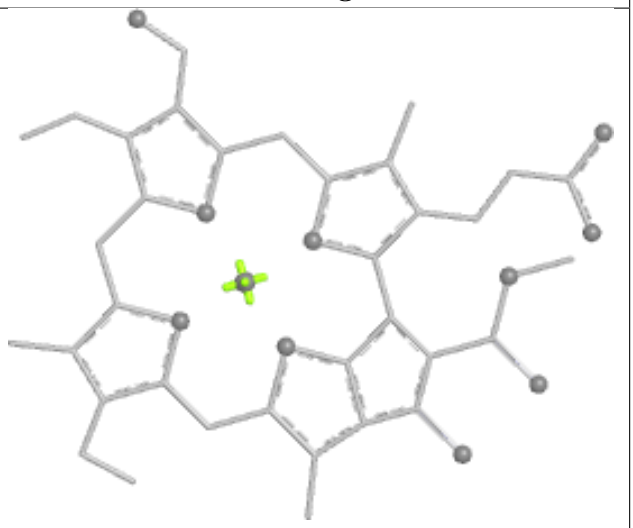
Bond lengths



Bond angles

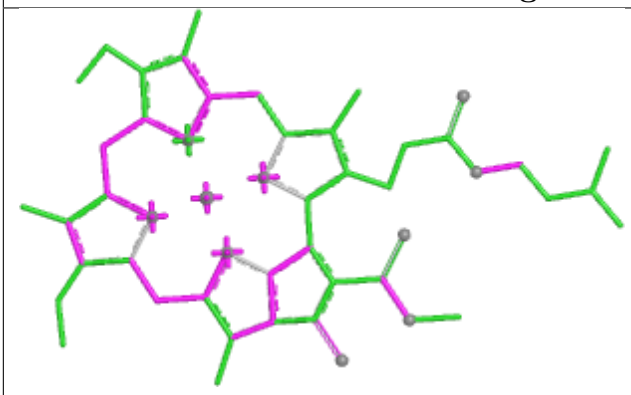


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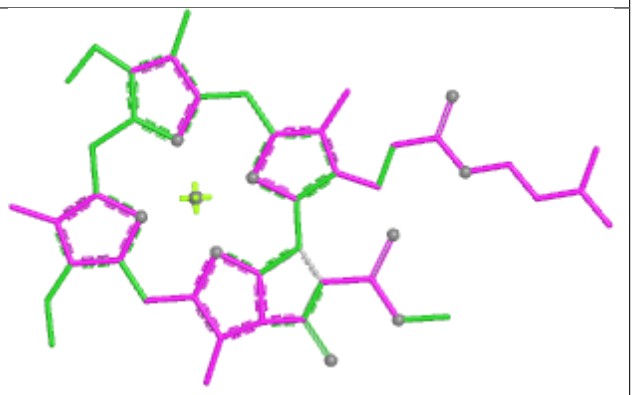


Rings

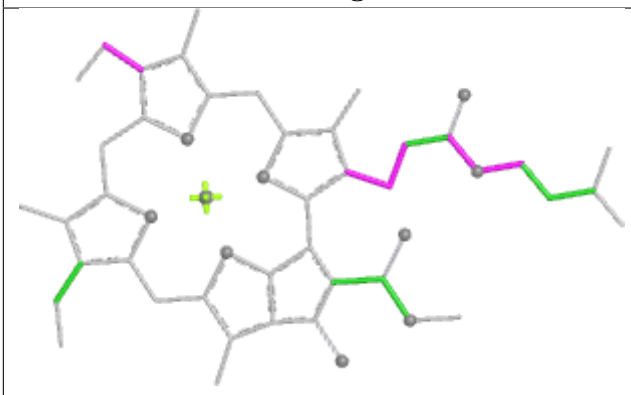
Ligand CLA a 1129



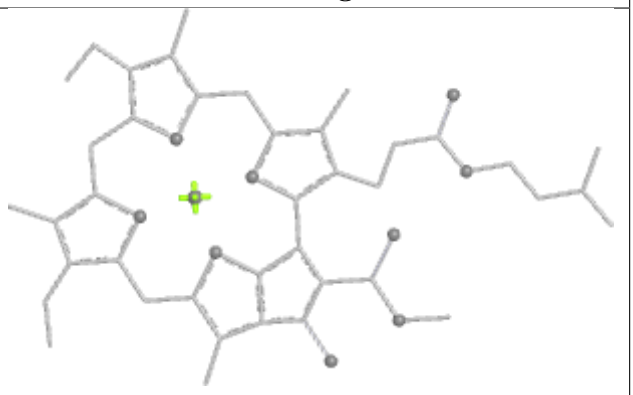
Bond lengths



Bond angles

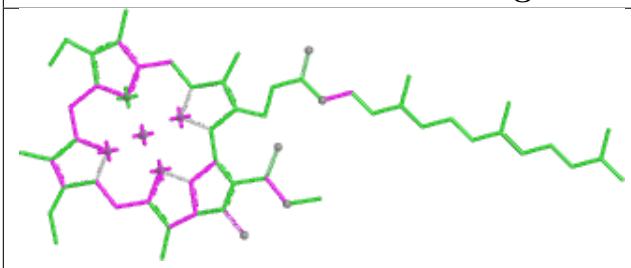


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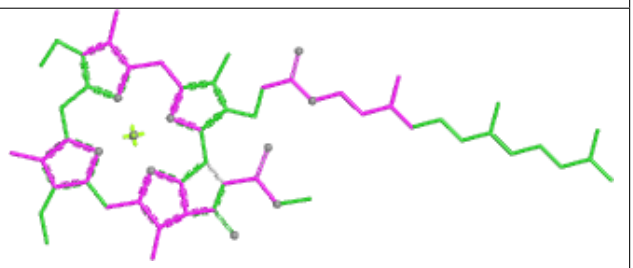


Rings

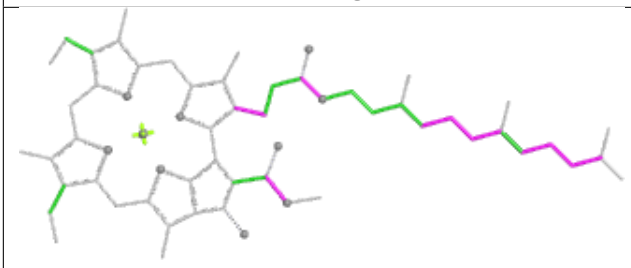
Ligand CLA G 1102



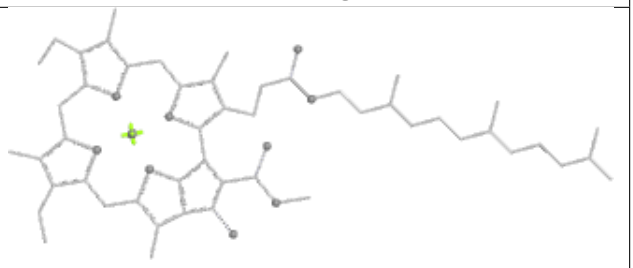
Bond lengths



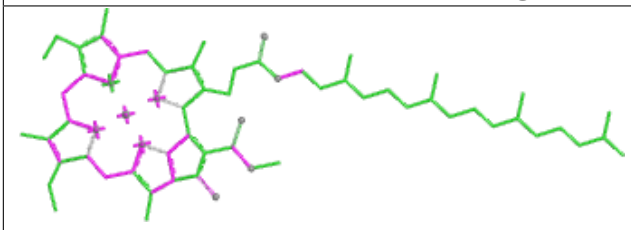
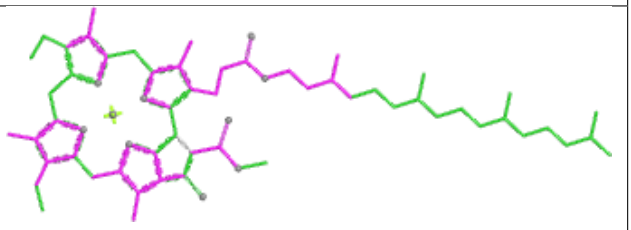
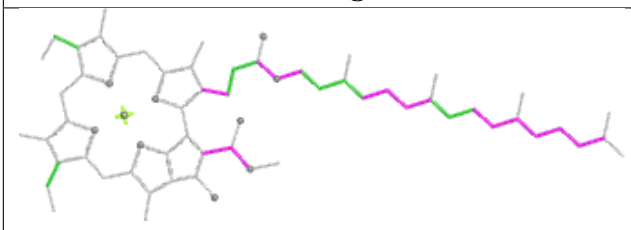
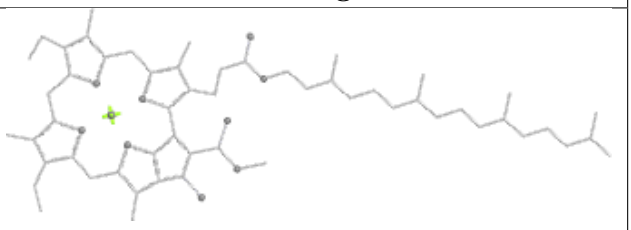
Bond angles

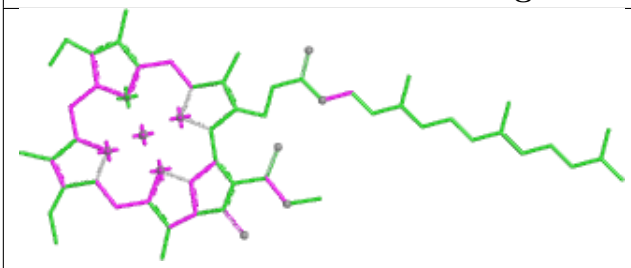
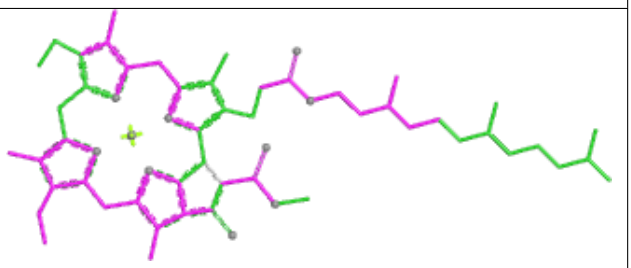
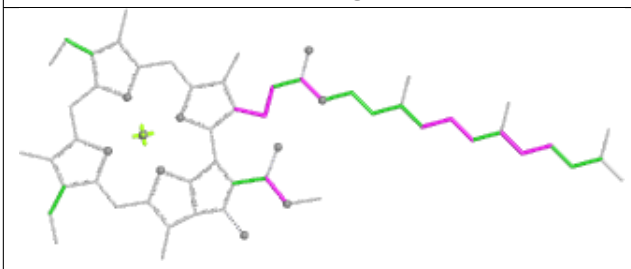
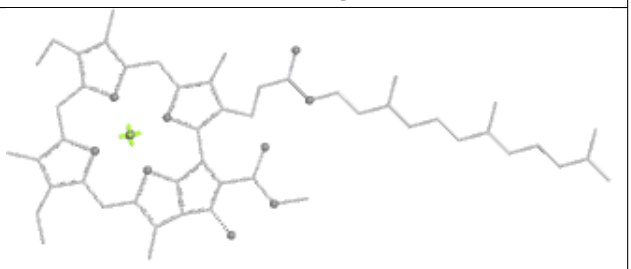


Torsions

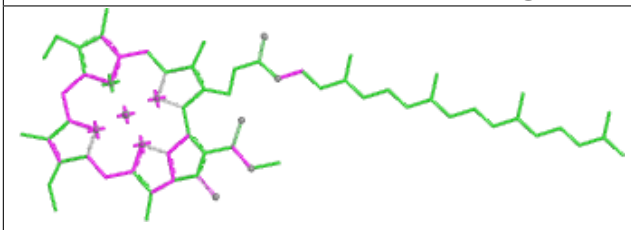


Rings

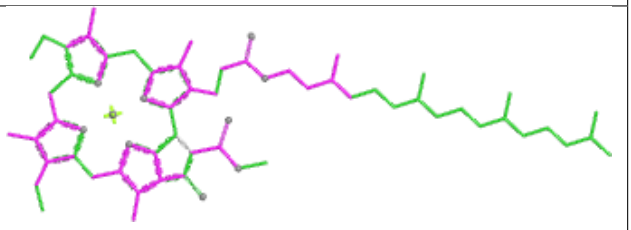
Ligand CLA G 1115	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 1013	
 Bond lengths	 Bond angles
 Torsions	 Rings

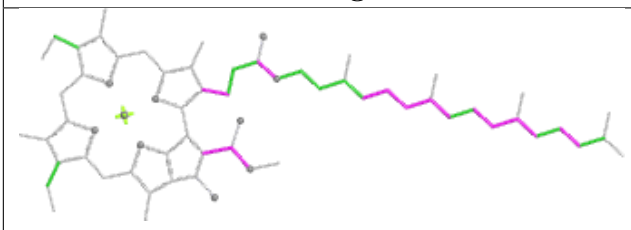
Ligand CLA a 1117



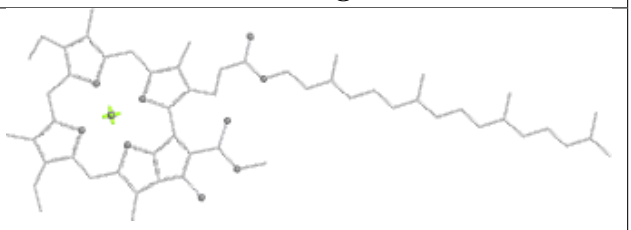
Bond lengths



Bond angles

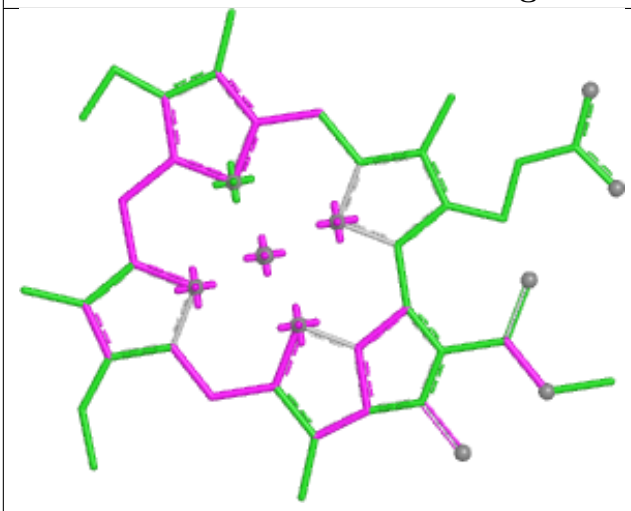


Torsions

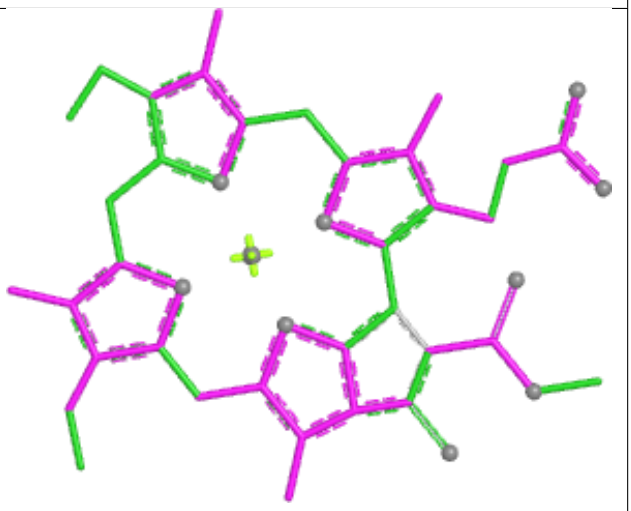


Rings

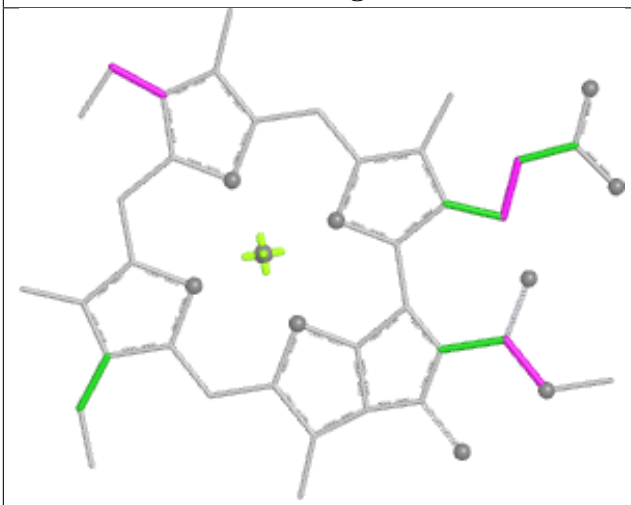
Ligand CLA a 1139



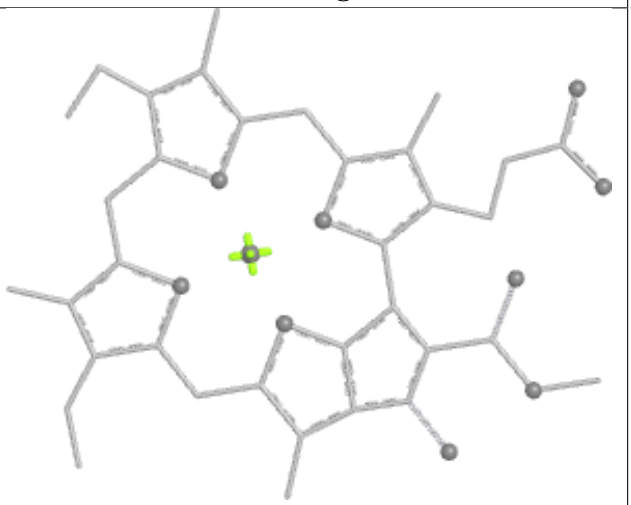
Bond lengths



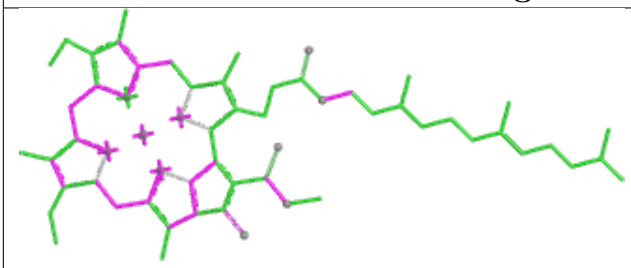
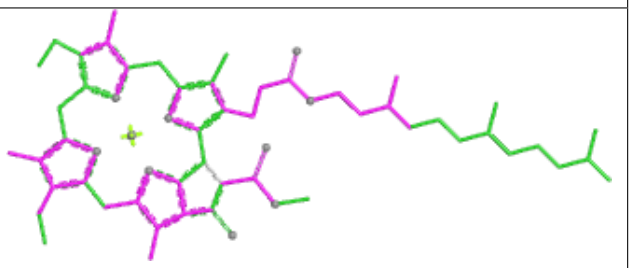
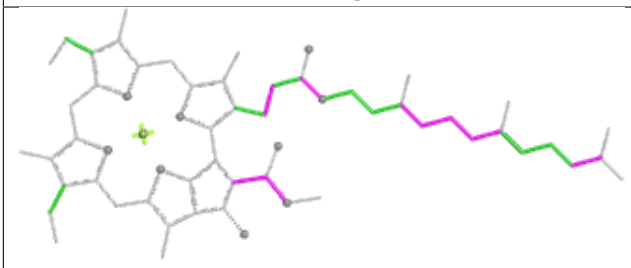
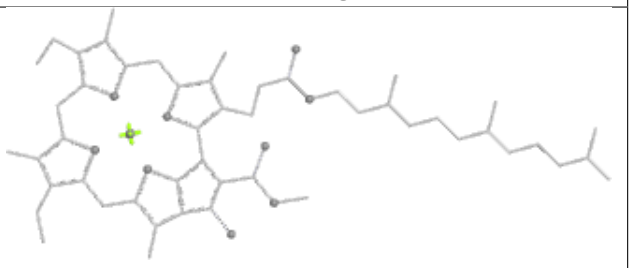
Bond angles

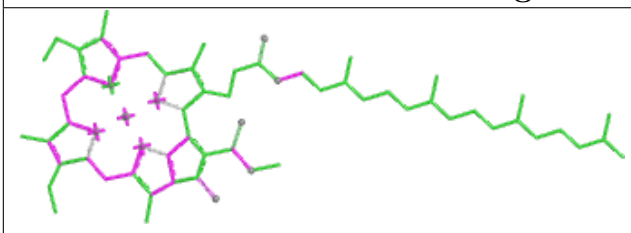
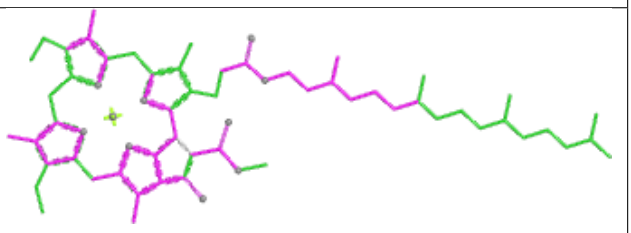
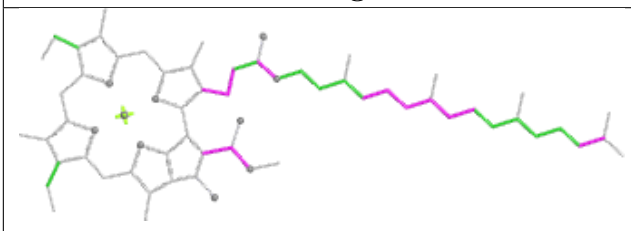
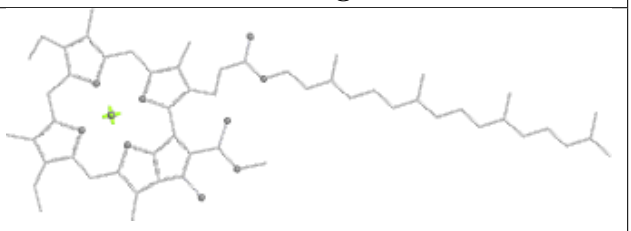


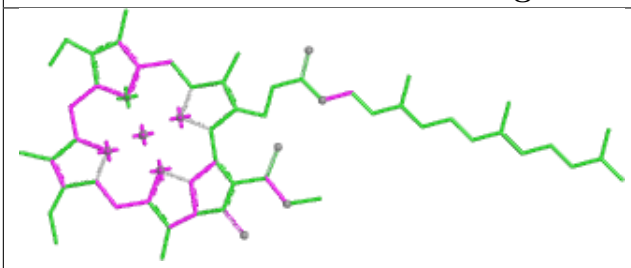
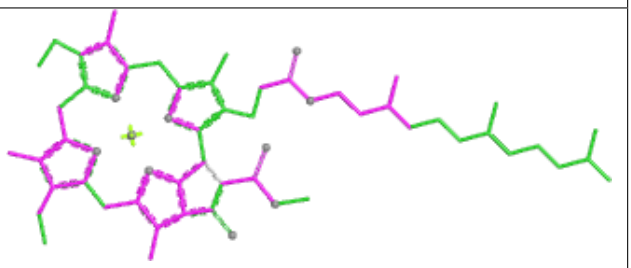
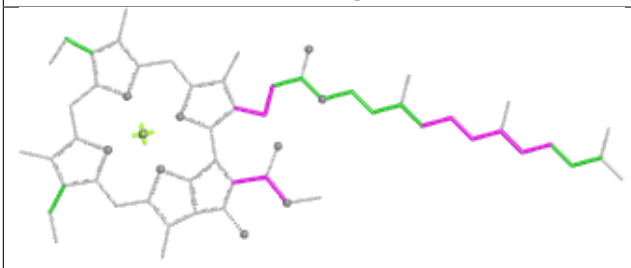
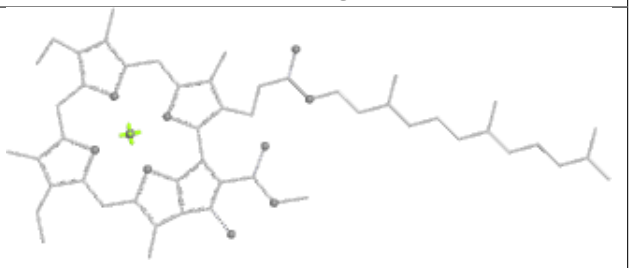
Torsions

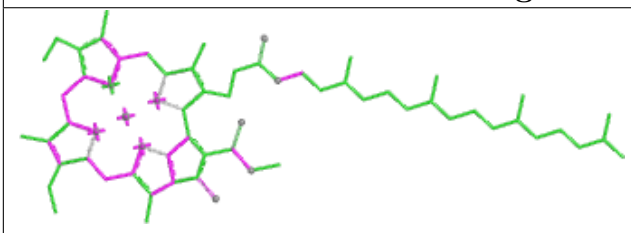
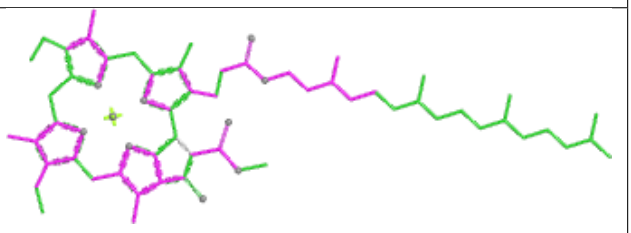
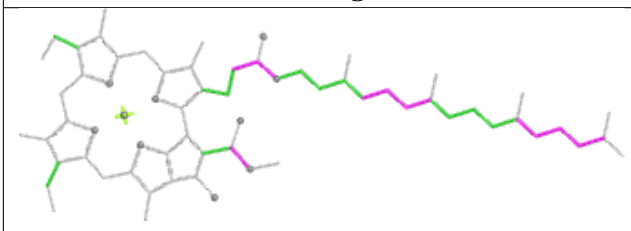
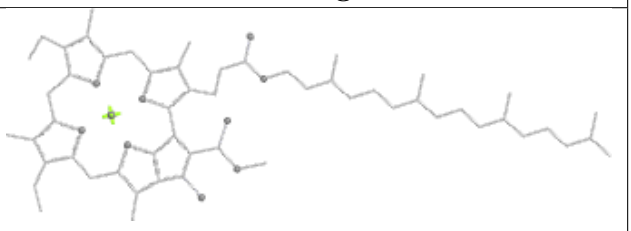


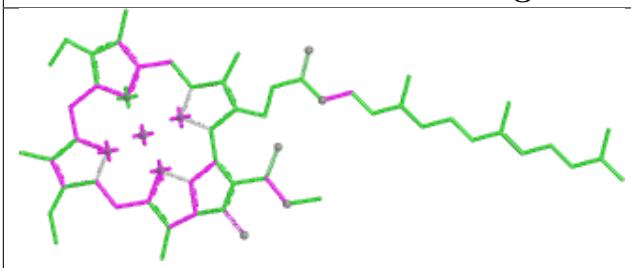
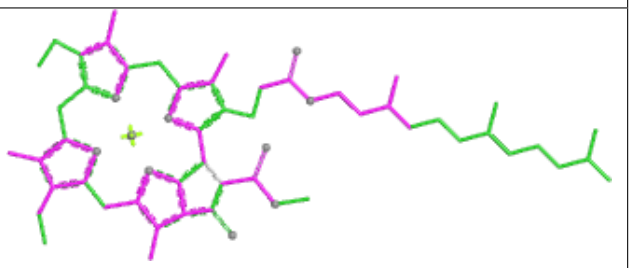
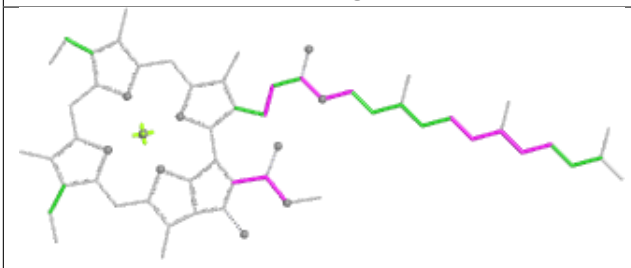
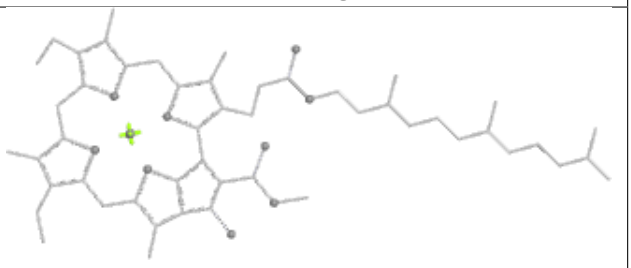
Rings

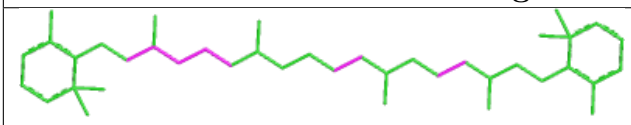
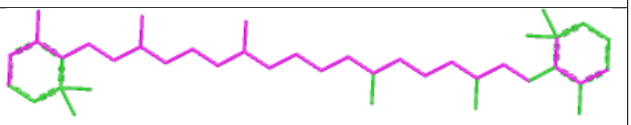
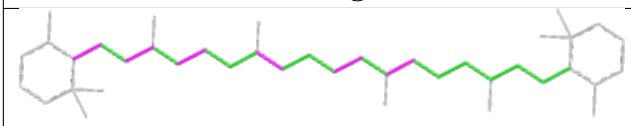
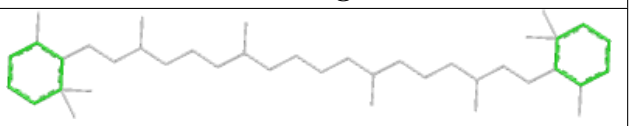
Ligand CLA G 1111	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

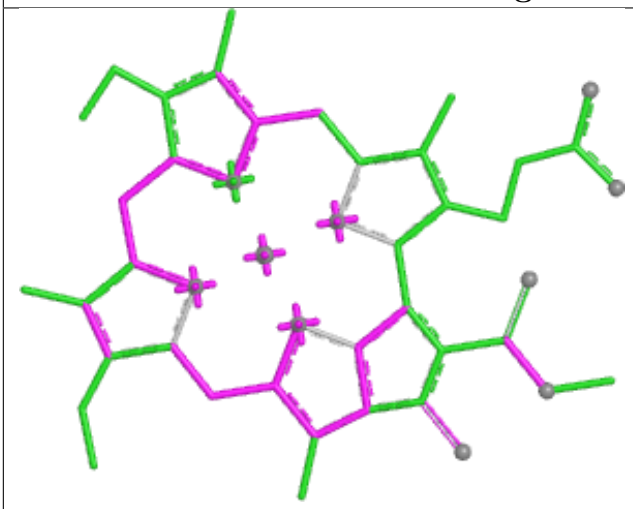
Ligand CLA G 1135	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1208	
	
Bond lengths	Bond angles
	
Torsions	Rings

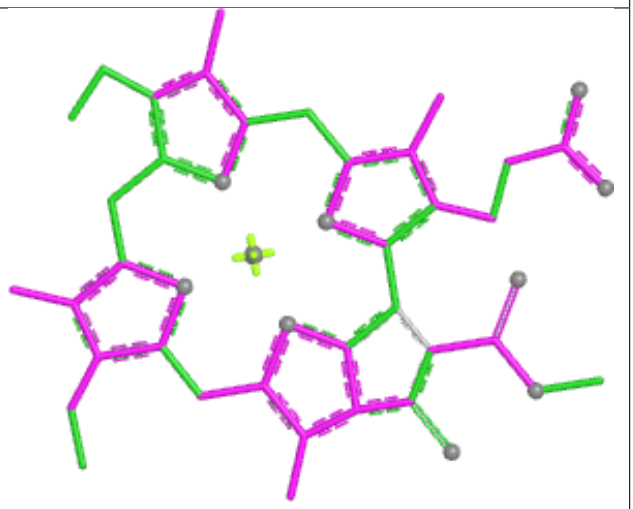
Ligand CLA G 1123	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 4016	
	
Bond lengths	Bond angles
	
Torsions	Rings

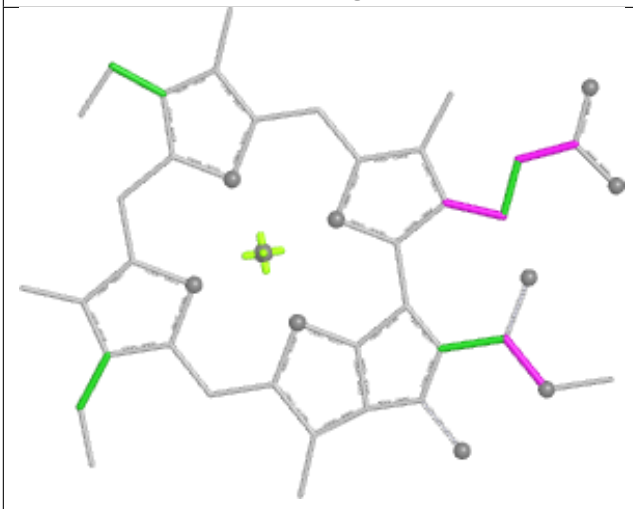
Ligand CLA A 1105



Bond lengths



Bond angles

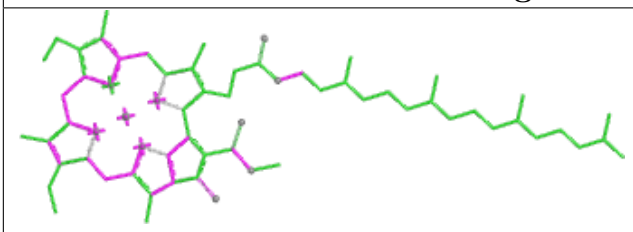


Torsions

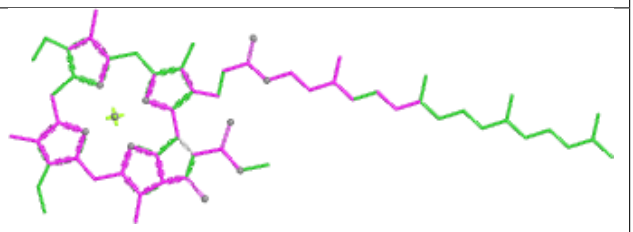


Rings

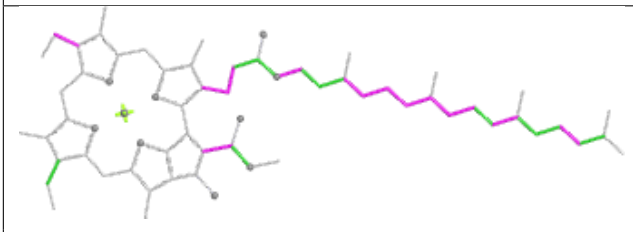
Ligand CLA H 1022



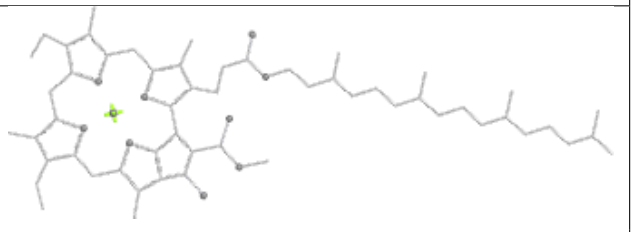
Bond lengths



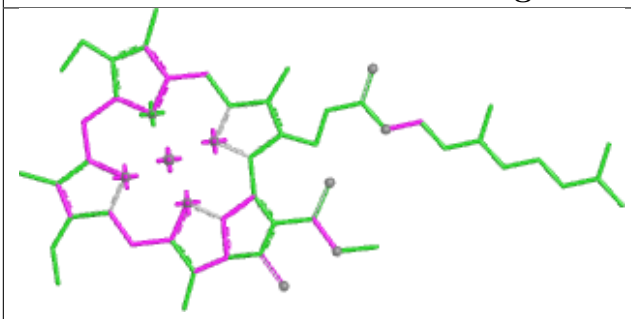
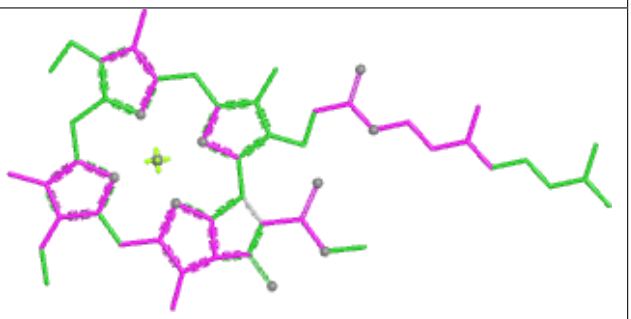
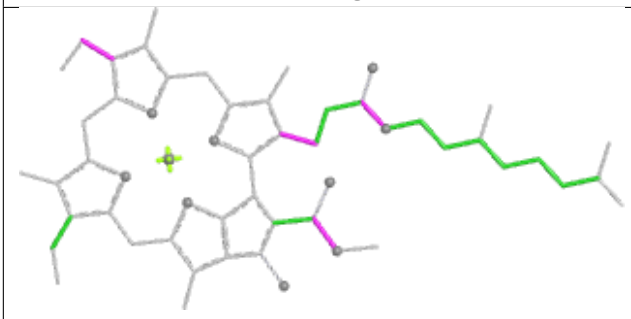
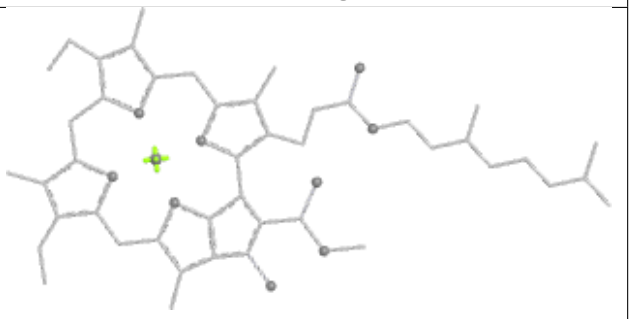
Bond angles

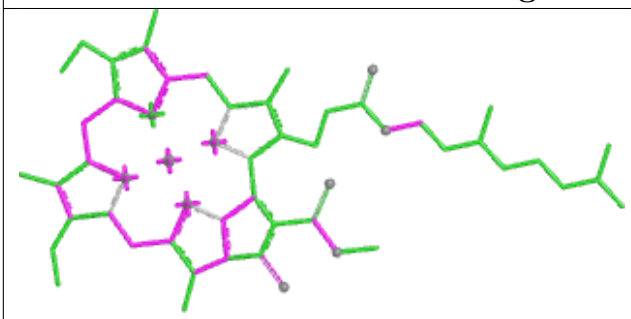
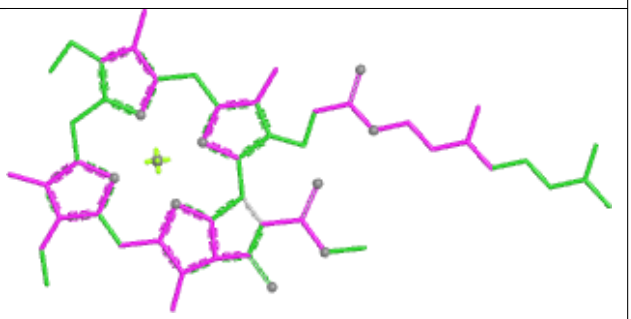
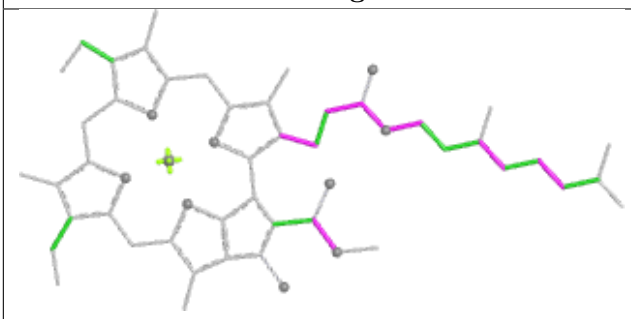
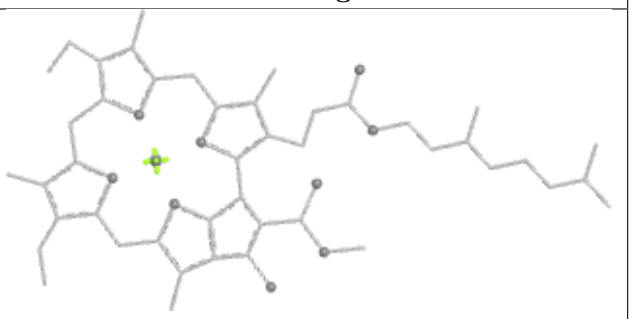


Torsions

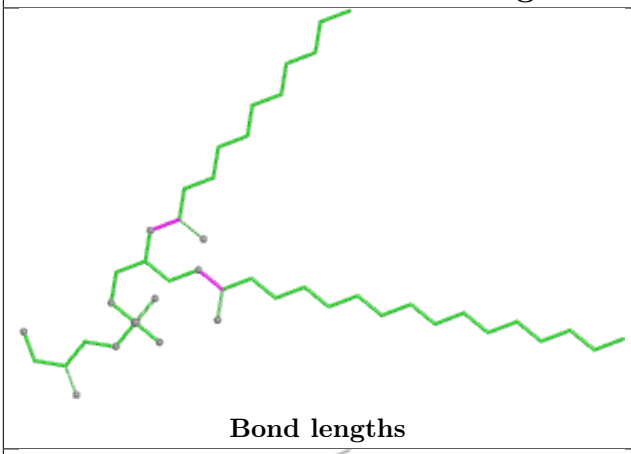


Rings

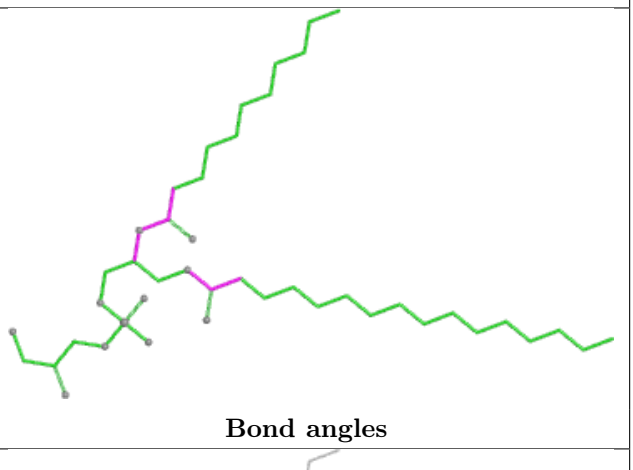
Ligand CLA H 1231	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA x 1701	
 Bond lengths	 Bond angles
 Torsions	 Rings

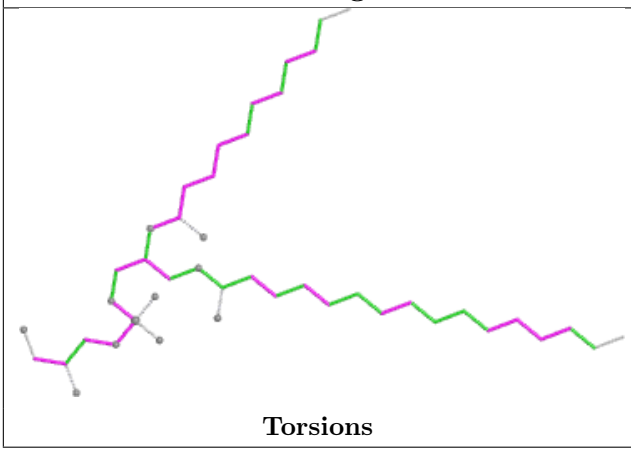
Ligand LHG b 5004



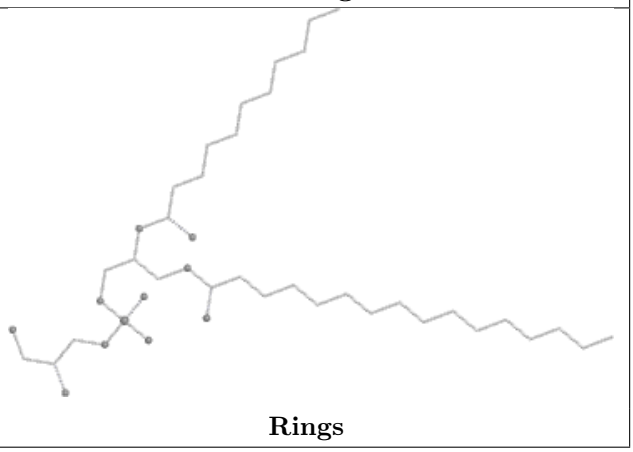
Bond lengths



Bond angles

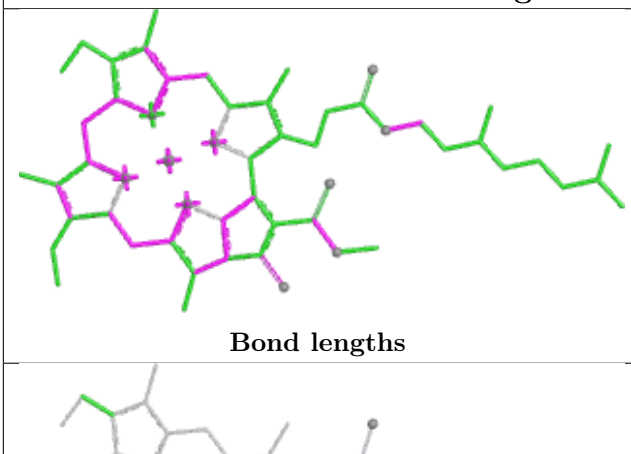


Torsions

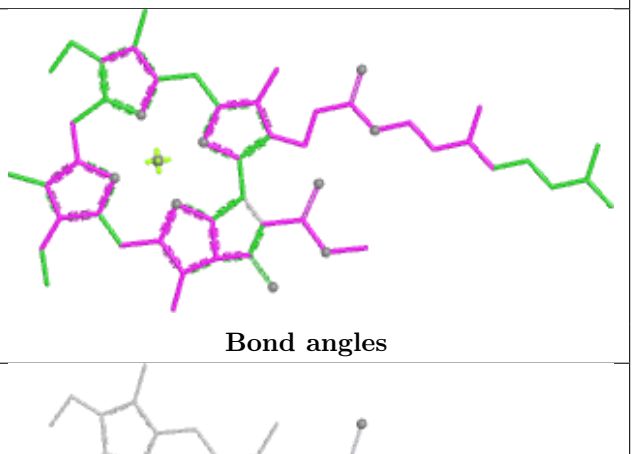


Rings

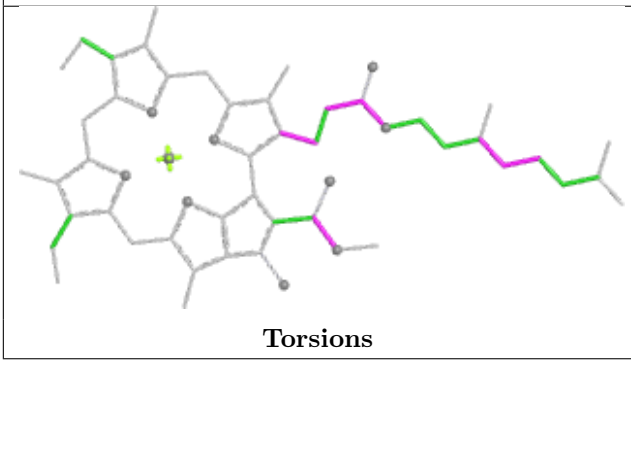
Ligand CLA H 1220



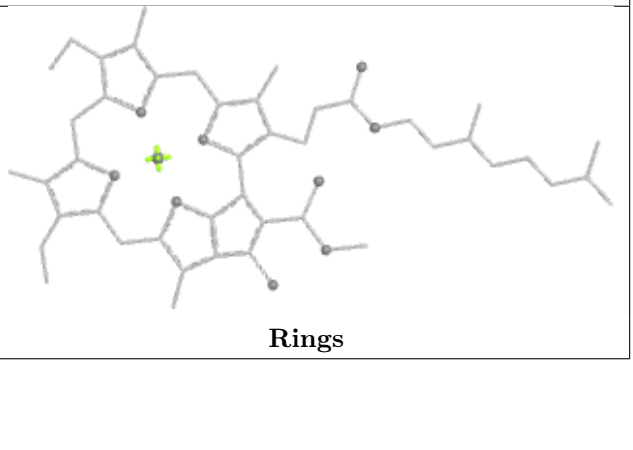
Bond lengths



Bond angles

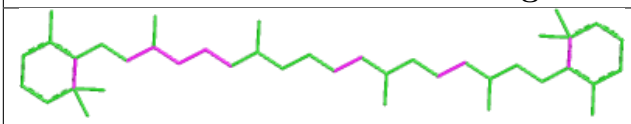


Torsions

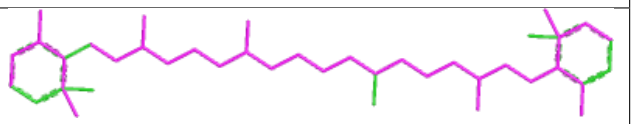


Rings

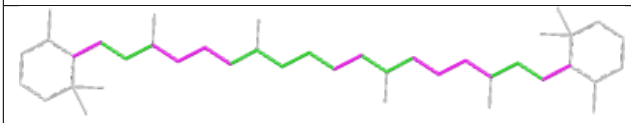
Ligand BCR i 4020



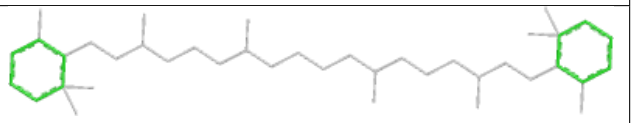
Bond lengths



Bond angles

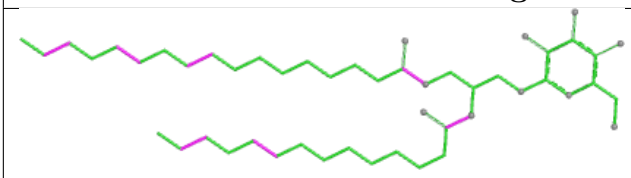


Torsions

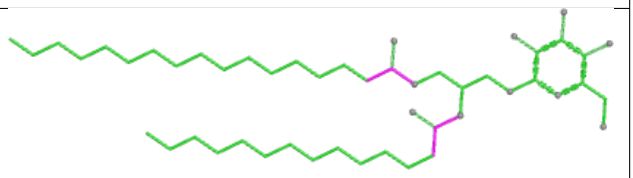


Rings

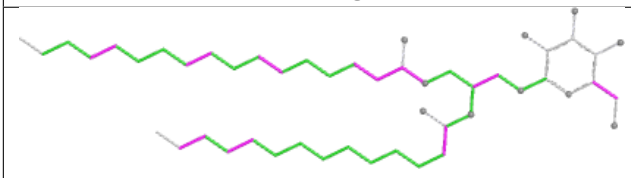
Ligand LMG U 5007



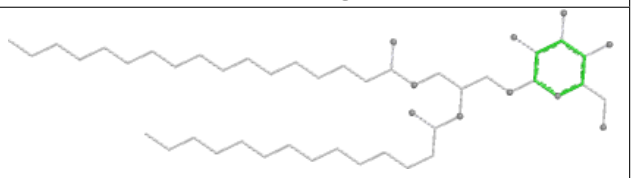
Bond lengths



Bond angles

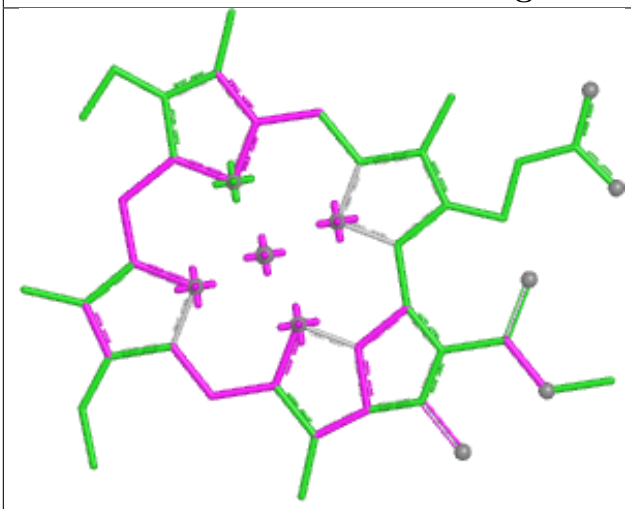


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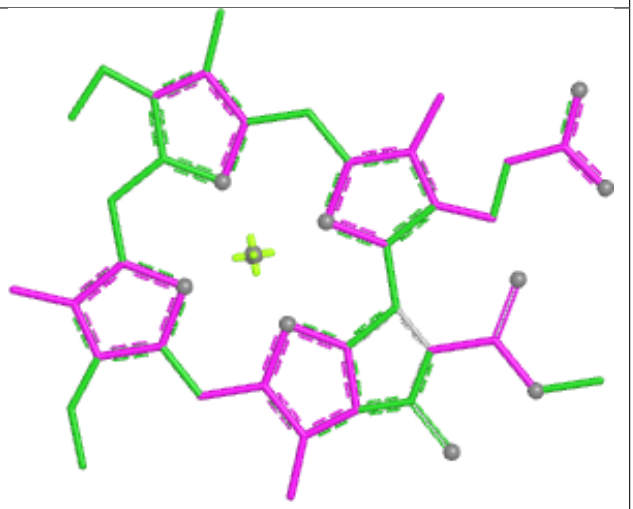


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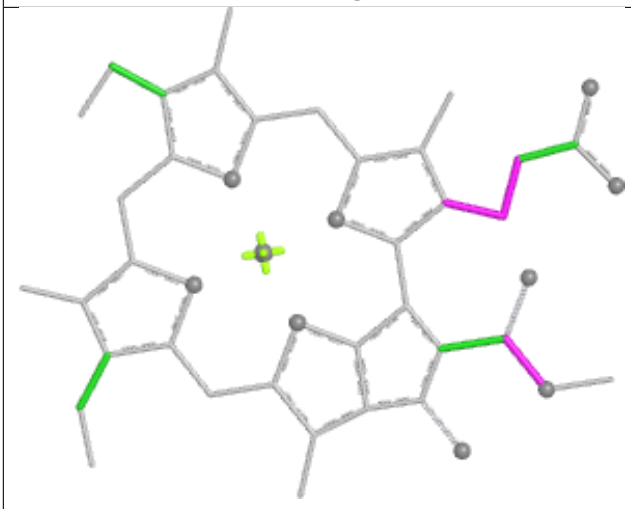
Ligand CLA B 1212



Bond lengths



Bond angles

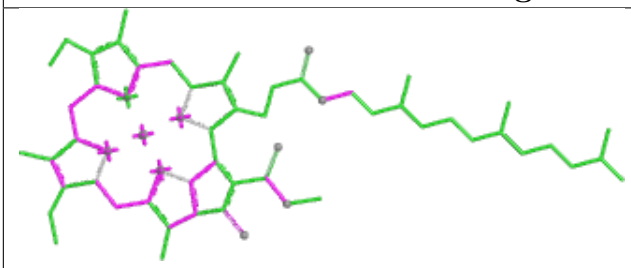


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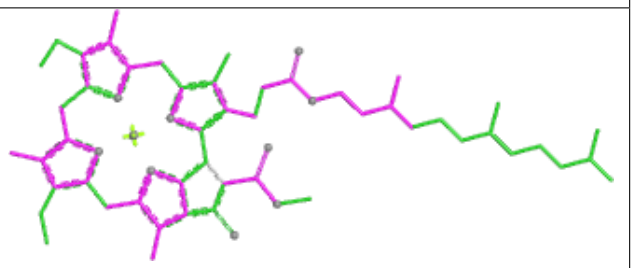


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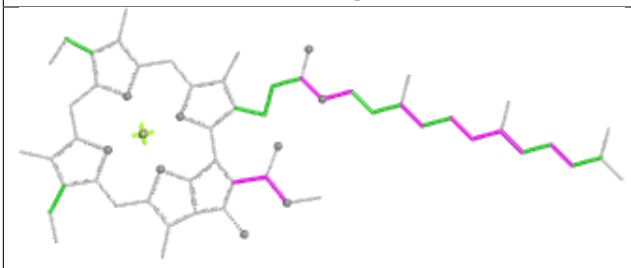
Ligand CLA A 1128



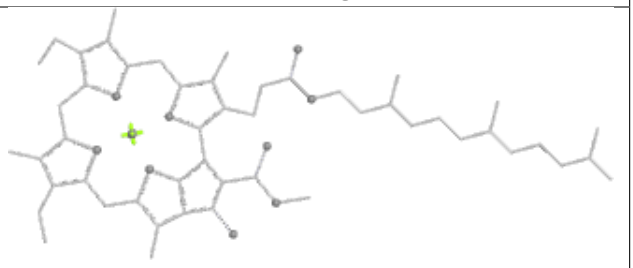
Bond lengths



Bond angles

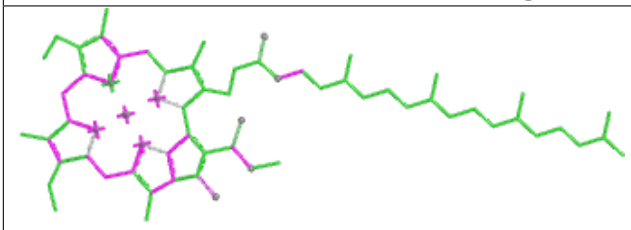


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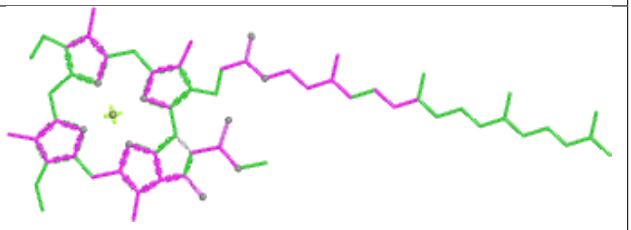


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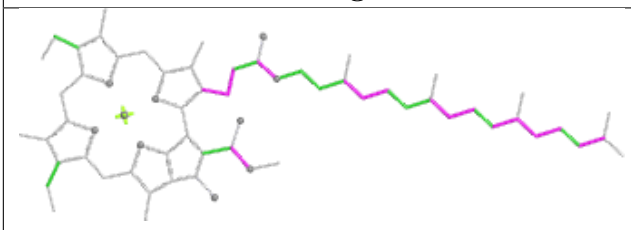
Ligand CLA a 1109



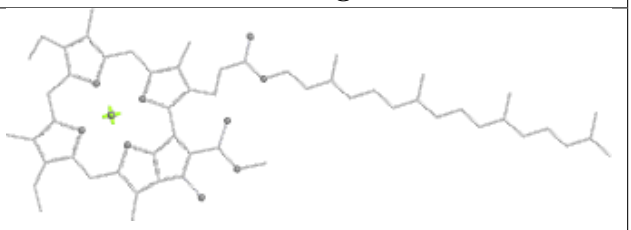
Bond lengths



Bond angles

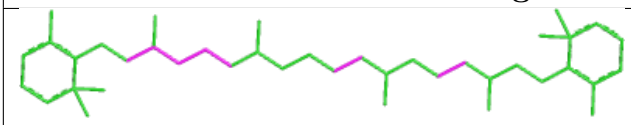


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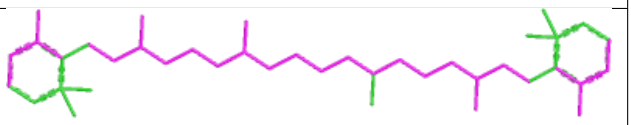


Rings

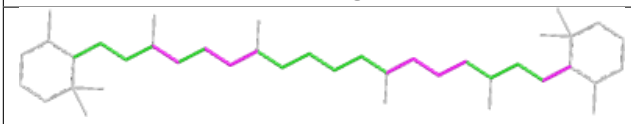
Ligand BCR H 4013



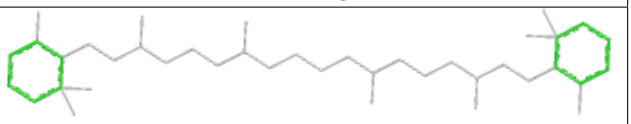
Bond lengths



Bond angles

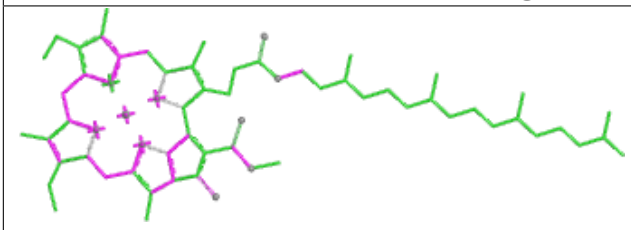


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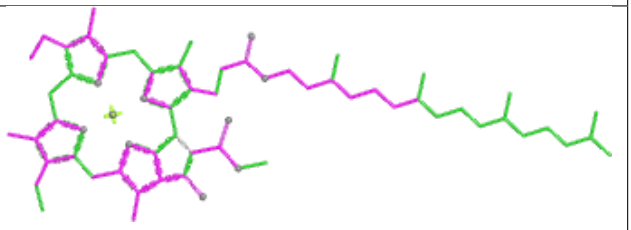


Rings

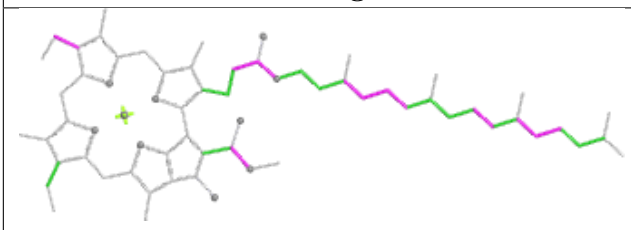
Ligand CLA b 1204



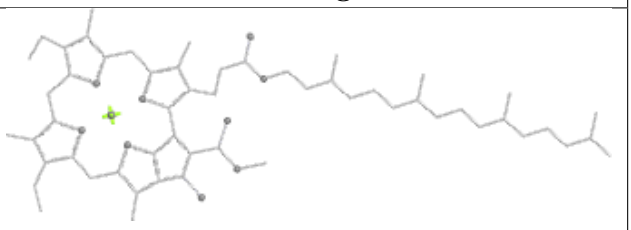
Bond lengths



Bond angles

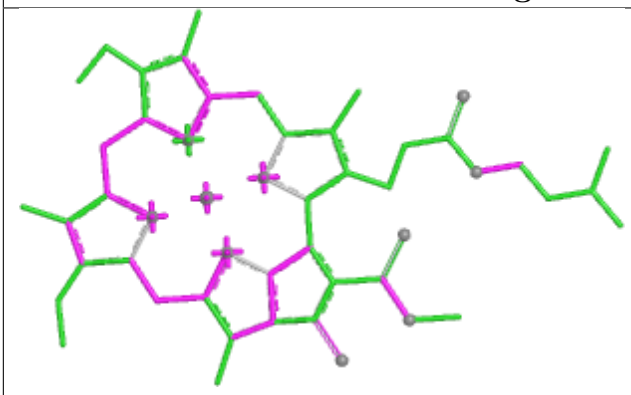


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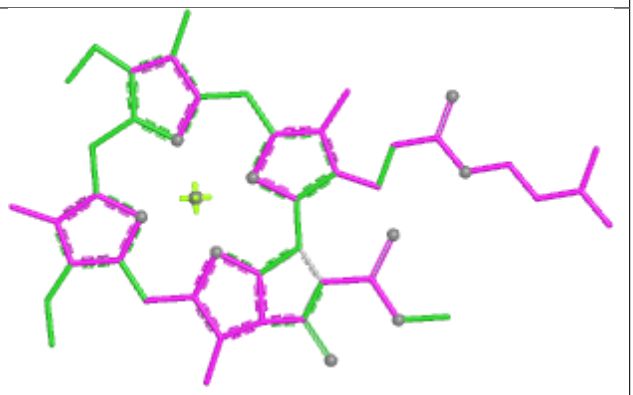


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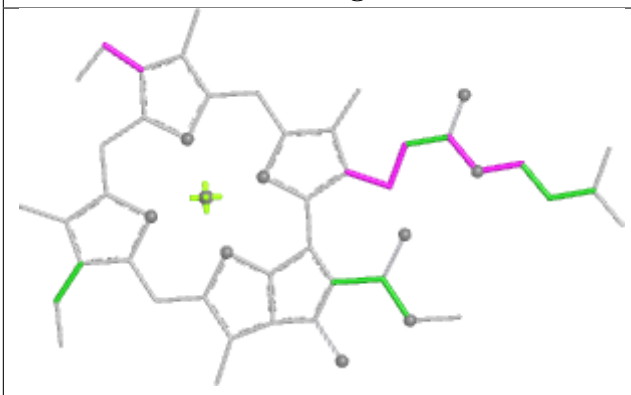
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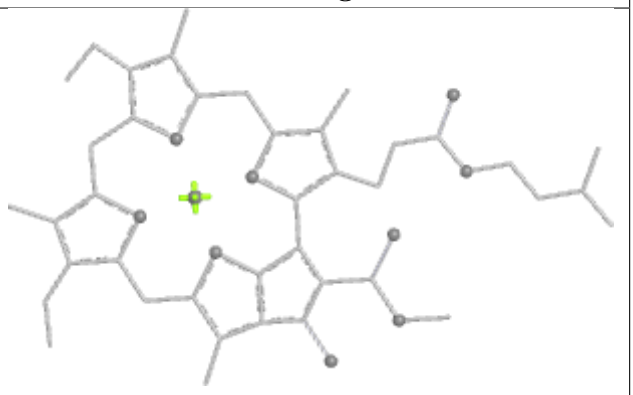
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Bond angles

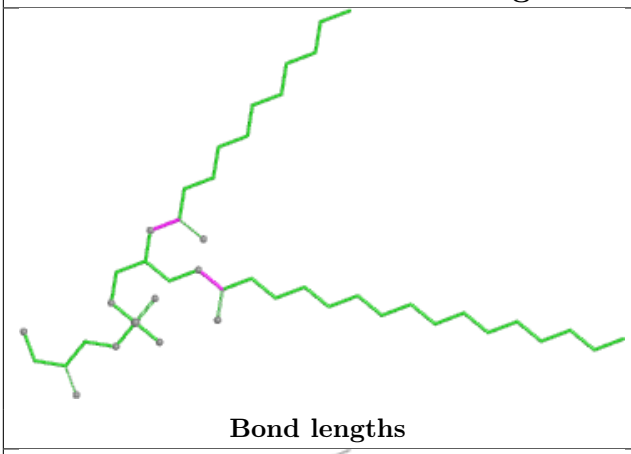


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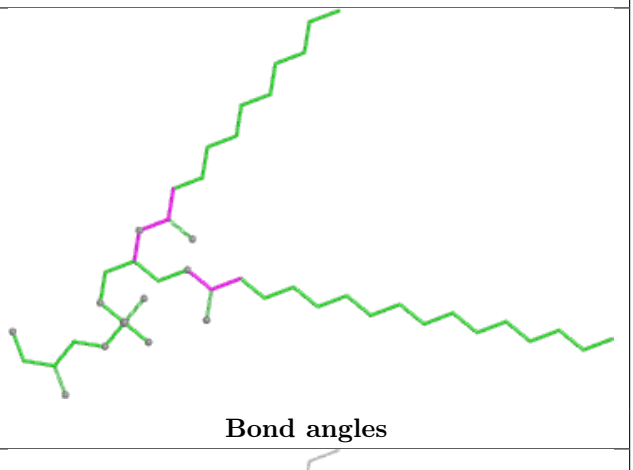


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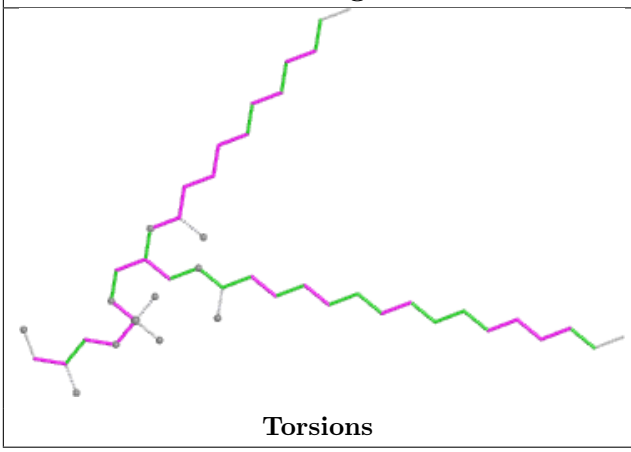
Ligand LHG H 5004



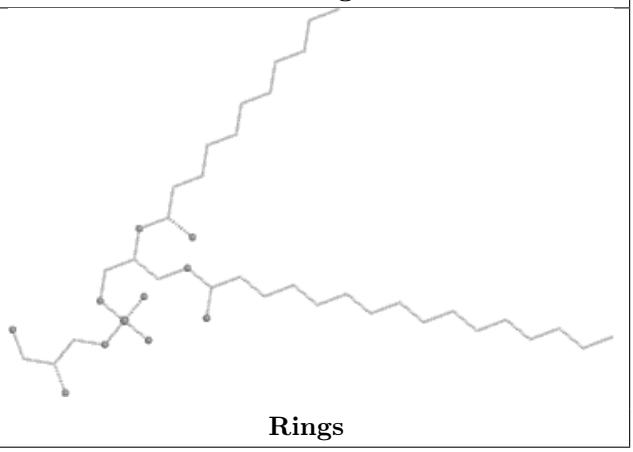
Bond lengths



Bond angles

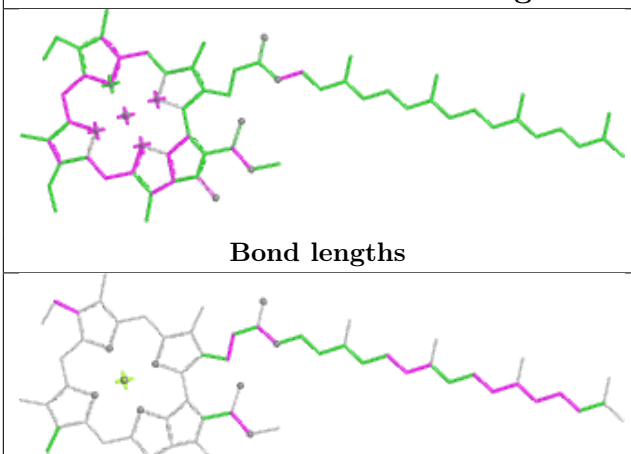


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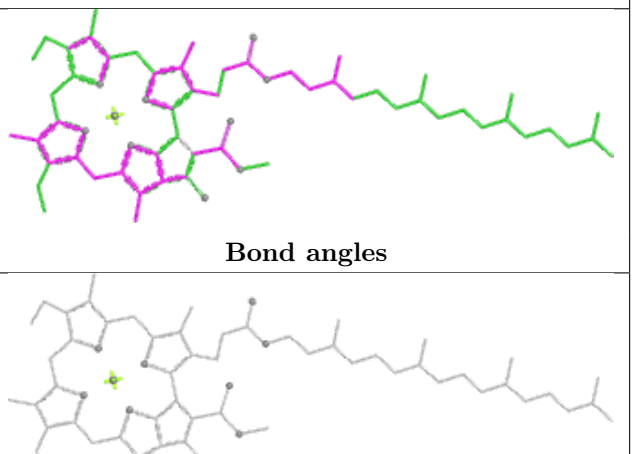


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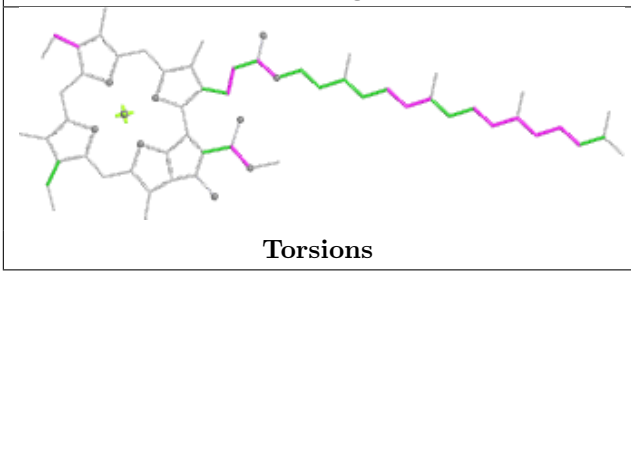
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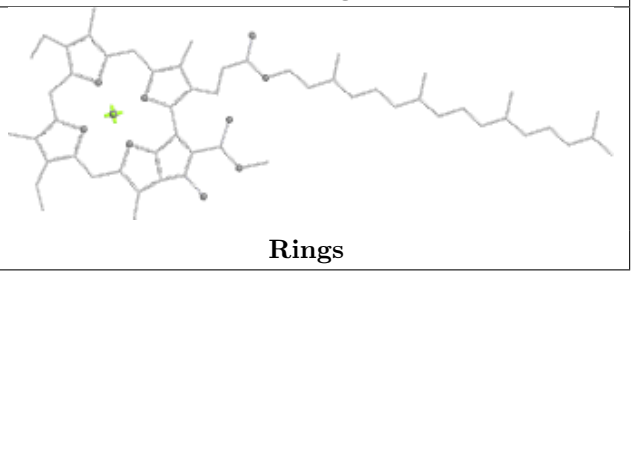
Bond lengths



Bond angles

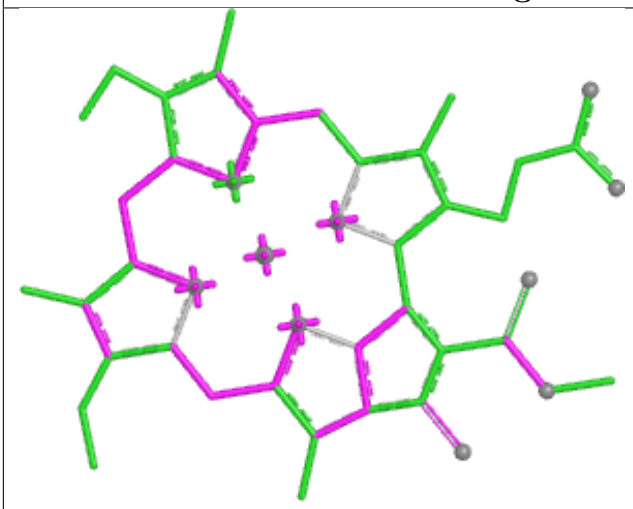


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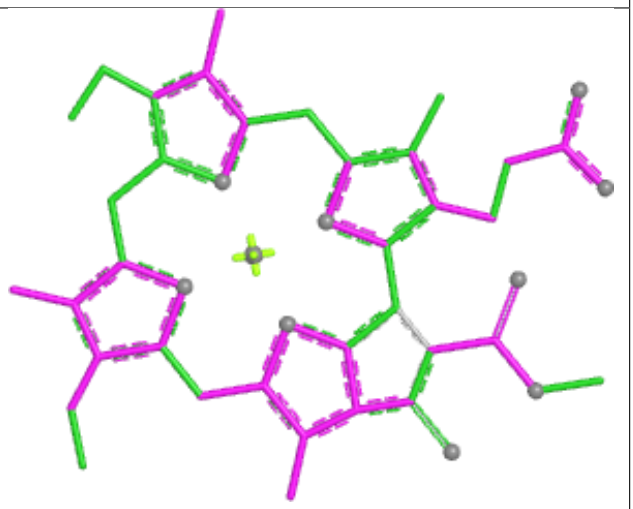


Rings

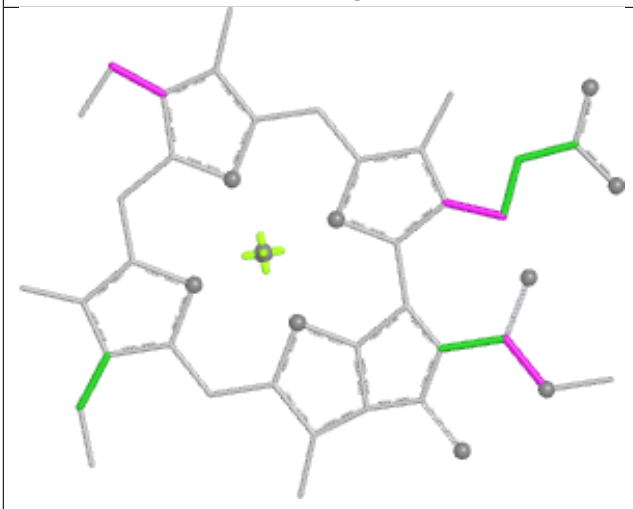
Ligand CLA G 1107



Bond lengths



Bond angles

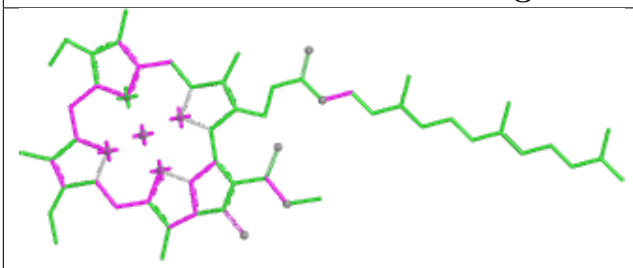


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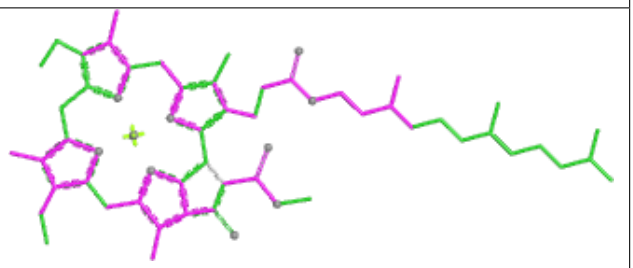


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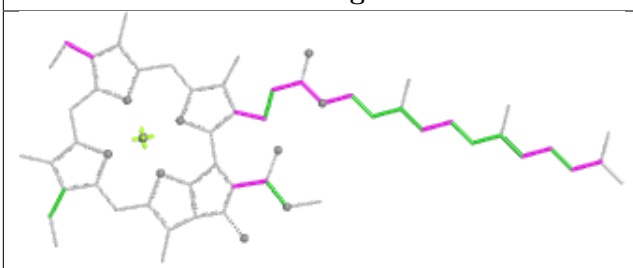
Ligand CLA H 1202



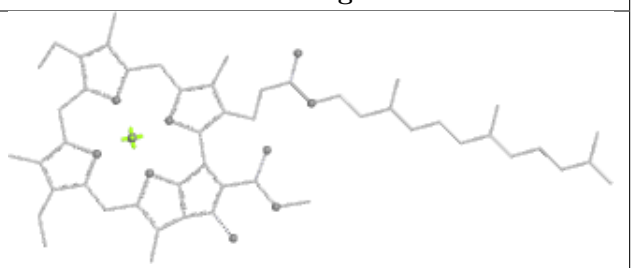
Bond lengths



Bond angles

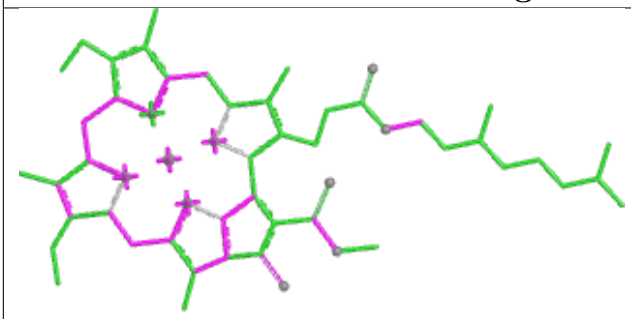


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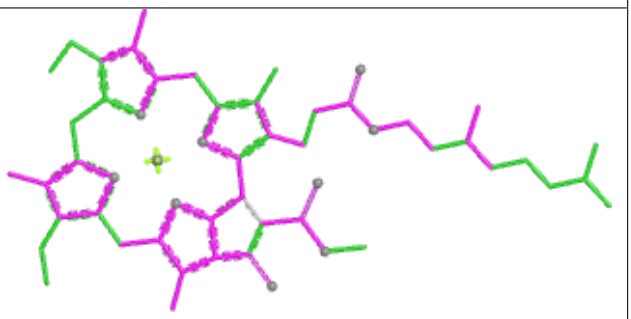


Rings

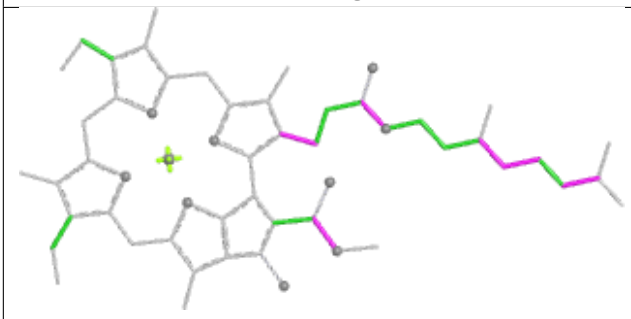
Ligand CLA A 1130



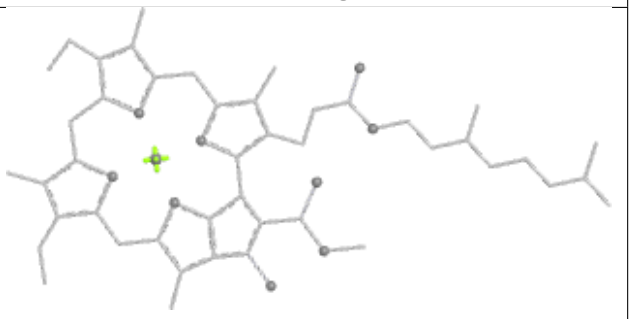
Bond lengths



Bond angles

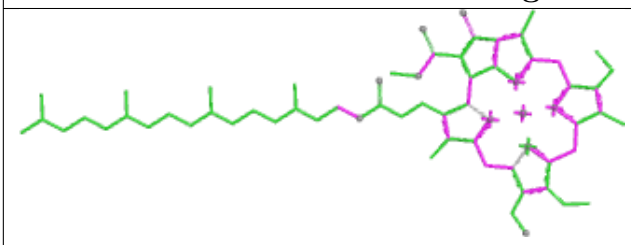


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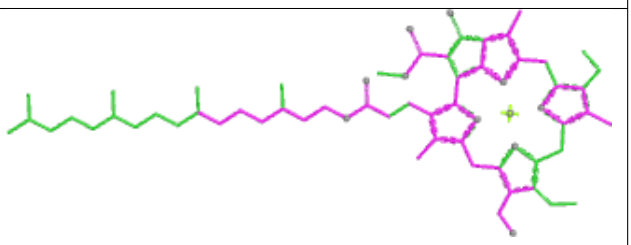


Rings

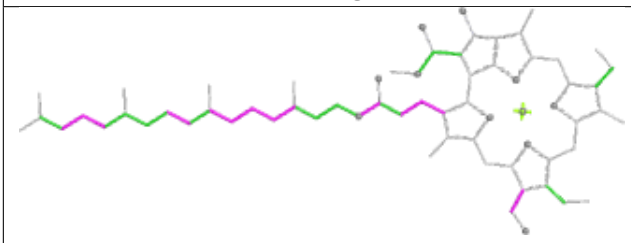
Ligand F6C b 1238



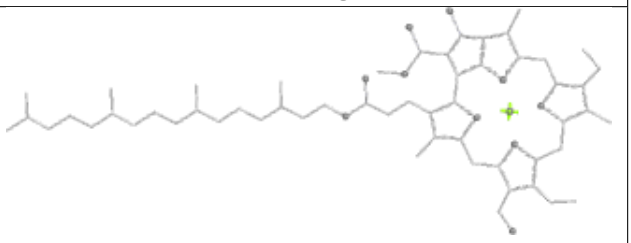
Bond lengths



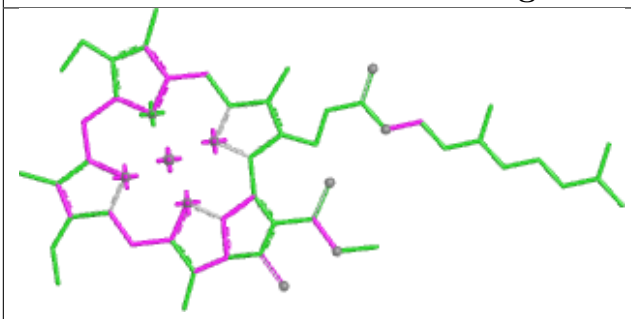
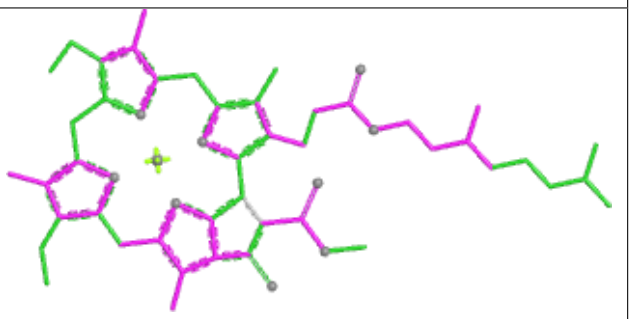
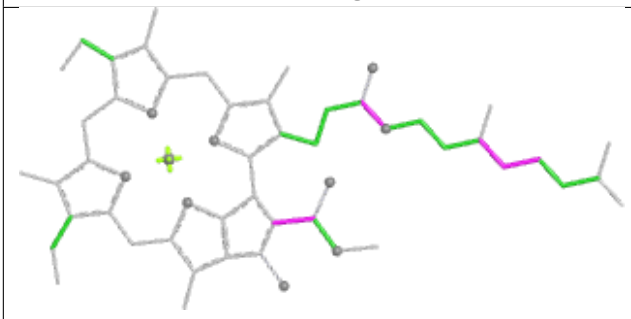
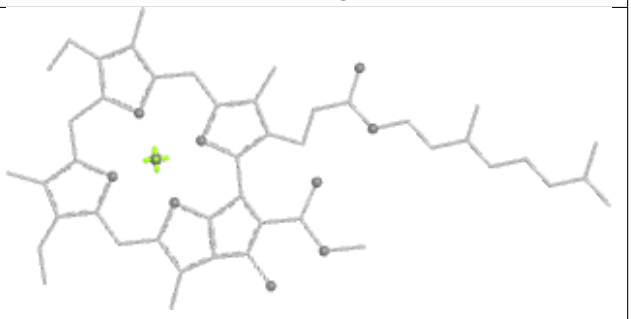
Bond angles

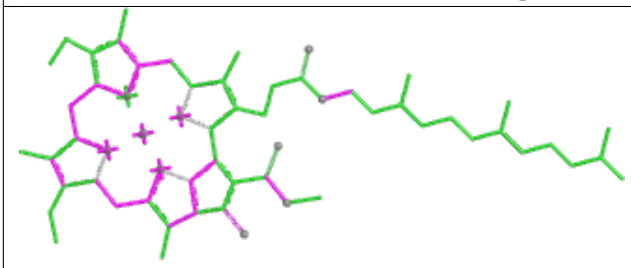
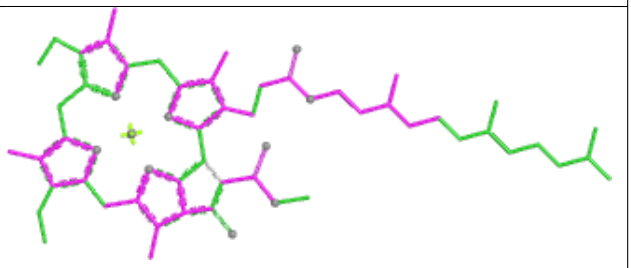
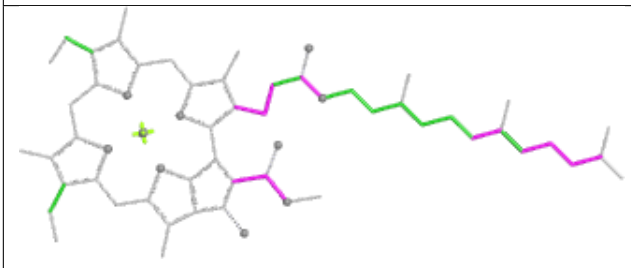
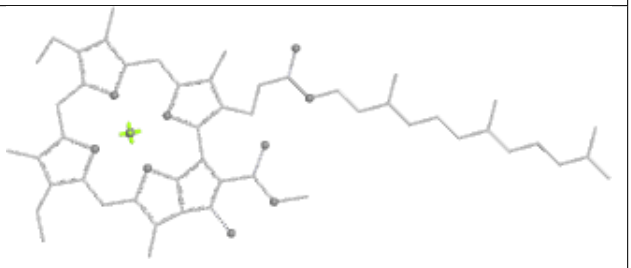


Torsions

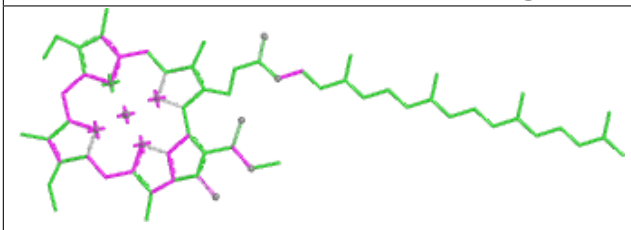


Rings

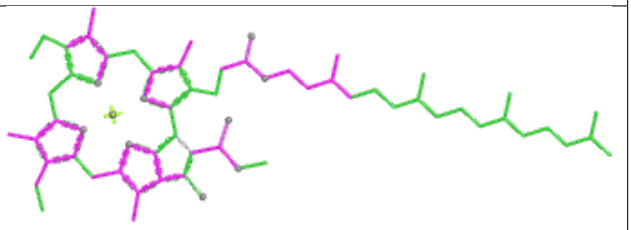
Ligand CLA b 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1106	
	
Bond lengths	Bond angles
	
Torsions	Rings

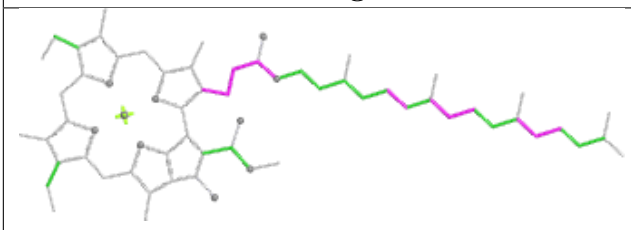
Ligand CLA a 1127



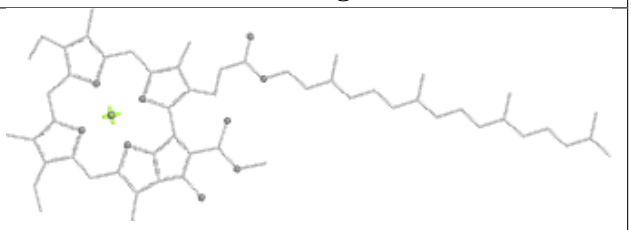
Bond lengths



Bond angles

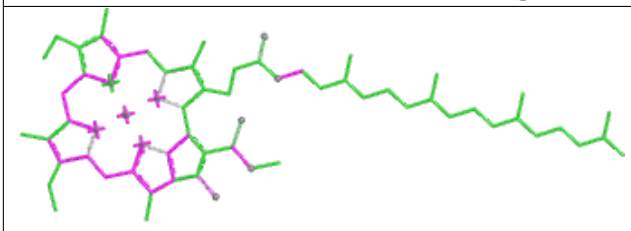


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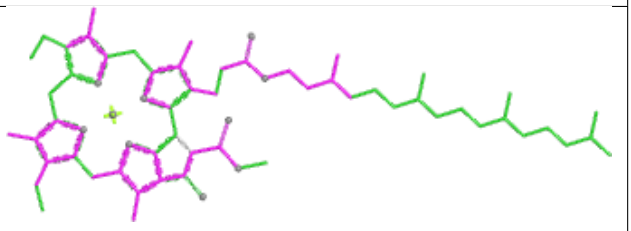


Rings

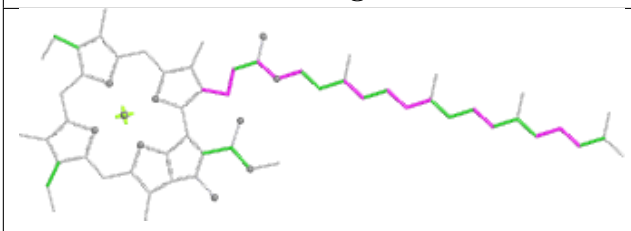
Ligand CLA H 1210



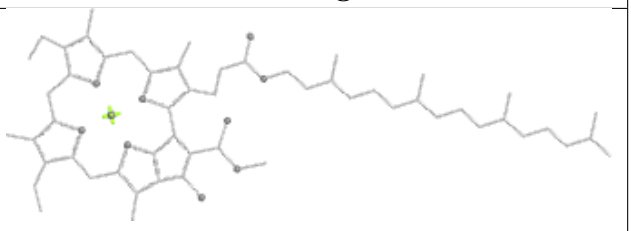
Bond lengths



Bond angles

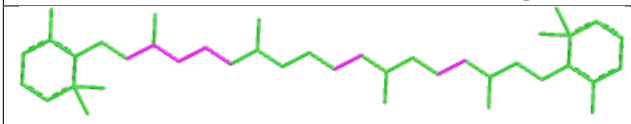


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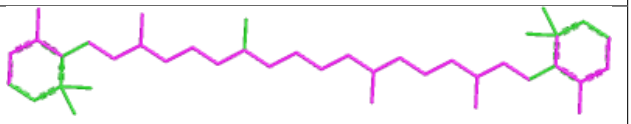


Rings

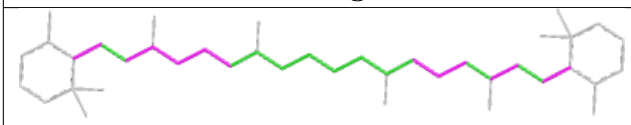
Ligand BCR a 4003



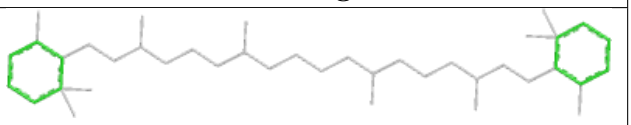
Bond lengths



Bond angles

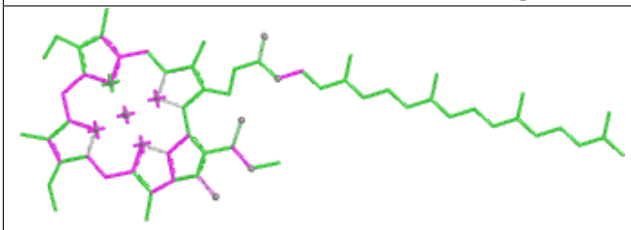


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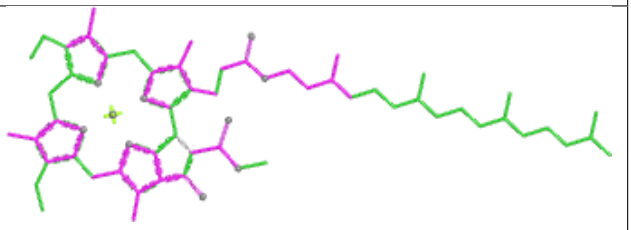


Rings

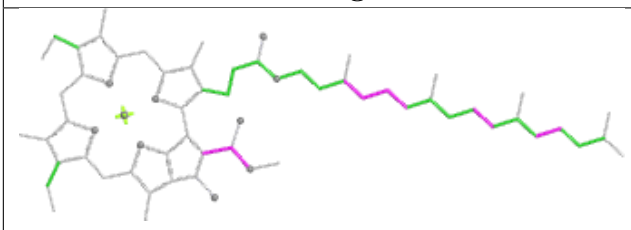
Ligand CLA H 1205



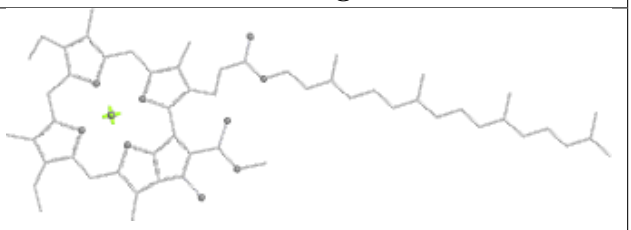
Bond lengths



Bond angles

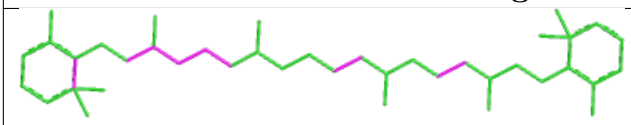


Torsions

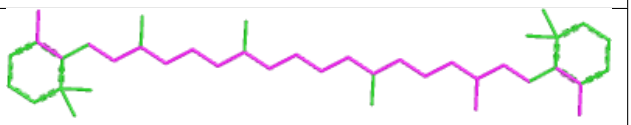


Rings

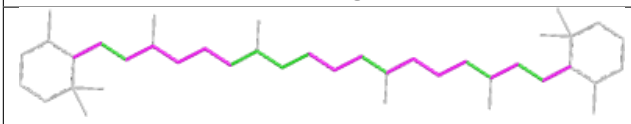
Ligand BCR m 4021



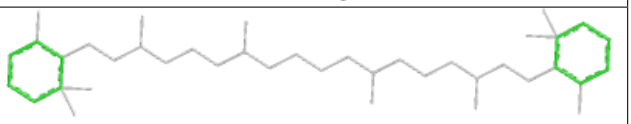
Bond lengths



Bond angles

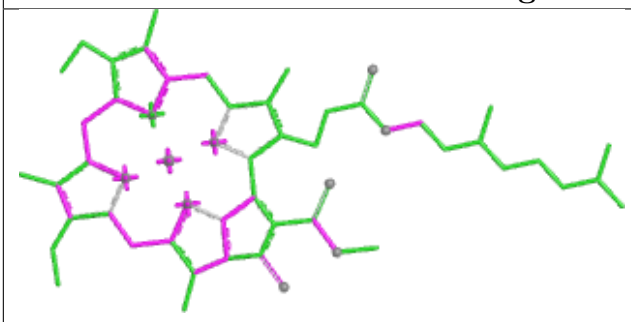


Torsions

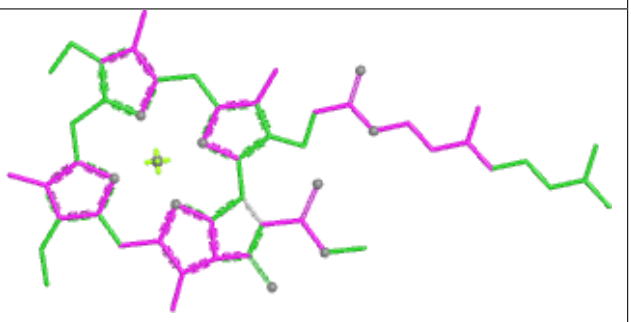


Rings

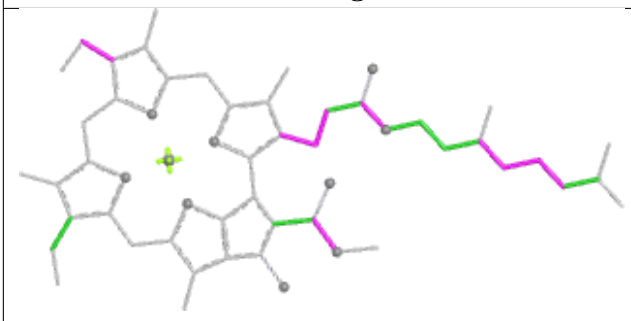
Ligand CLA b 1217



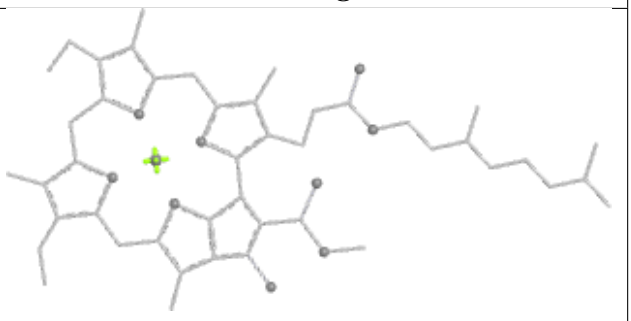
Bond lengths



Bond angles

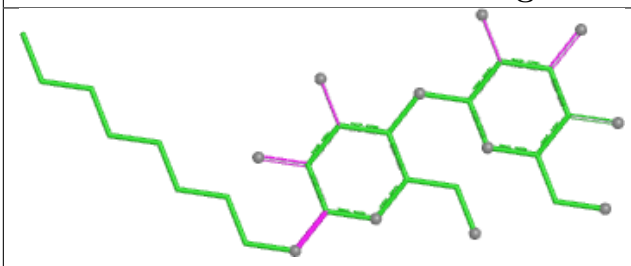


Torsions

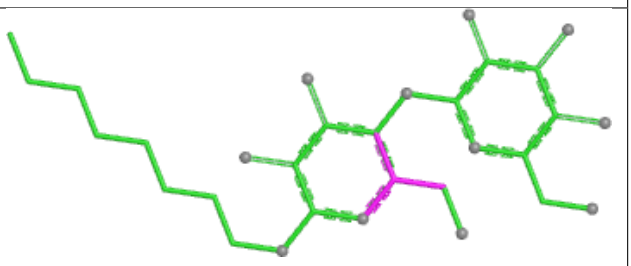


Rings

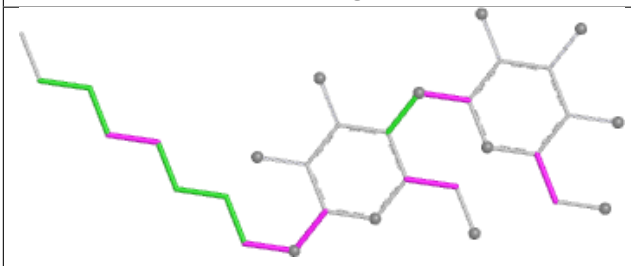
Ligand LMT a 6001



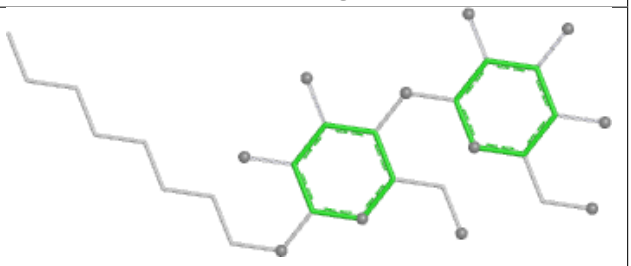
Bond lengths



Bond angles

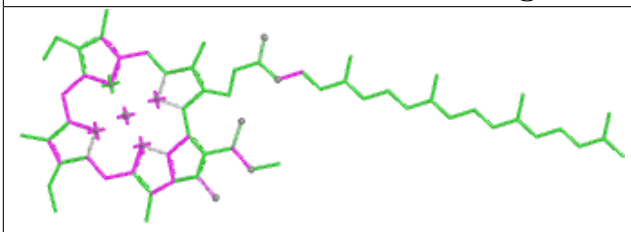


Torsions

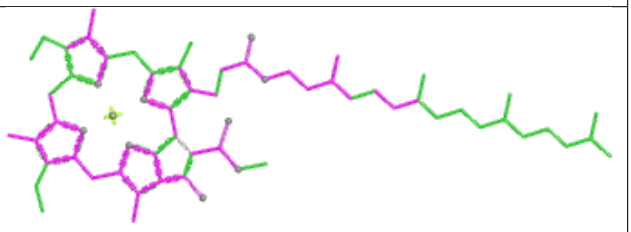


Rings

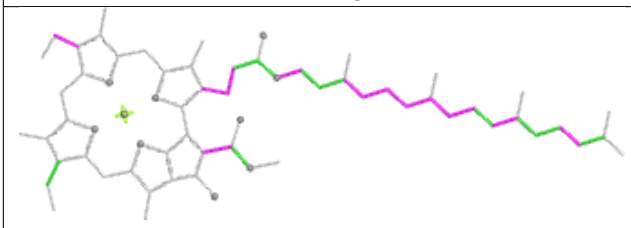
Ligand CLA b 1022



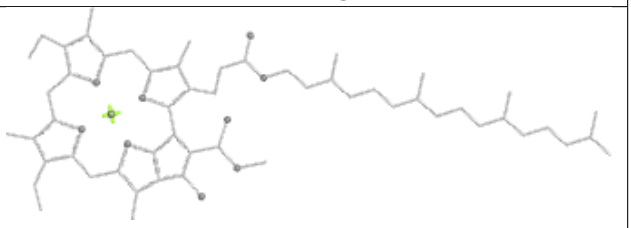
Bond lengths



Bond angles

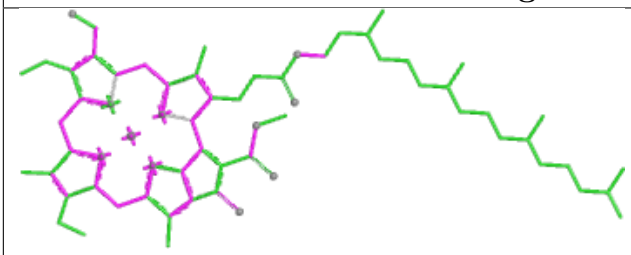


Torsions

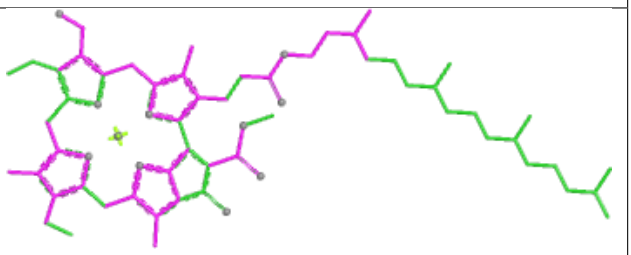


Rings

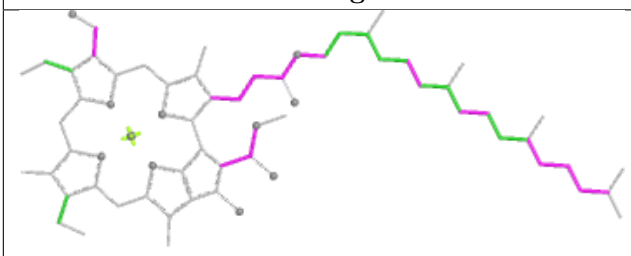
Ligand F6C H 1207



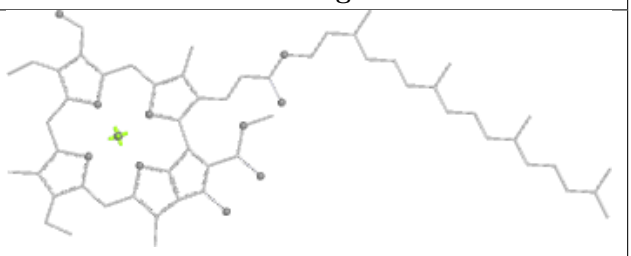
Bond lengths



Bond angles

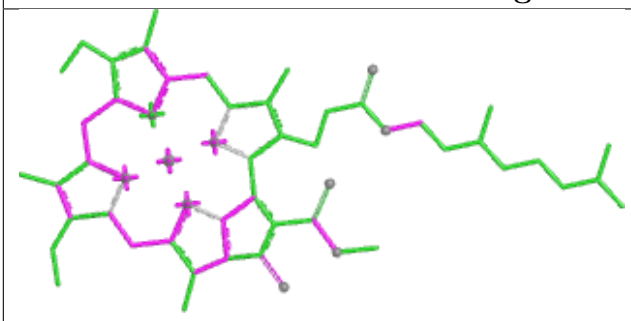


Torsions

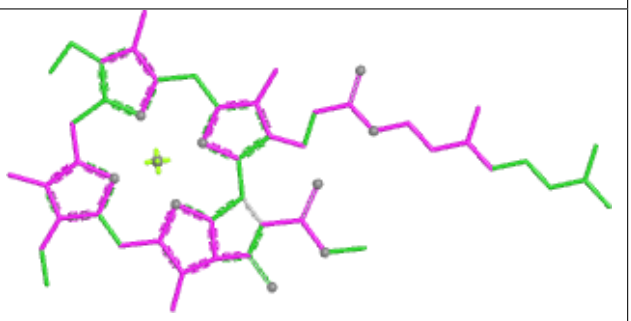


Rings

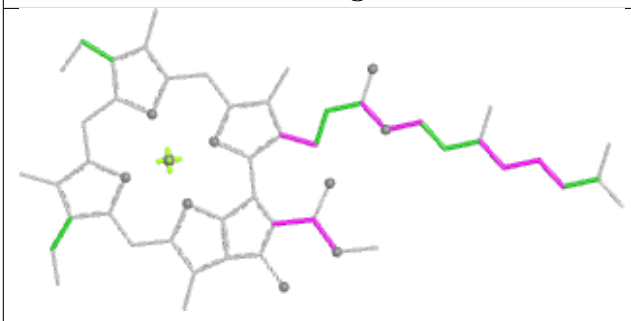
Ligand CLA G 1122



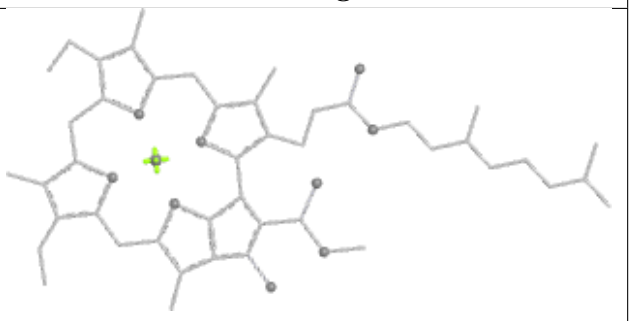
Bond lengths



Bond angles

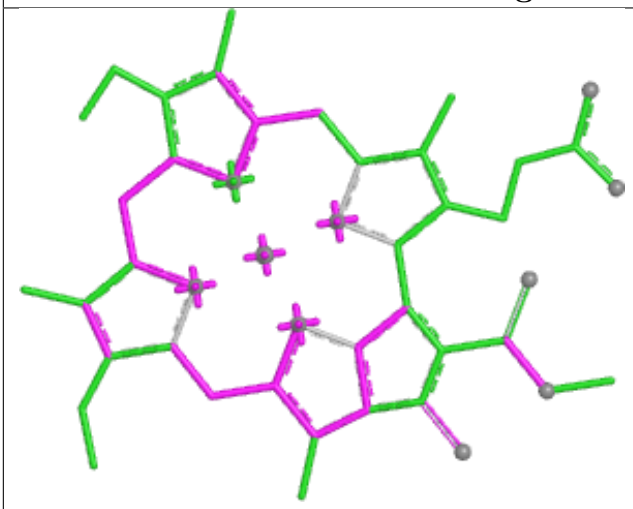


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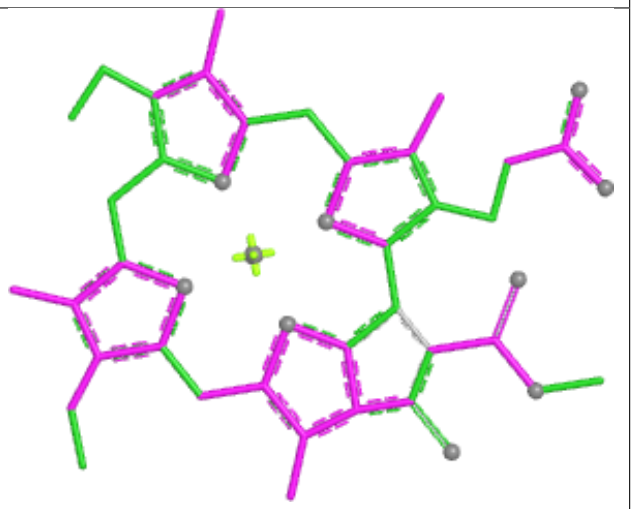


Rings

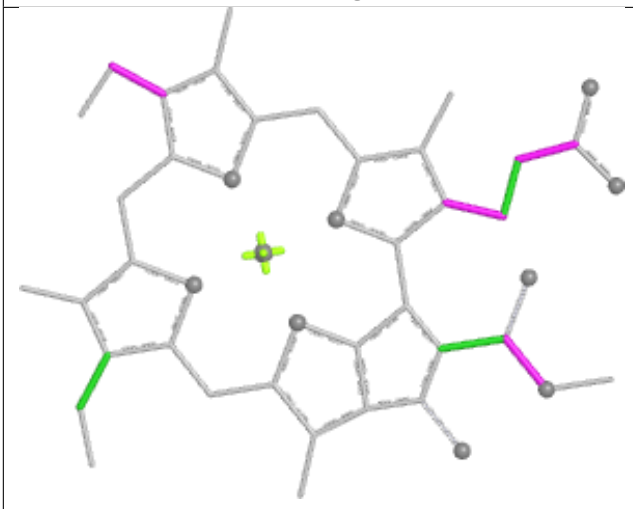
Ligand CLA B 1233



Bond lengths



Bond angles

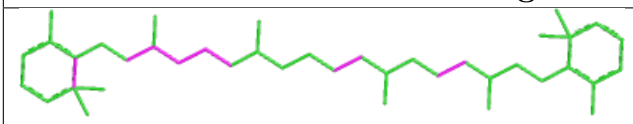


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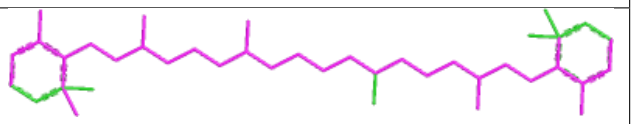


Rings

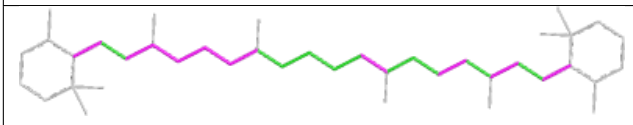
Ligand BCR a 4011



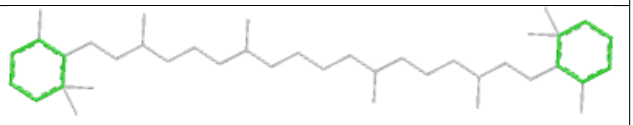
Bond lengths



Bond angles

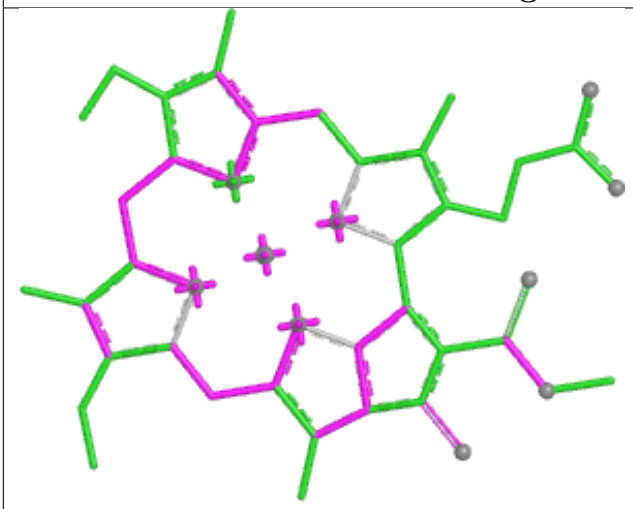


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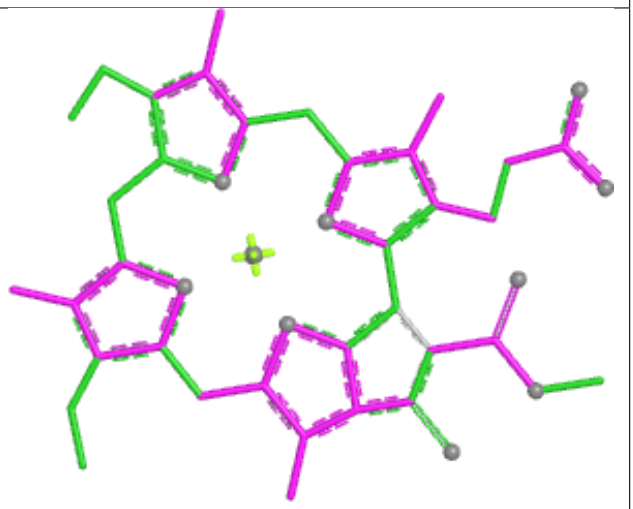


Rings

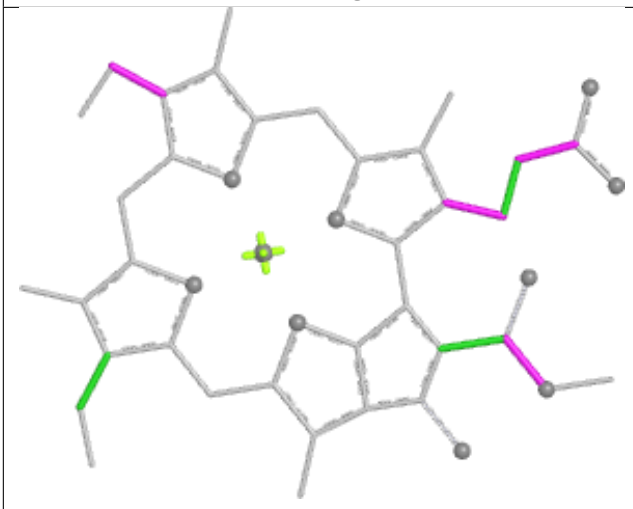
Ligand CLA a 1110



Bond lengths



Bond angles

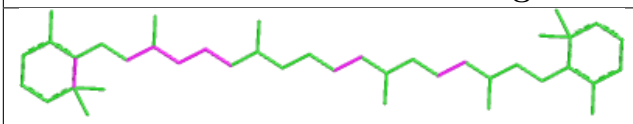


Torsions

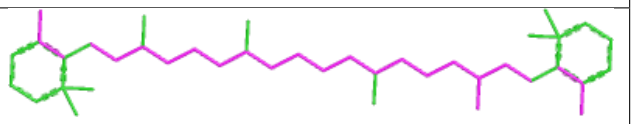


Rings

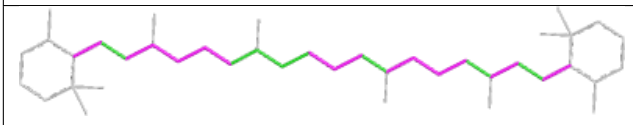
Ligand BCR V 4021



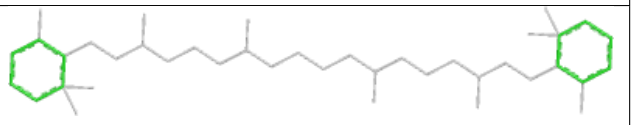
Bond lengths



Bond angles

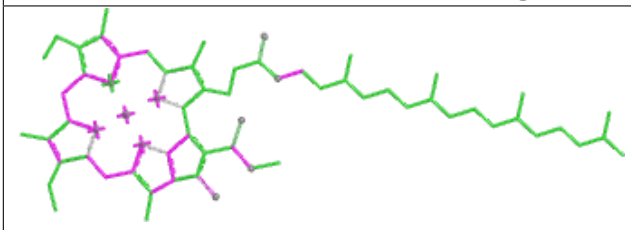


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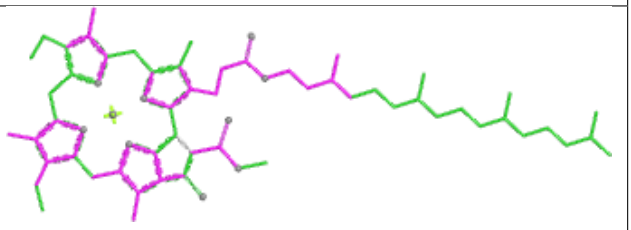


Rings

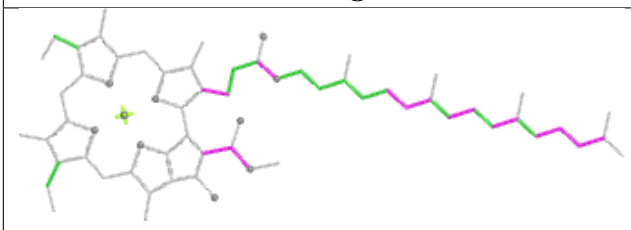
Ligand CLA H 1222



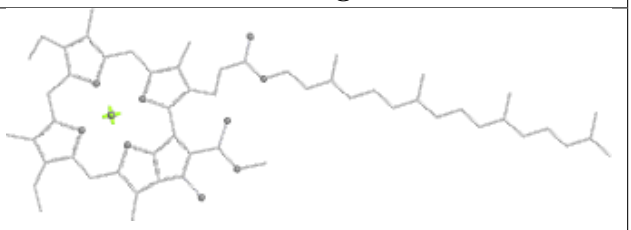
Bond lengths



Bond angles

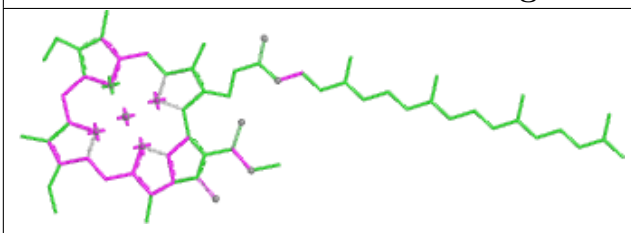


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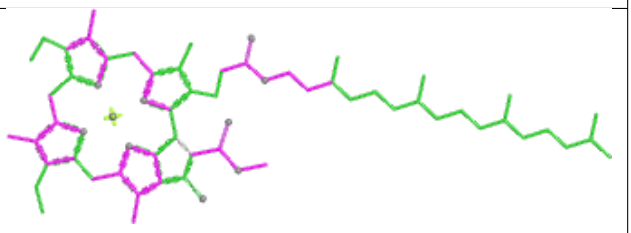


Rings

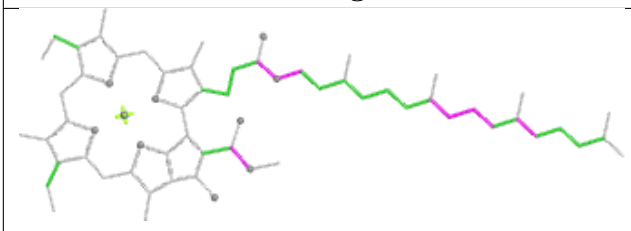
Ligand CLA a 1119



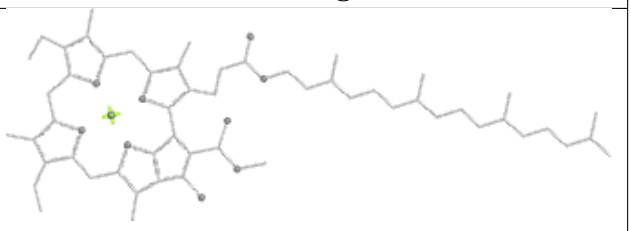
Bond lengths



Bond angles

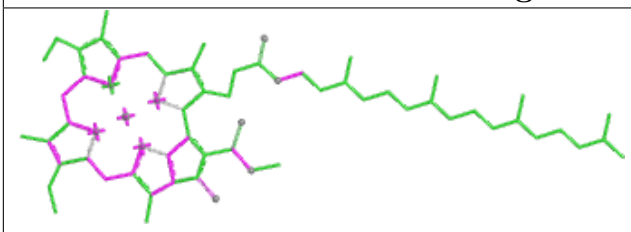


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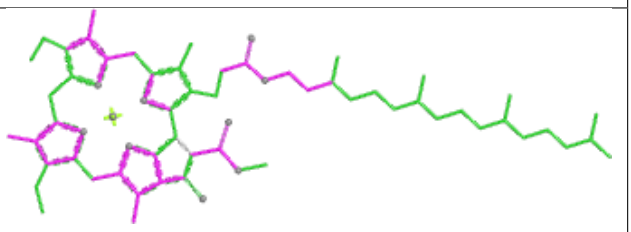


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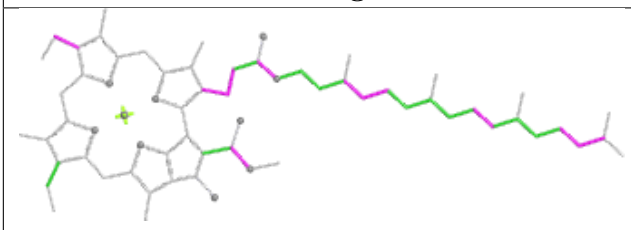
Ligand CLA B 1225



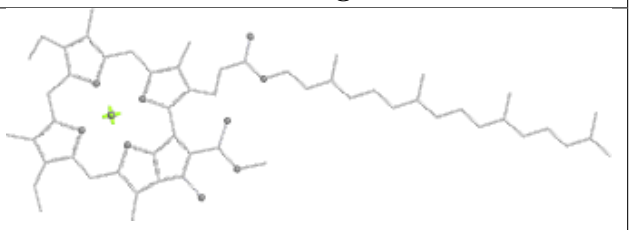
Bond lengths



Bond angles

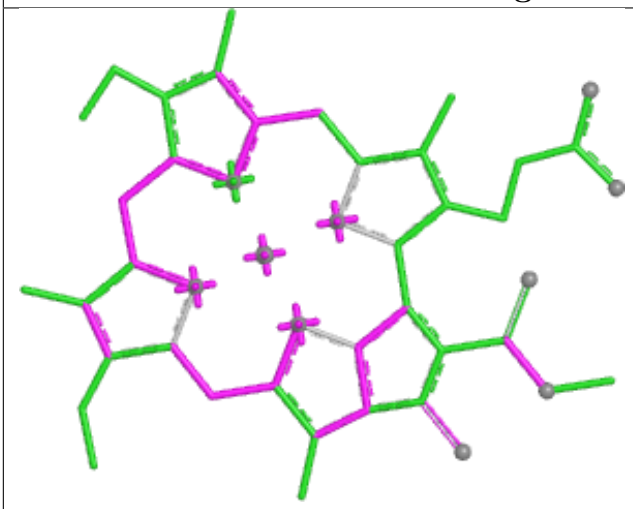


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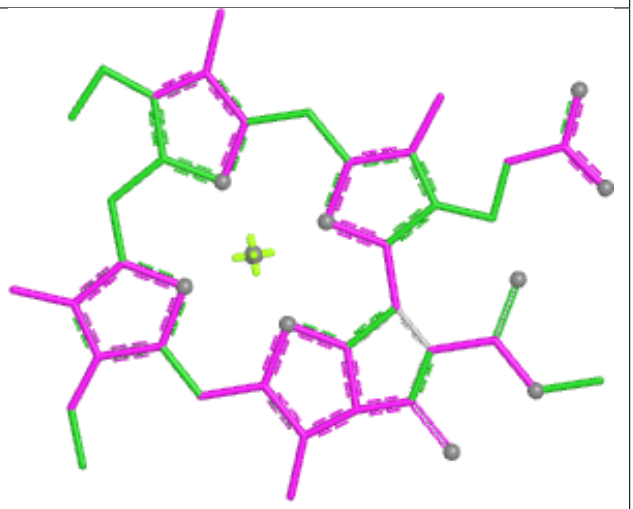


Rings

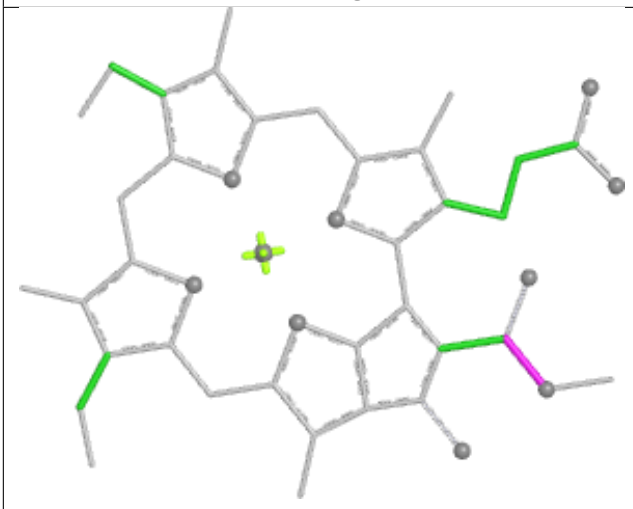
Ligand CLA H 1232



Bond lengths



Bond angles

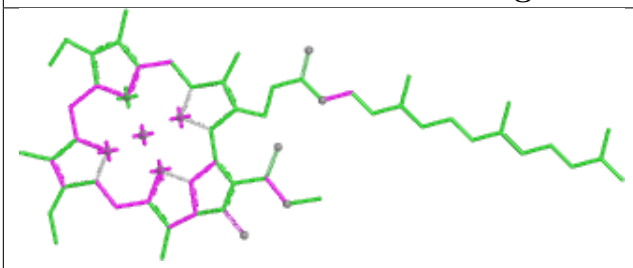


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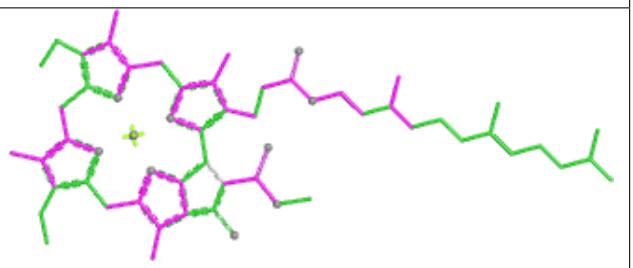


Rings

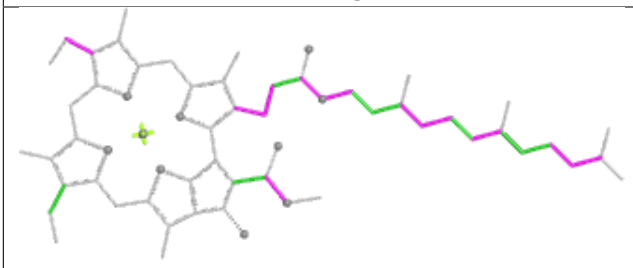
Ligand CLA H 1215



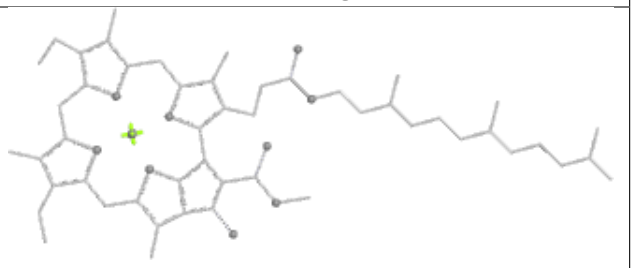
Bond lengths



Bond angles

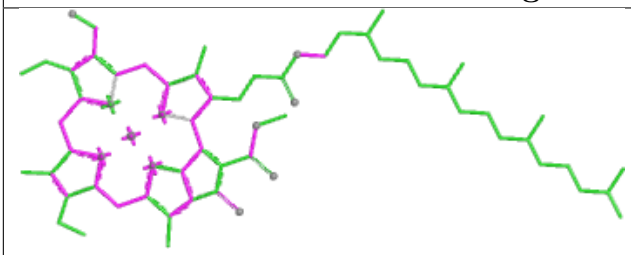


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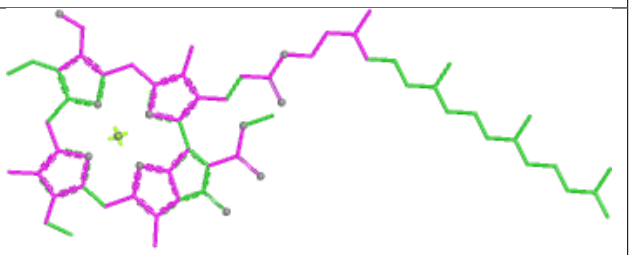


Rings

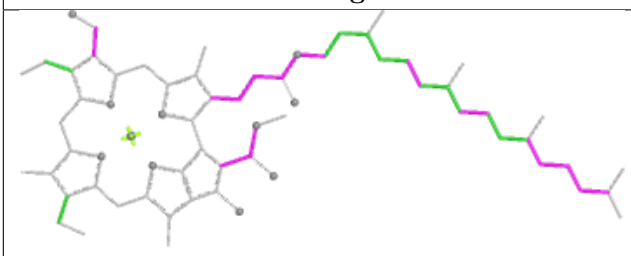
Ligand F6C b 1207



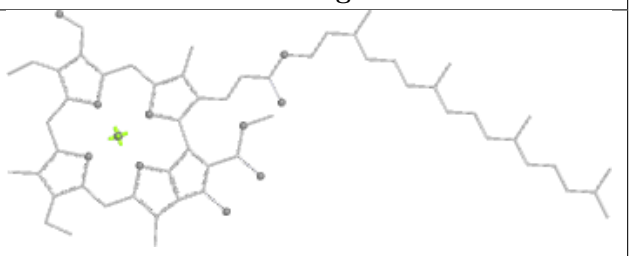
Bond lengths



Bond angles

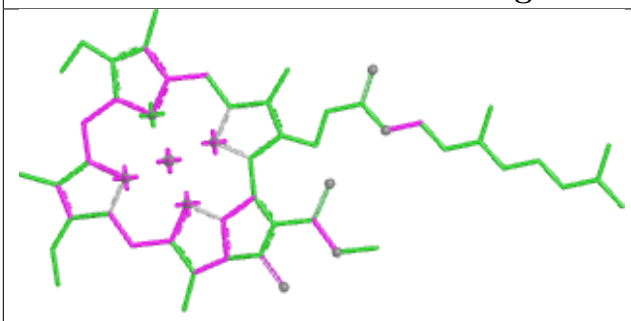


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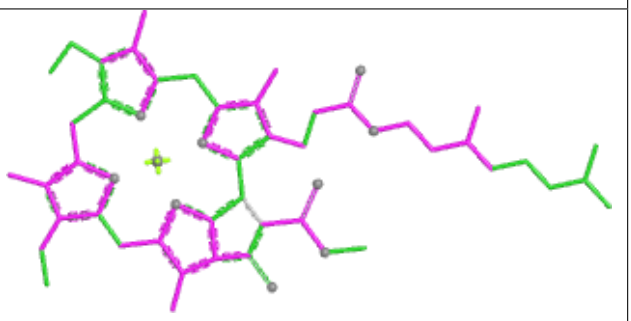


Rings

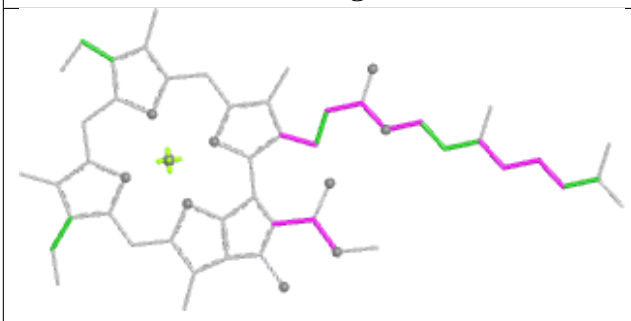
Ligand CLA A 1122



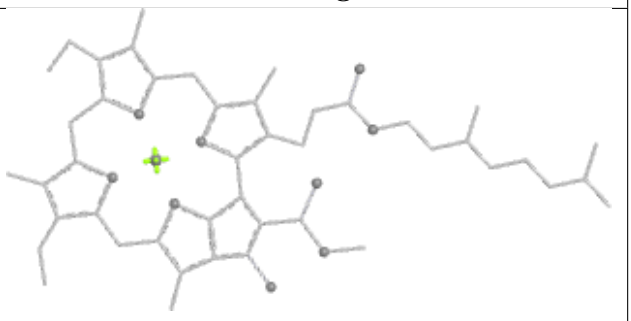
Bond lengths



Bond angles

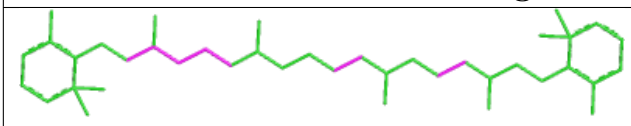


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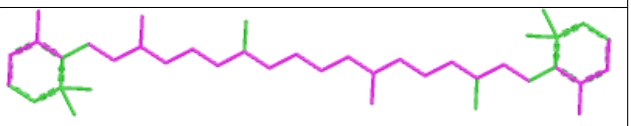


Rings

Ligand BCR B 4010



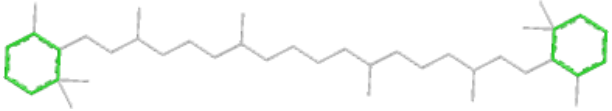
Bond lengths



Bond angles

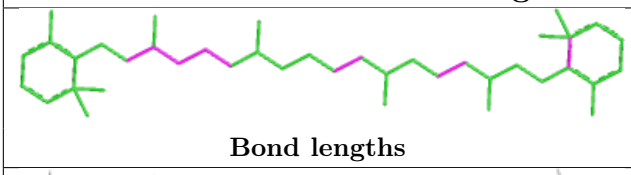


Torsions

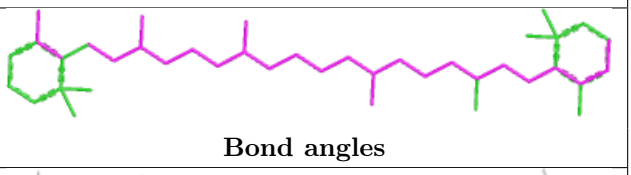


Rings

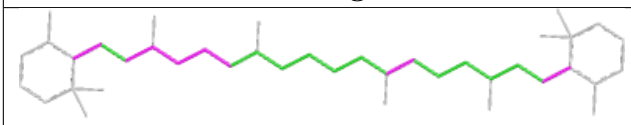
Ligand BCR G 4008



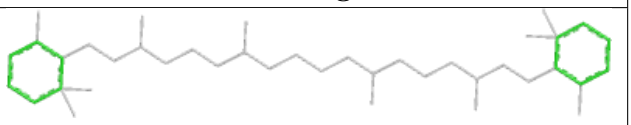
Bond lengths



Bond angles

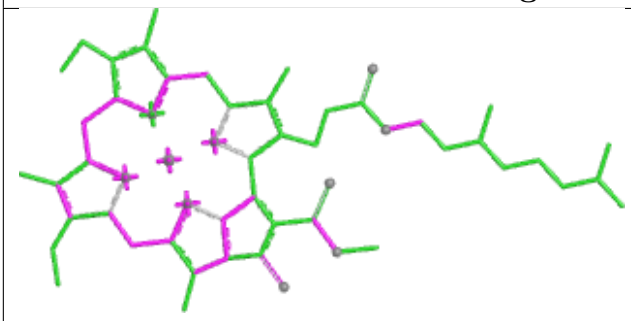


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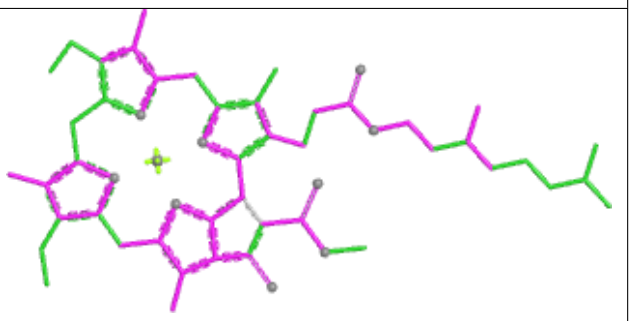


Rings

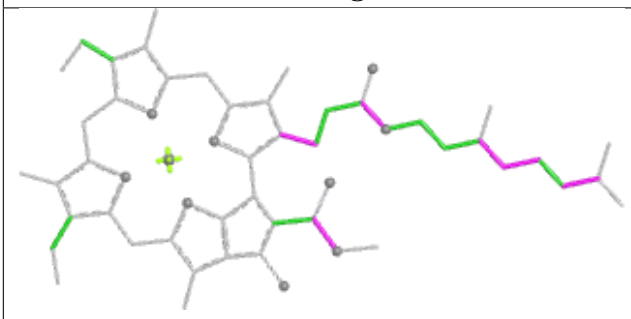
Ligand CLA a 1130



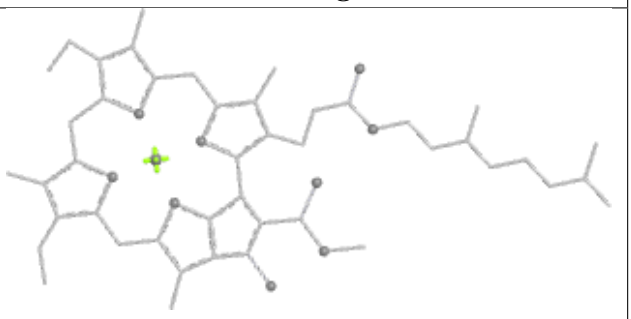
Bond lengths



Bond angles

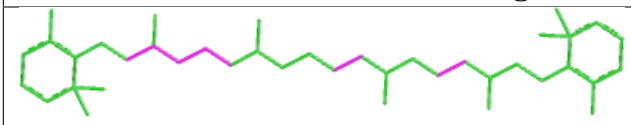


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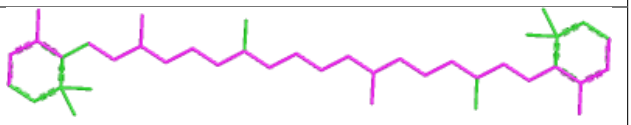


Rings

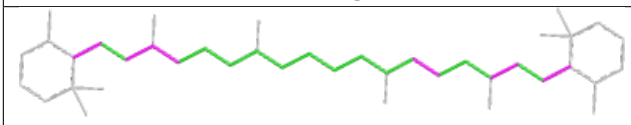
Ligand BCR H 4006



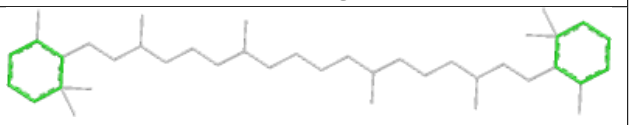
Bond lengths



Bond angles

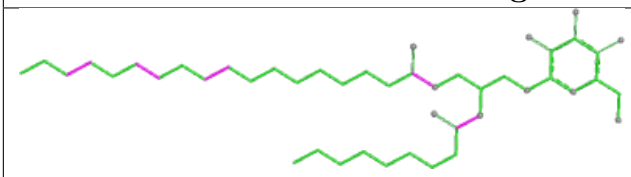


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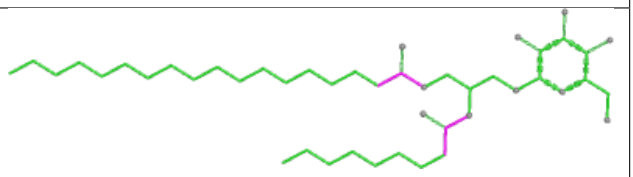


Rings

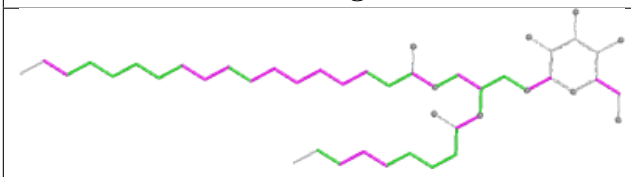
Ligand LMG A 5005



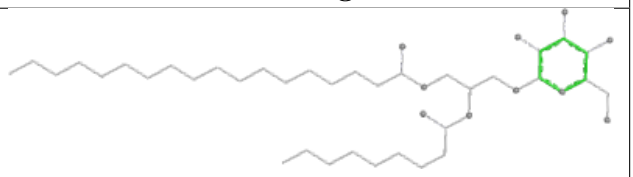
Bond lengths



Bond angles

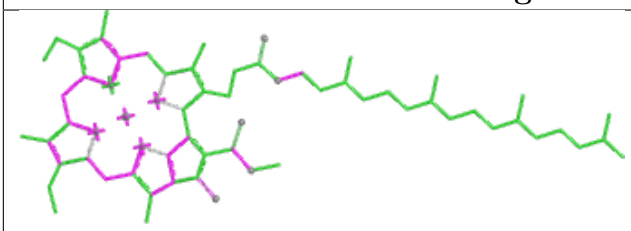


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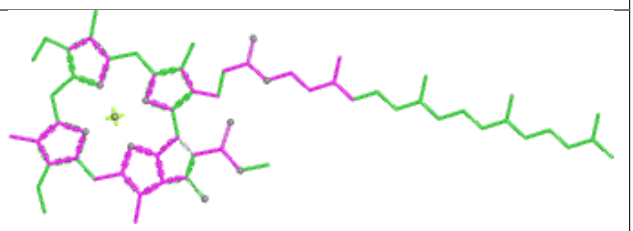


Rings

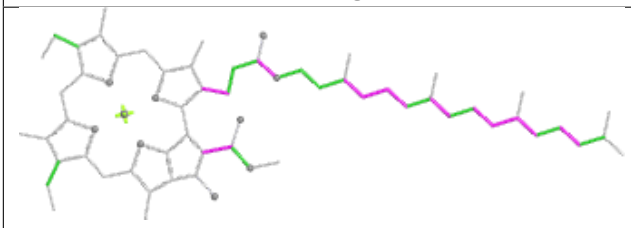
Ligand CLA H 1203



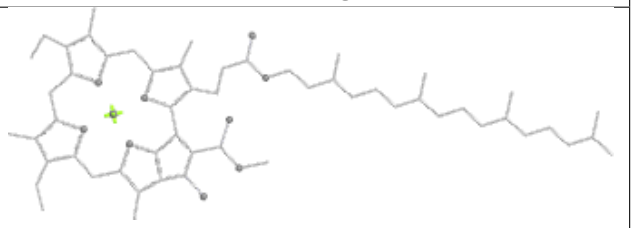
Bond lengths



Bond angles

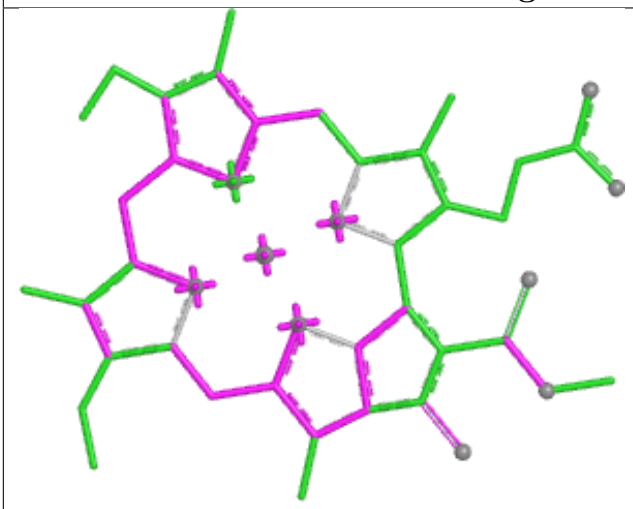


Torsions

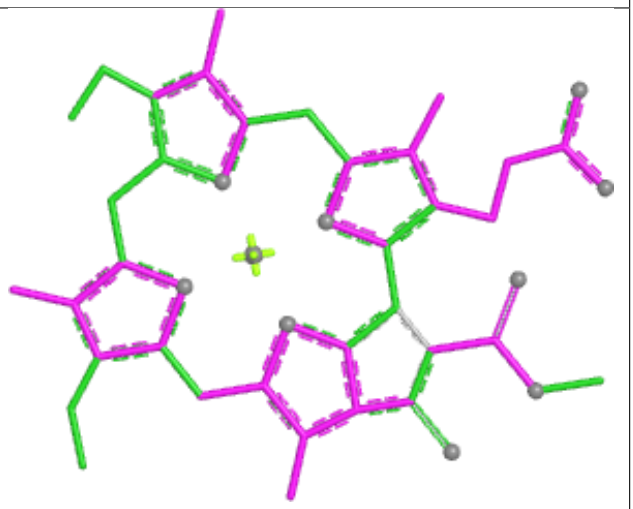


Rings

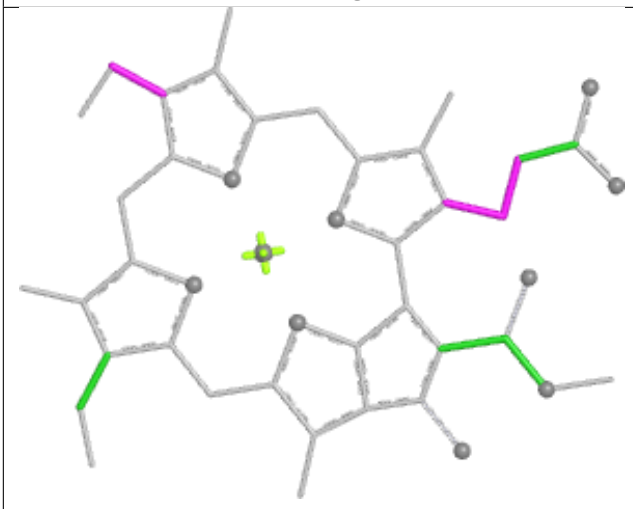
Ligand CLA b 1209



Bond lengths



Bond angles

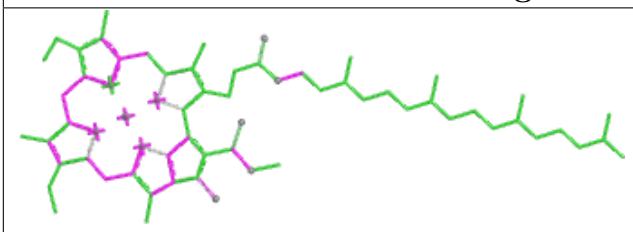


Torsions

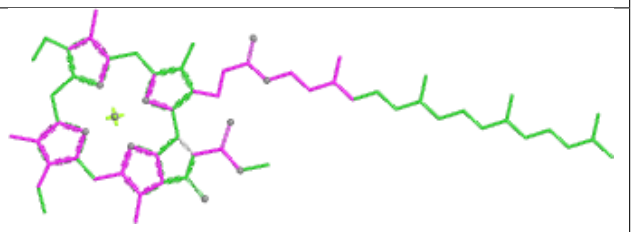


Rings

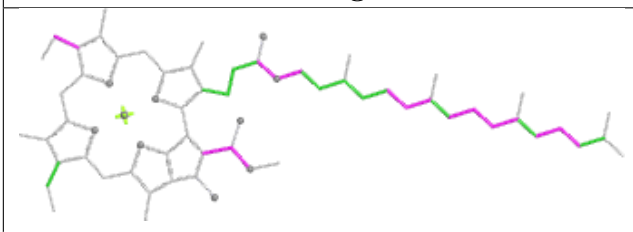
Ligand CLA H 1234



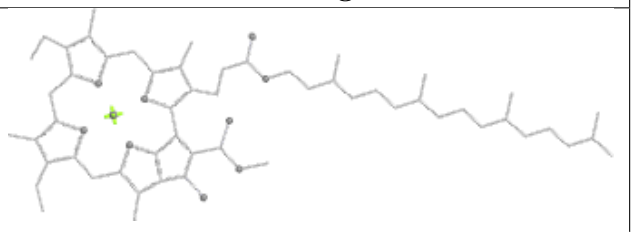
Bond lengths



Bond angles

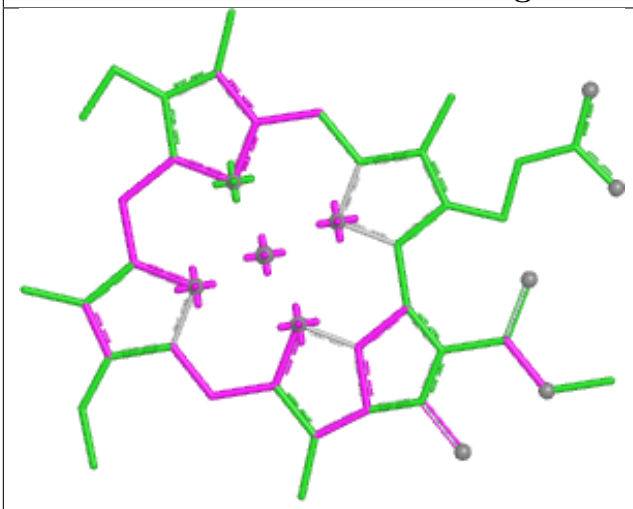


Torsions

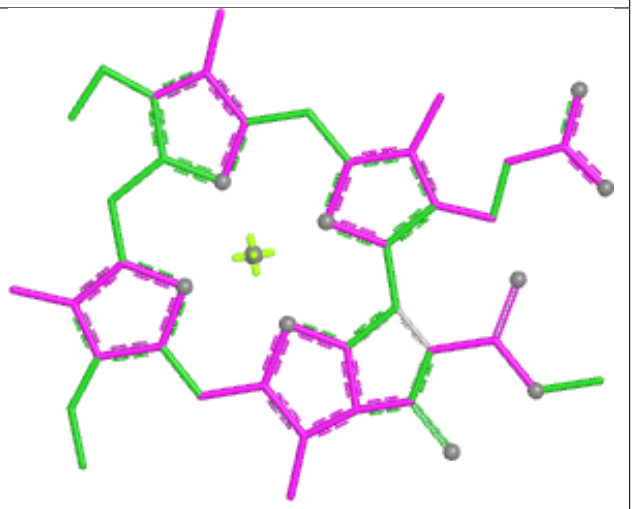


Rings

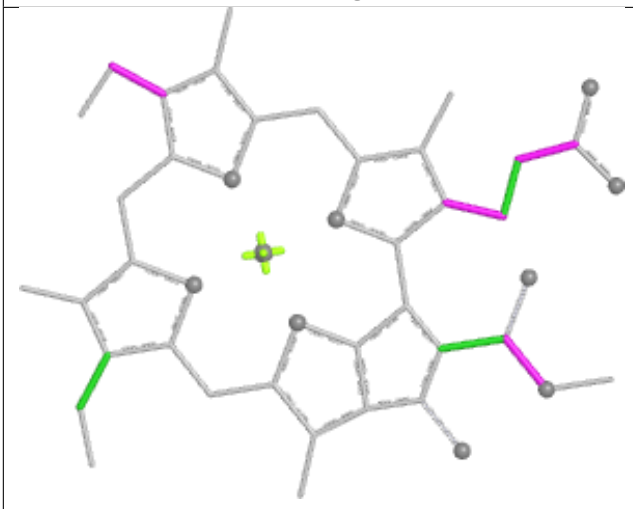
Ligand CLA G 1110



Bond lengths



Bond angles

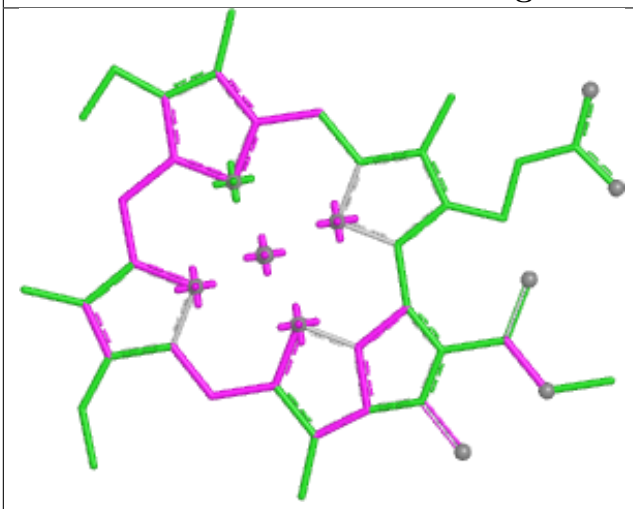


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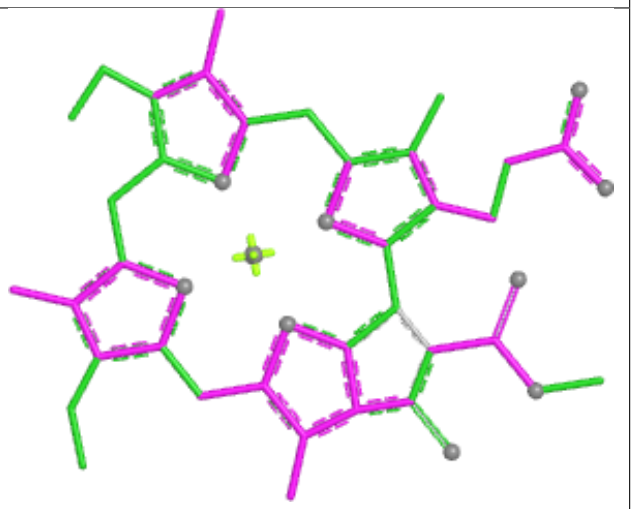


Rings

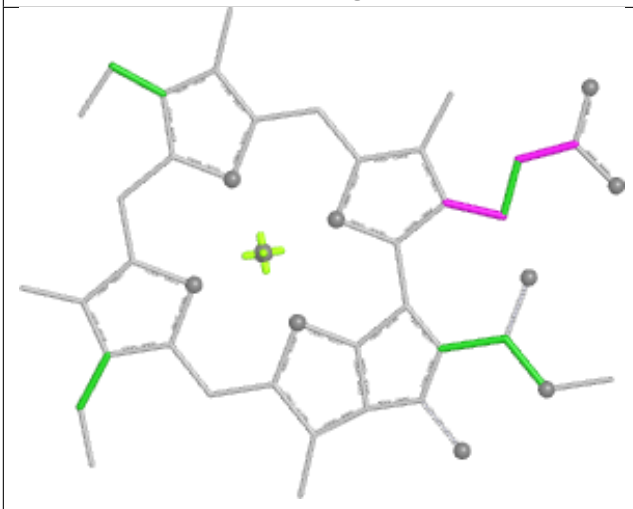
Ligand CLA B 1236



Bond lengths



Bond angles

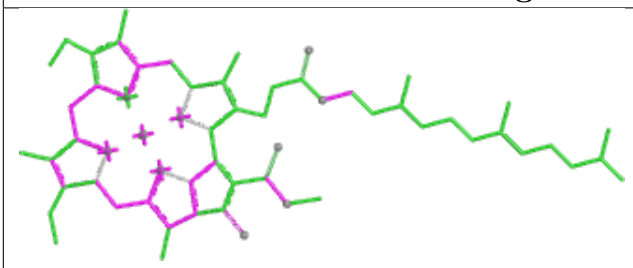


Torsions

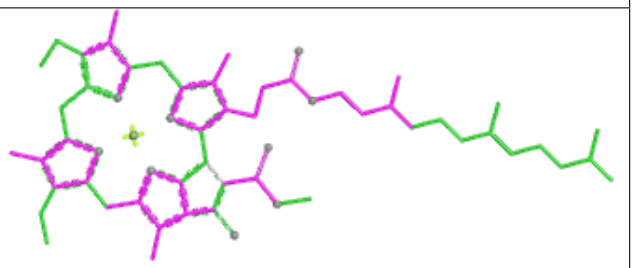


Rings

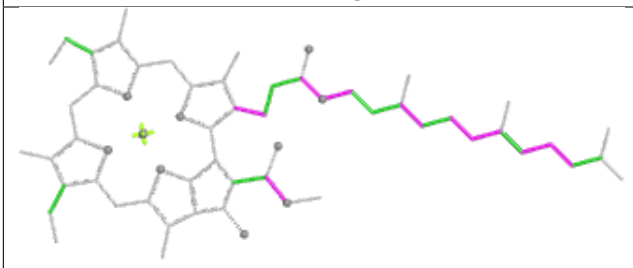
Ligand CLA B 1229



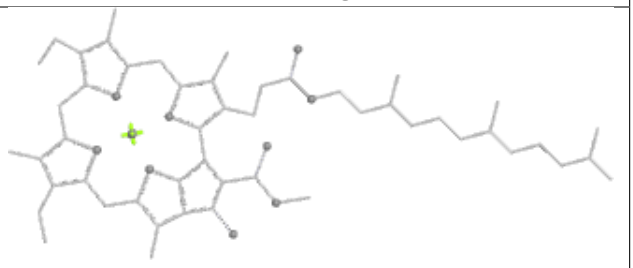
Bond lengths



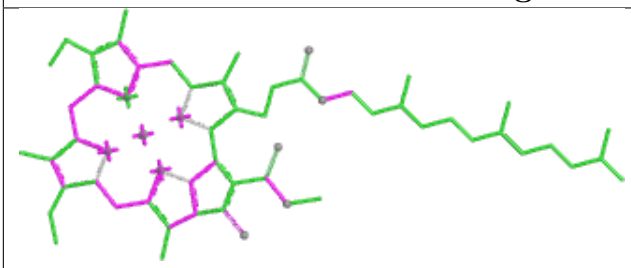
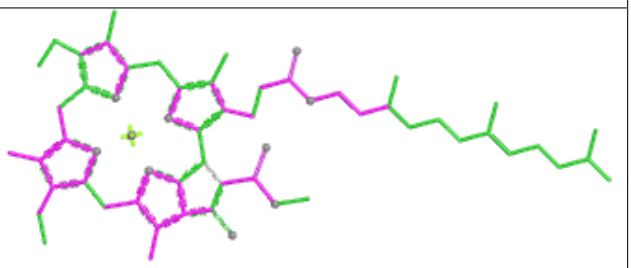
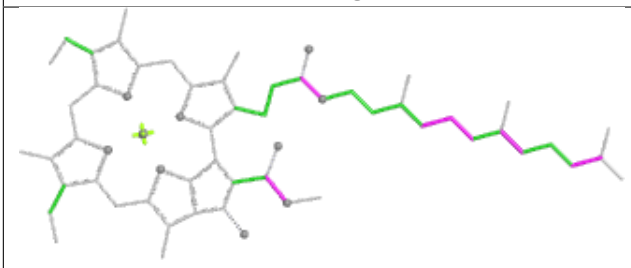
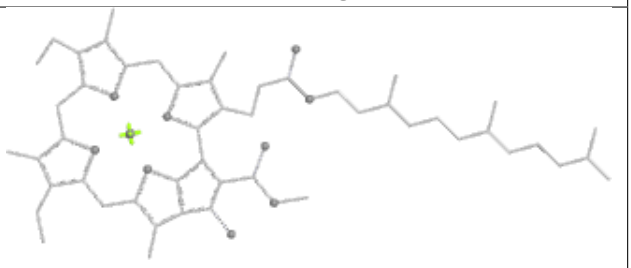
Bond angles

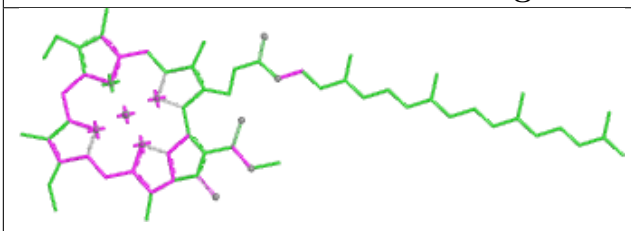
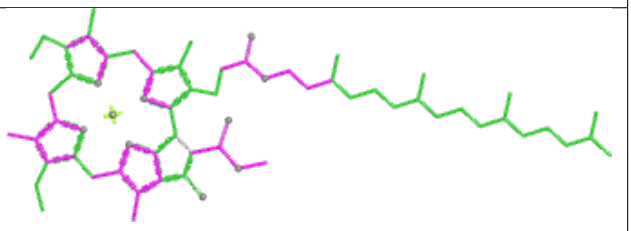
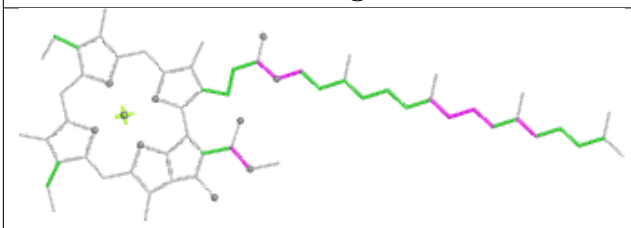
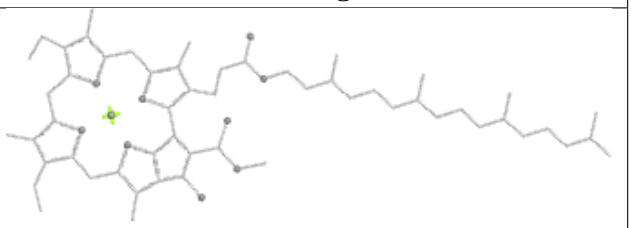


Torsions

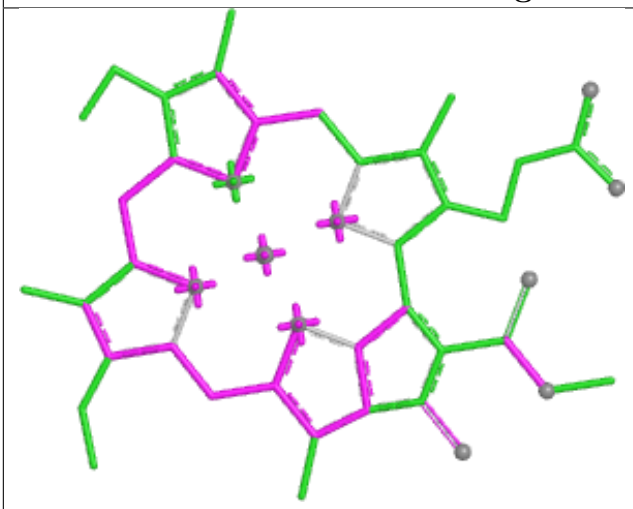


Rings

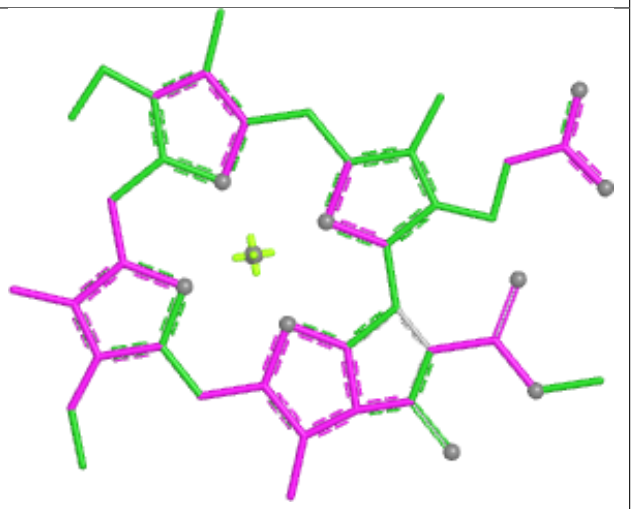
Ligand CLA A 1133	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1119	
 Bond lengths	 Bond angles
 Torsions	 Rings

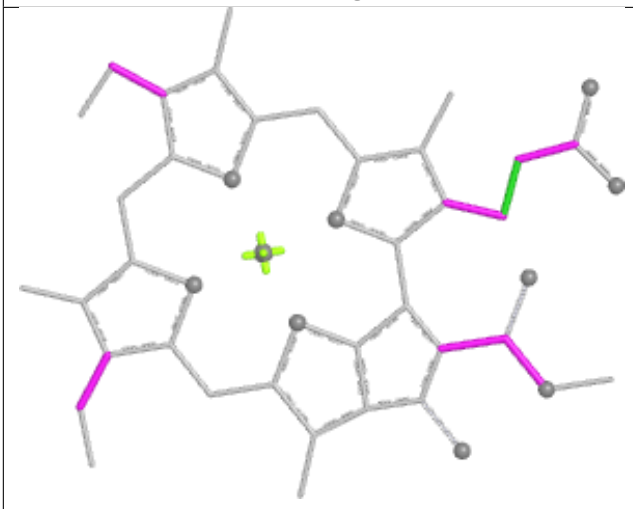
Ligand CLA A 1114



Bond lengths



Bond angles

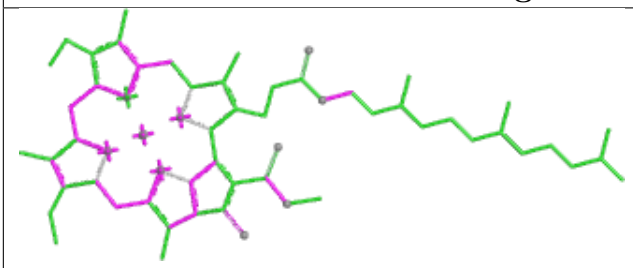


Torsions

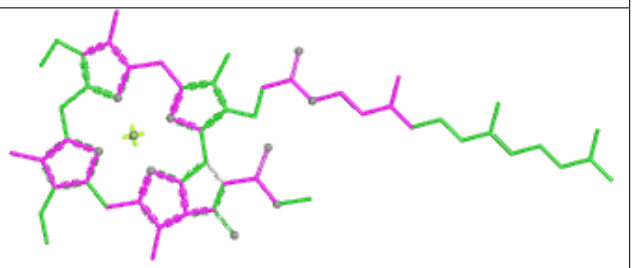


Rings

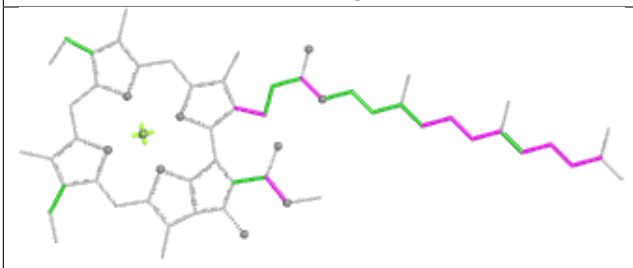
Ligand CLA A 1102



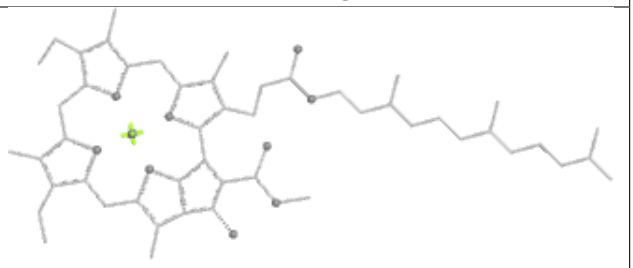
Bond lengths



Bond angles

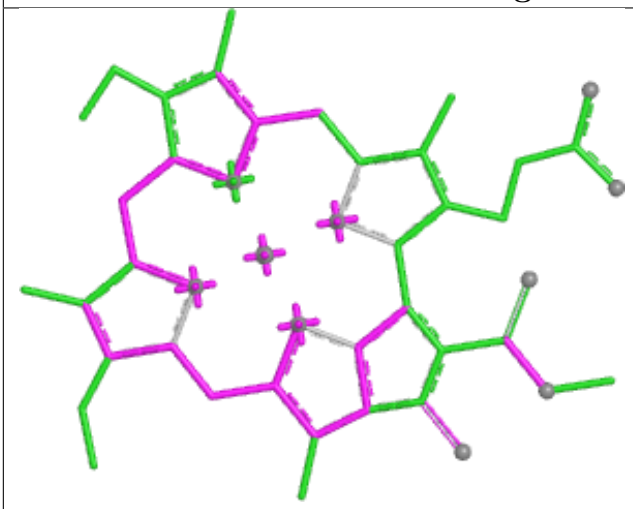


Torsions

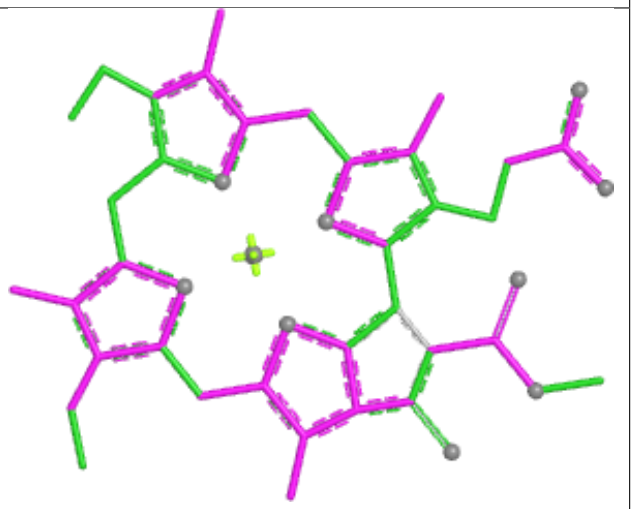


Rings

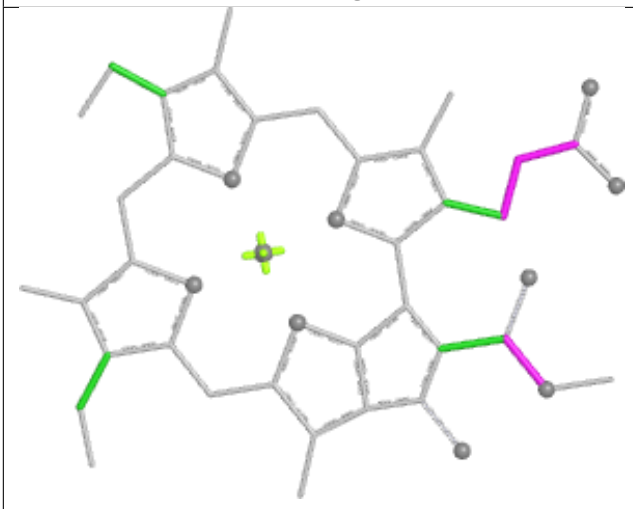
Ligand CLA G 1134



Bond lengths



Bond angles

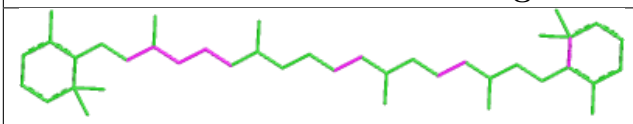


Torsions

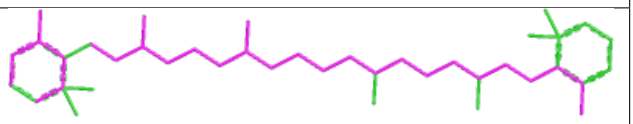


Rings

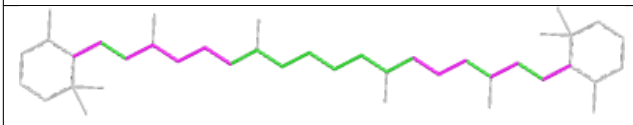
Ligand BCR B 4017



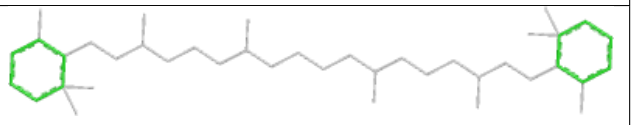
Bond lengths



Bond angles

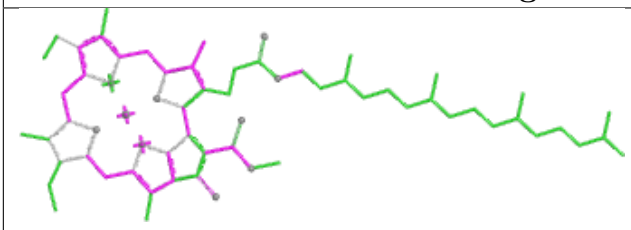


Torsions

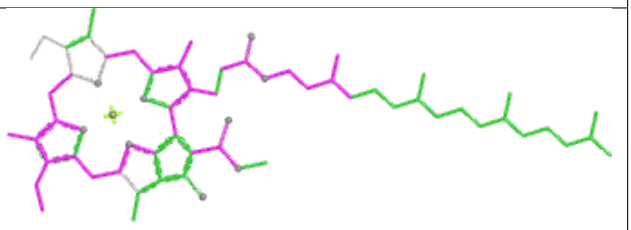


Rings

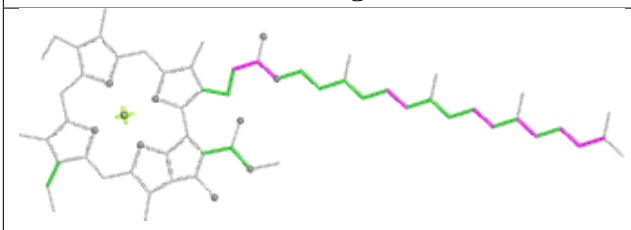
Ligand CL0 A 1011



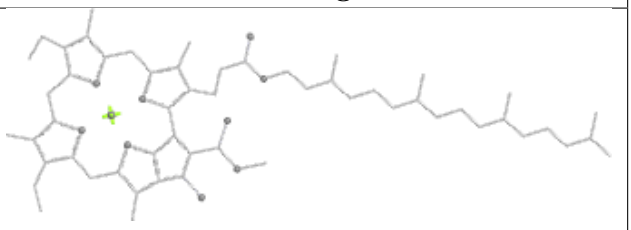
Bond lengths



Bond angles

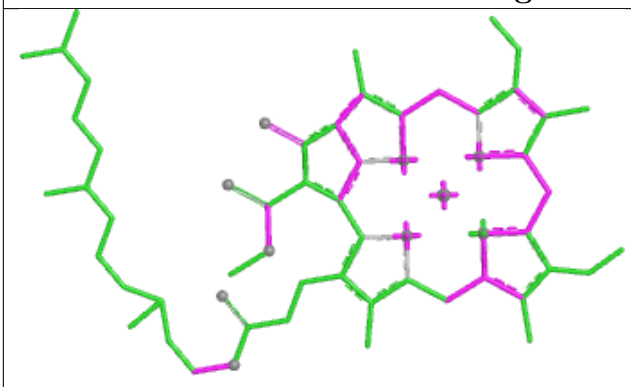


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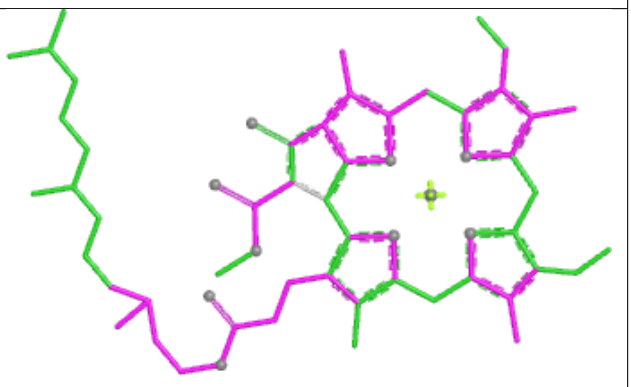


Rings

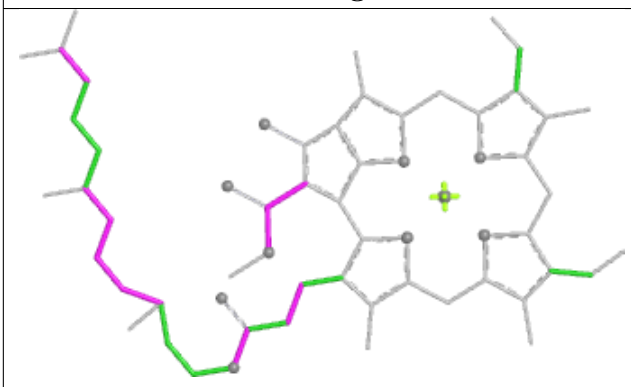
Ligand CLA A 1111



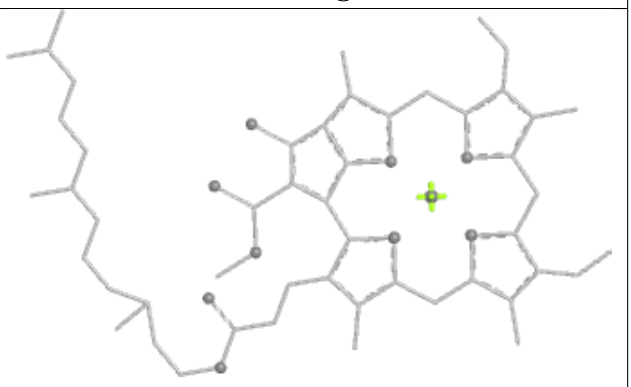
Bond lengths



Bond angles

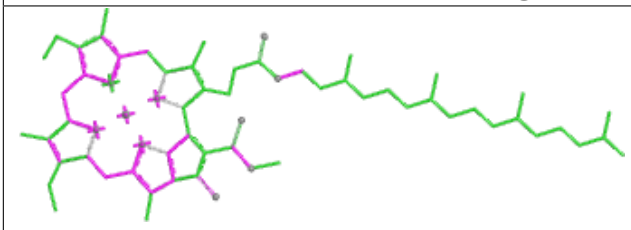


Torsions

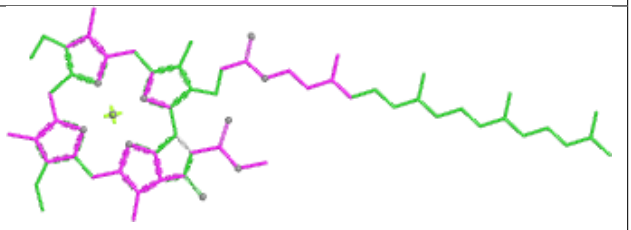


Rings

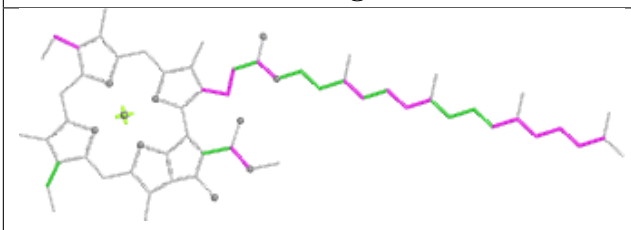
Ligand CLA B 1216



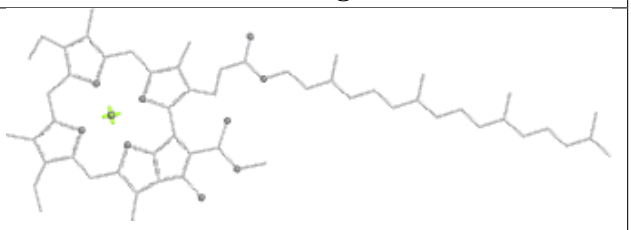
Bond lengths



Bond angles

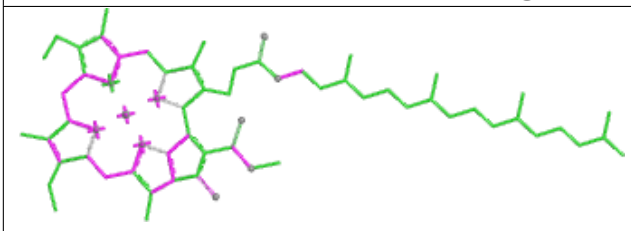


Torsions

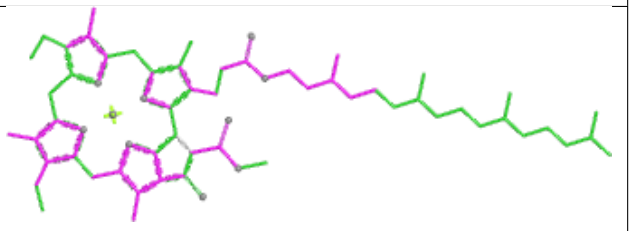


Rings

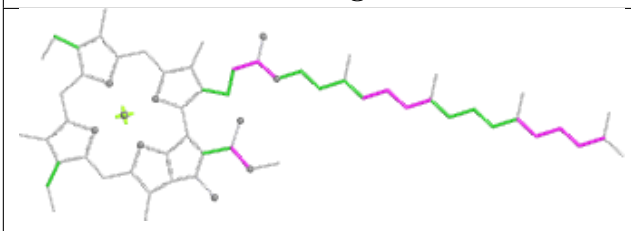
Ligand CLA b 1208



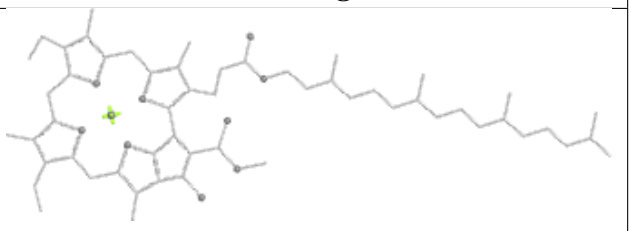
Bond lengths



Bond angles

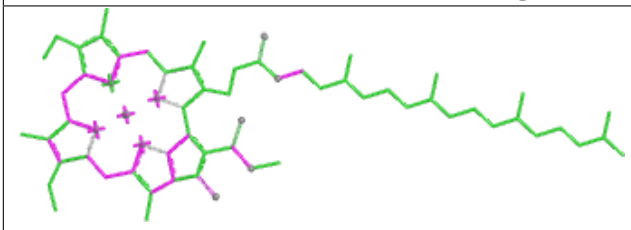


Torsions

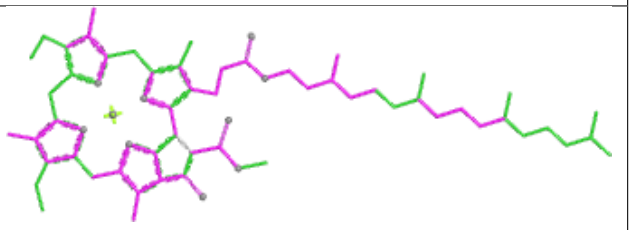


Rings

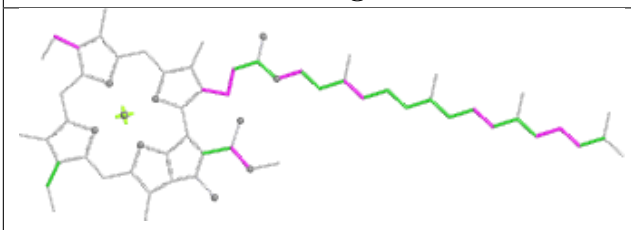
Ligand CLA G 1012



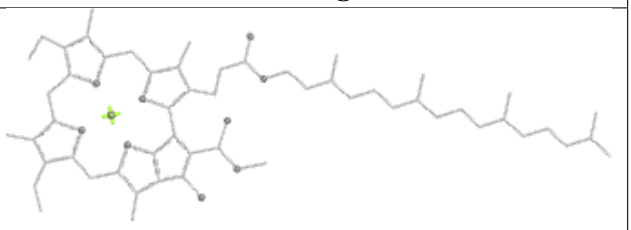
Bond lengths



Bond angles

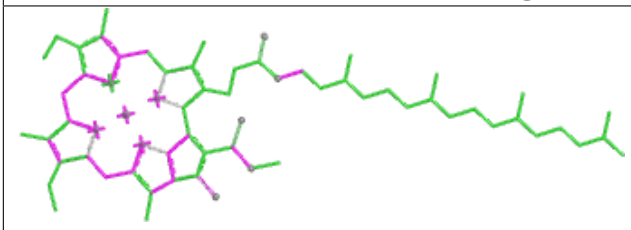


Torsions

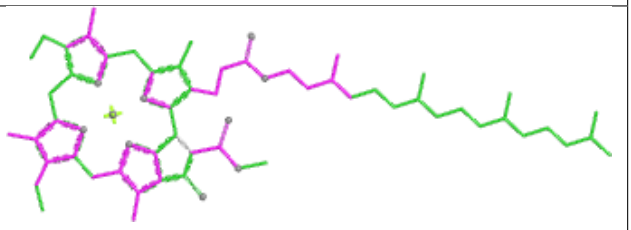


Rings

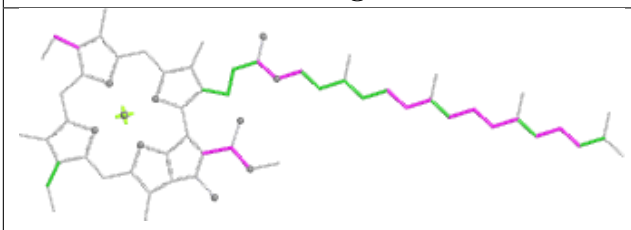
Ligand CLA b 1234



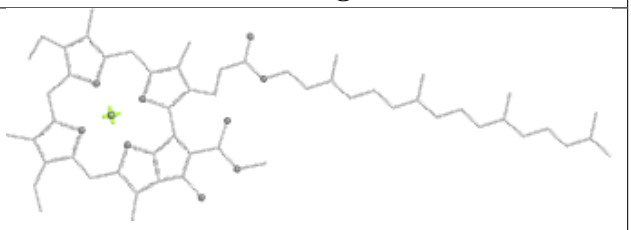
Bond lengths



Bond angles

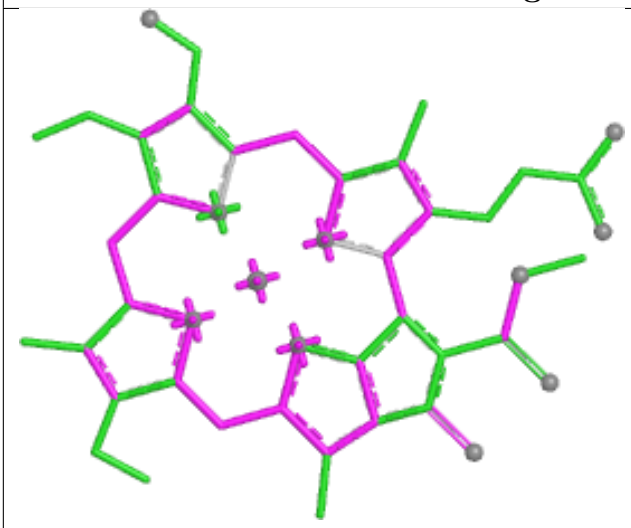


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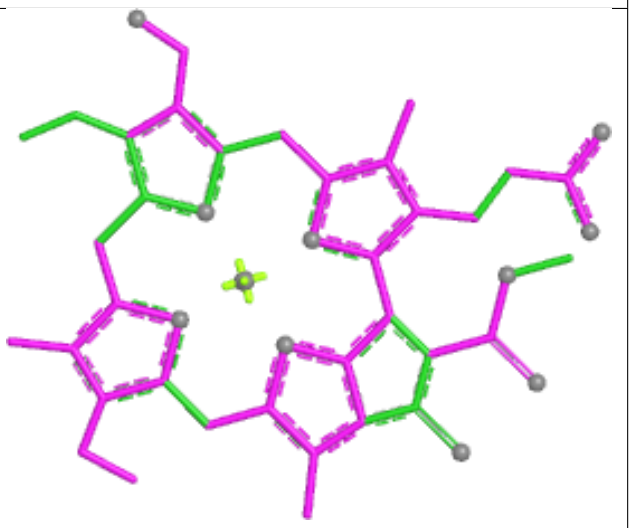


Rings

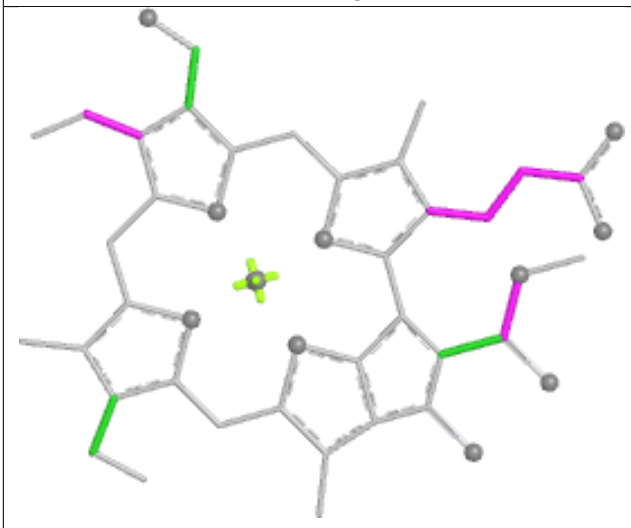
Ligand F6C a 1121



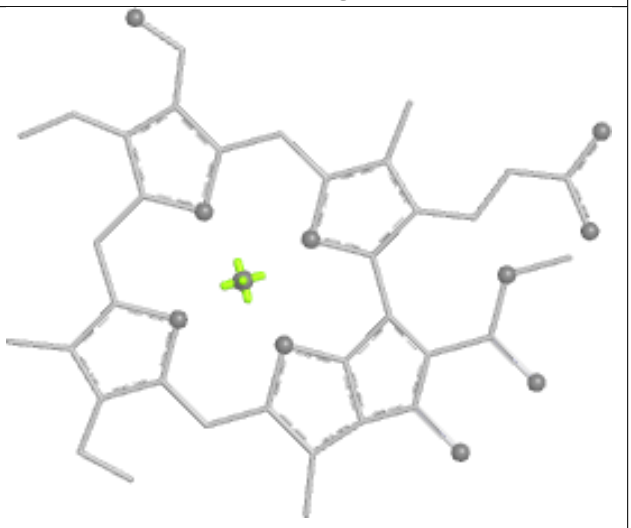
Bond lengths



Bond angles

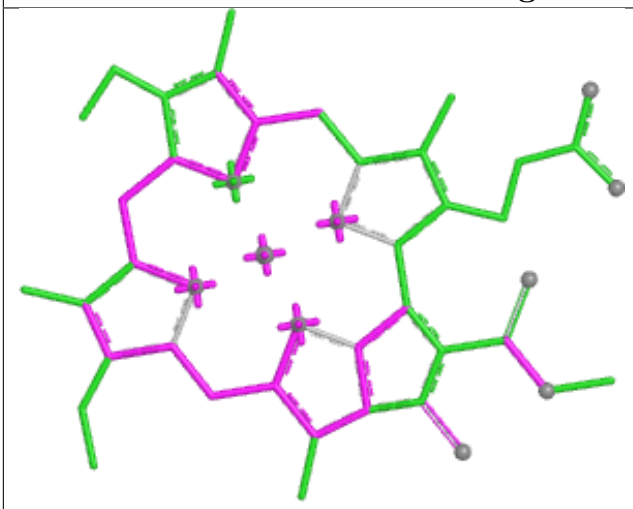


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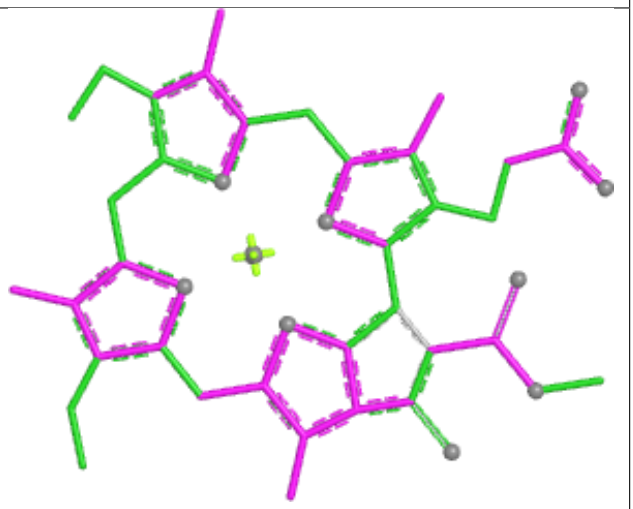


Rings

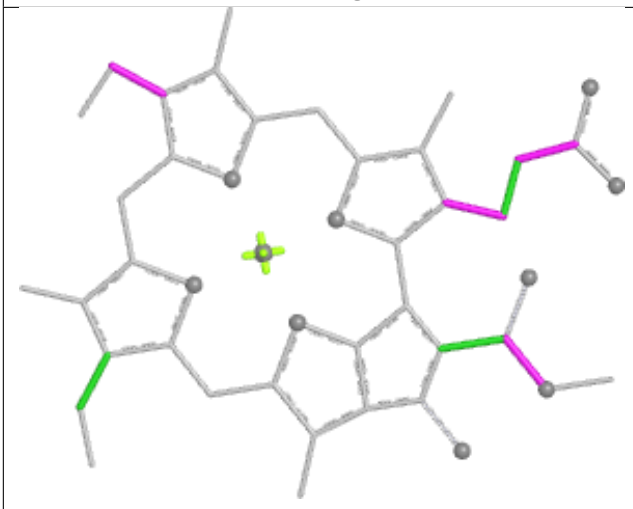
Ligand CLA b 1233



Bond lengths



Bond angles

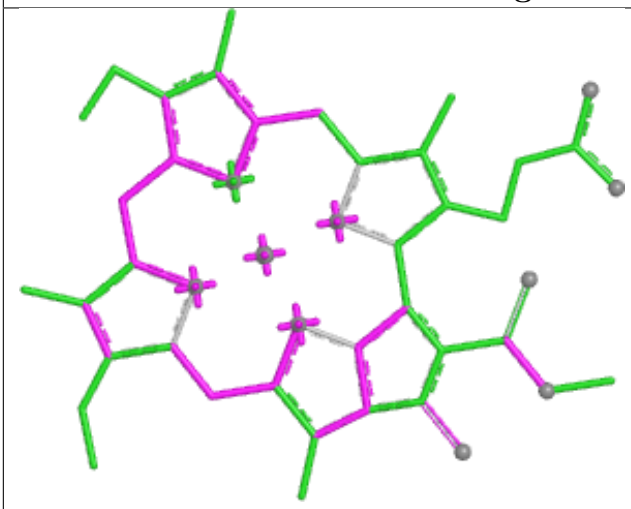


Torsions

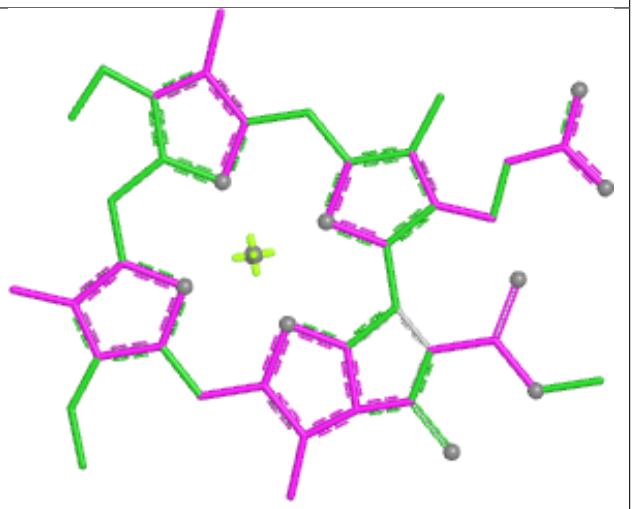


Rings

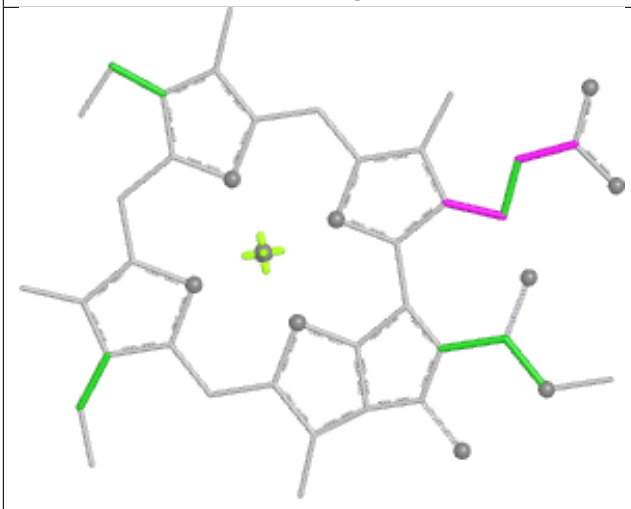
Ligand CLA H 1236



Bond lengths



Bond angles

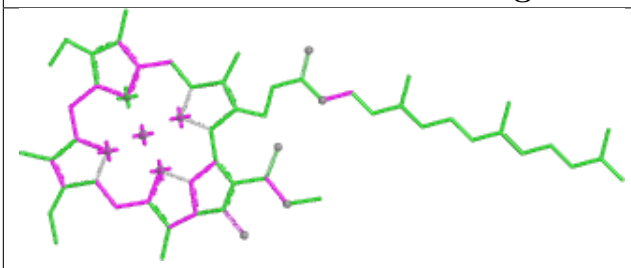


Torsions

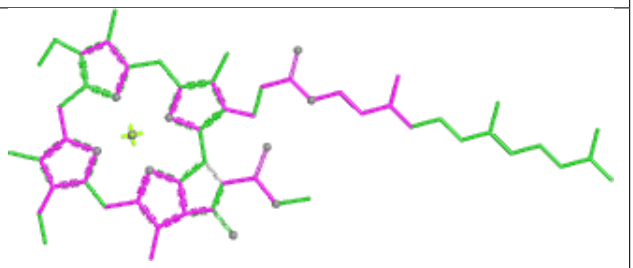


Rings

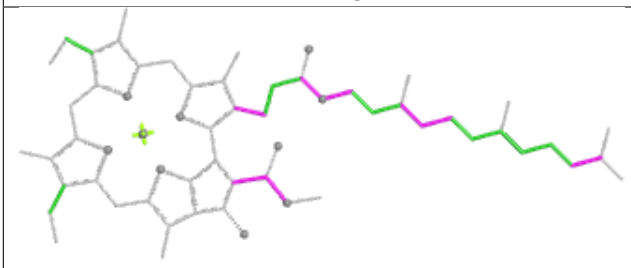
Ligand CLA G 1103



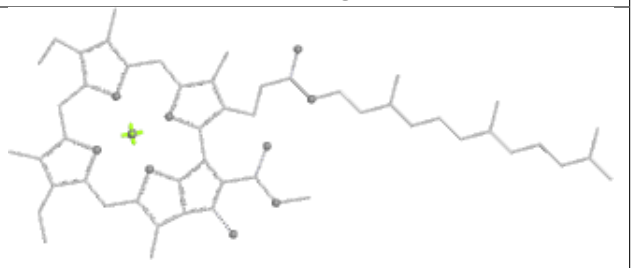
Bond lengths



Bond angles

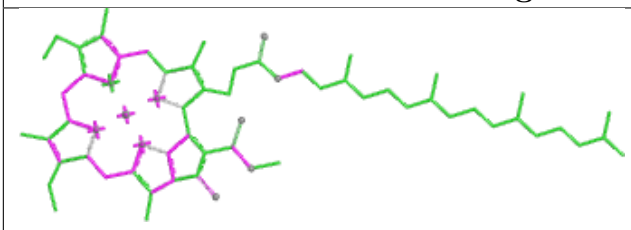


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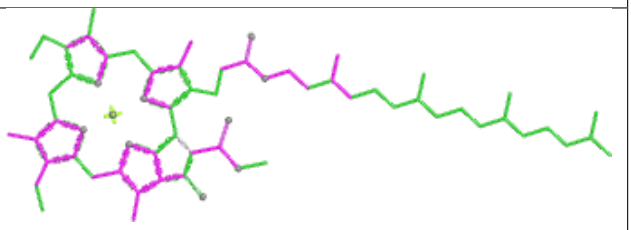


Rings

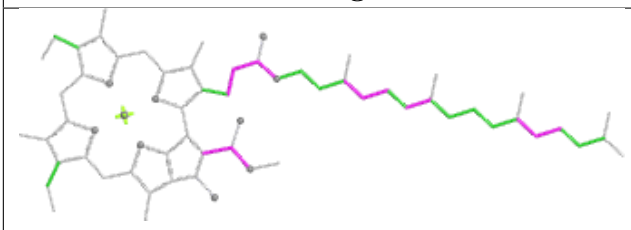
Ligand CLA B 1213



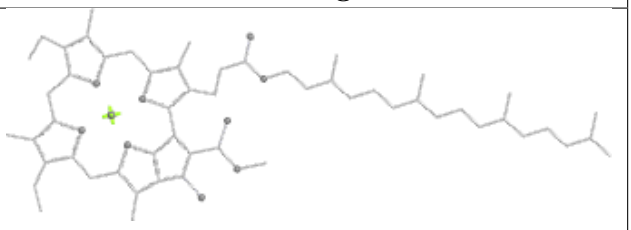
Bond lengths



Bond angles

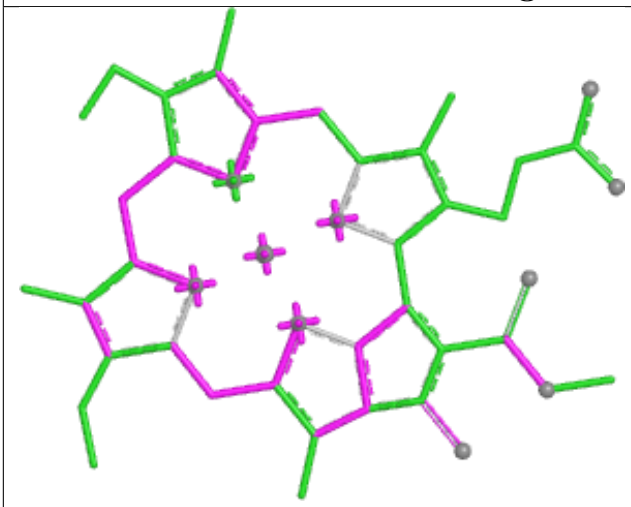


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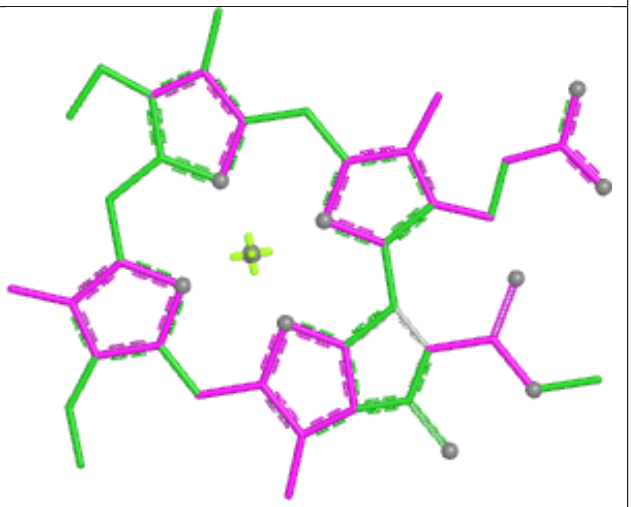


Rings

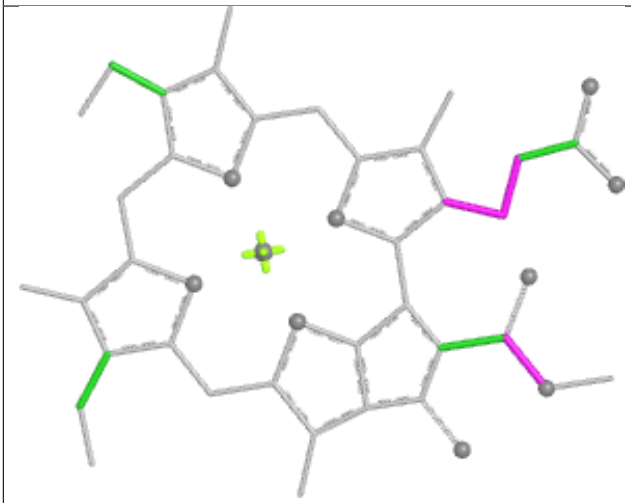
Ligand CLA b 1212



Bond lengths



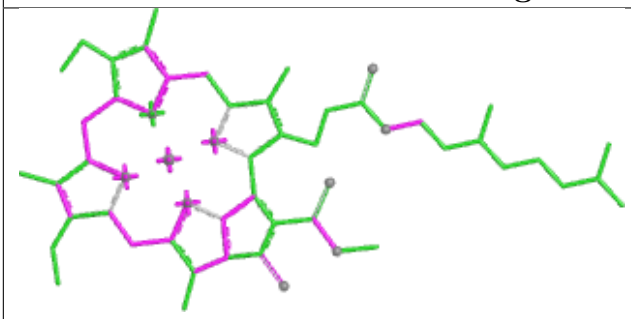
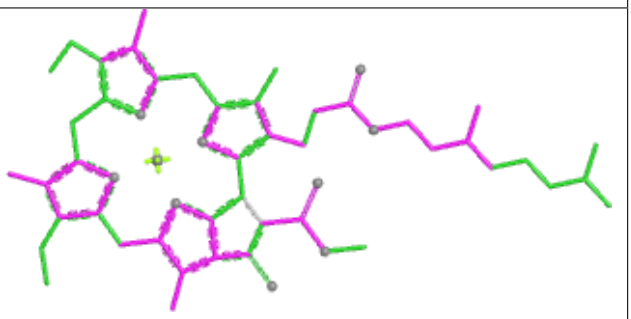
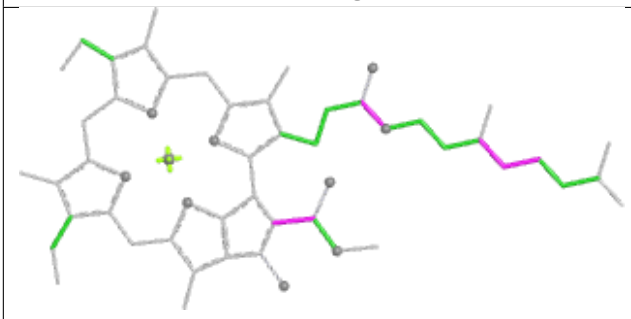
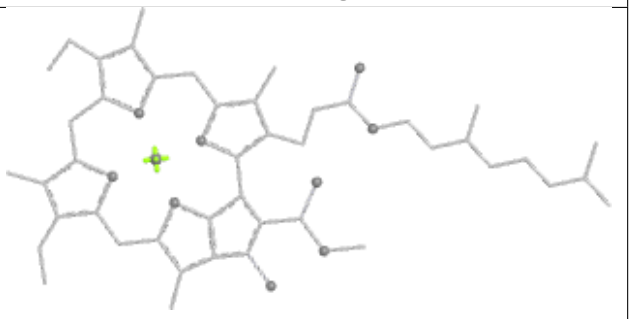
Bond angles

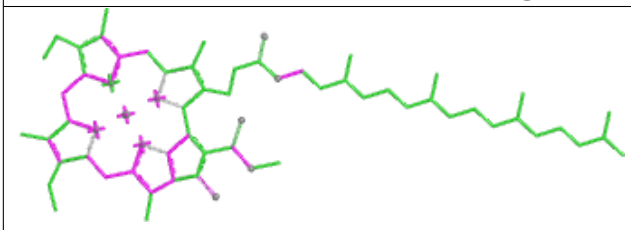
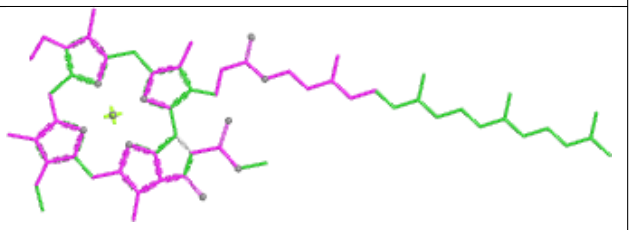
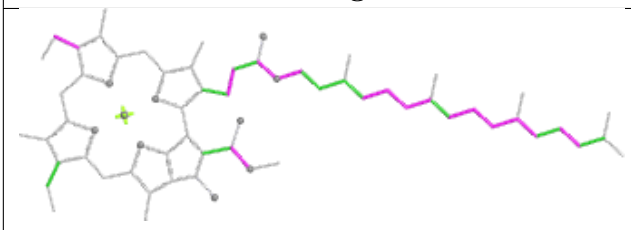
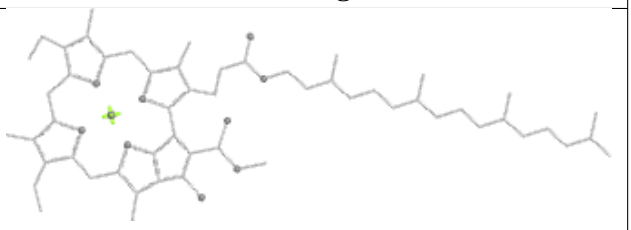


Torsions

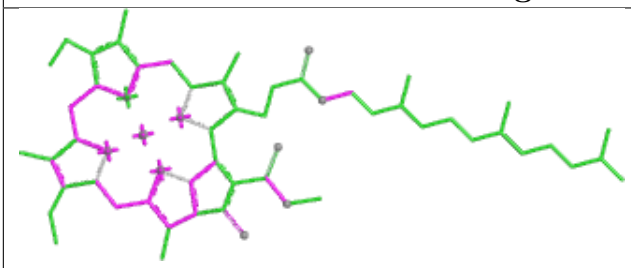


Rings

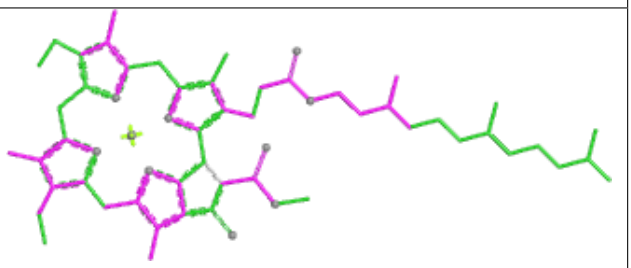
Ligand CLA H 1201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1214	
	
Bond lengths	Bond angles
	
Torsions	Rings

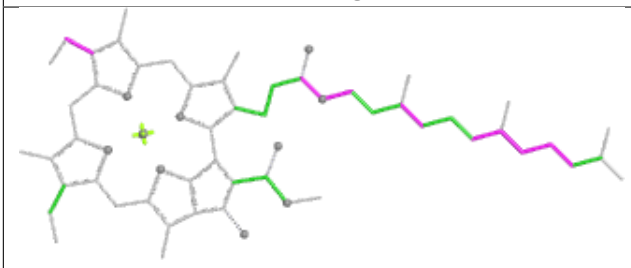
Ligand CLA U 1502



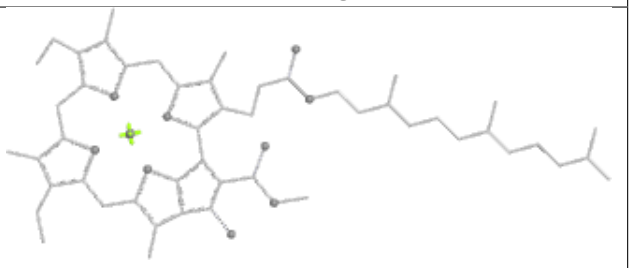
Bond lengths



Bond angles

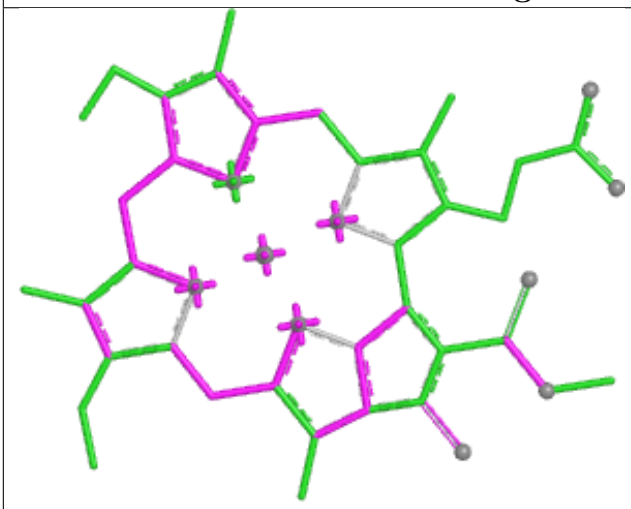


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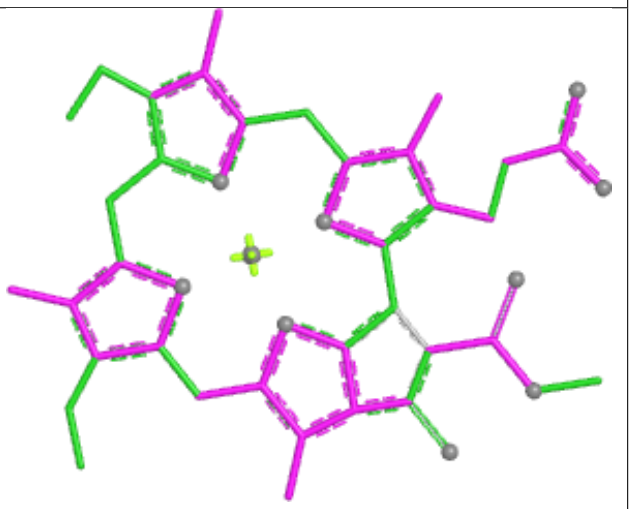


Rings

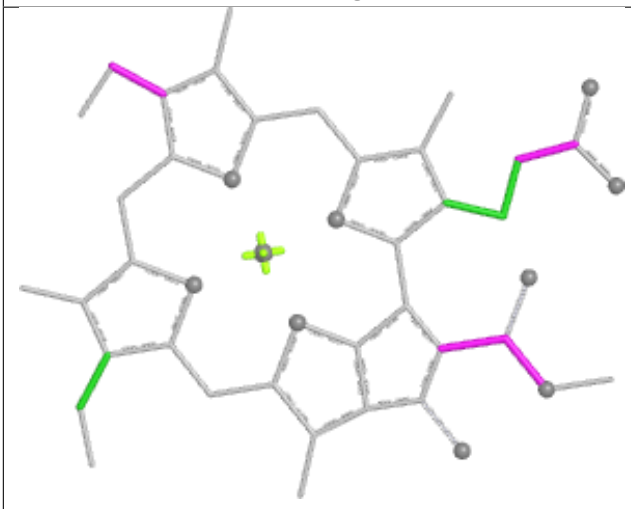
Ligand CLA G 1101



Bond lengths



Bond angles

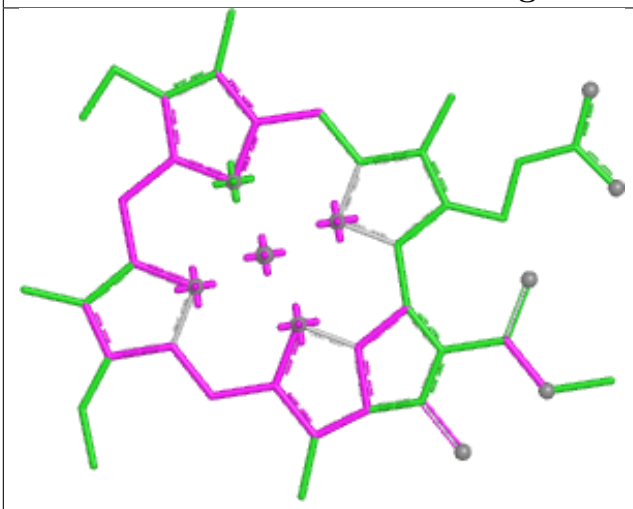


Torsions

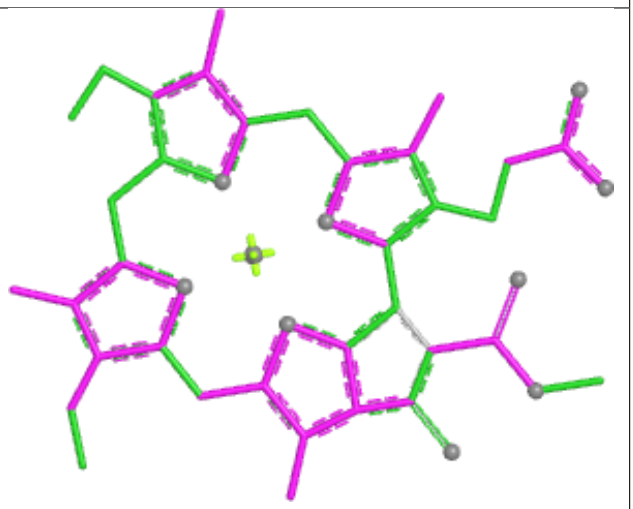


Rings

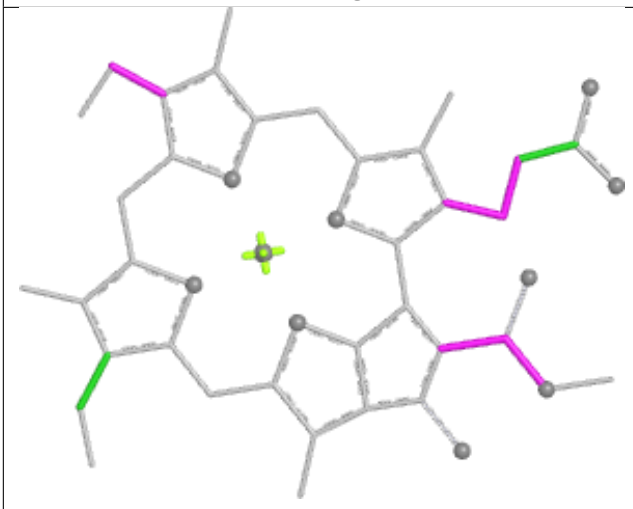
Ligand CLA k 1401



Bond lengths



Bond angles

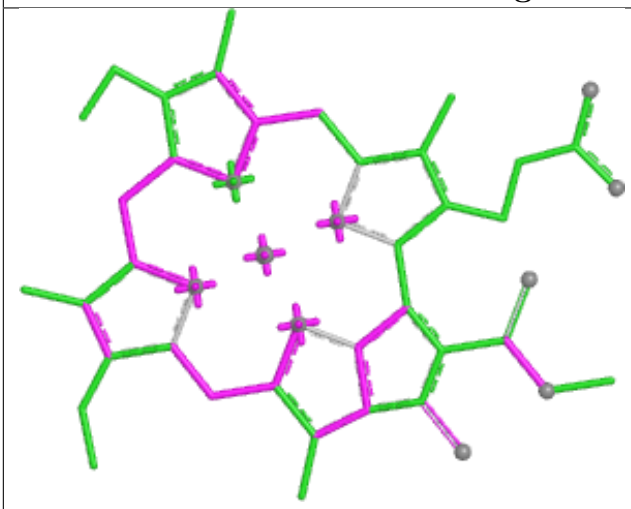


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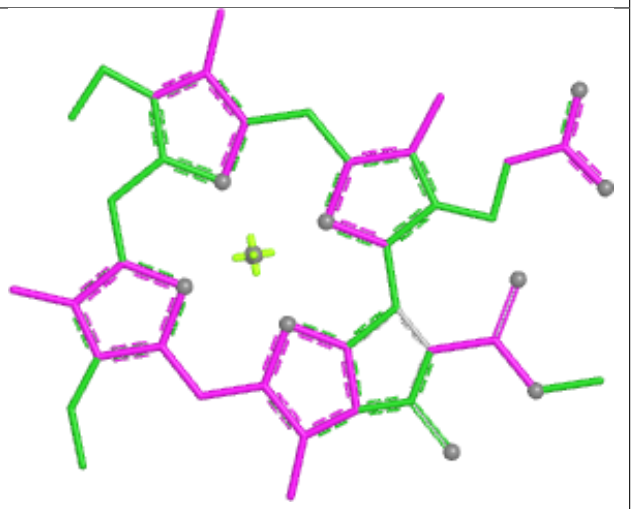


Rings

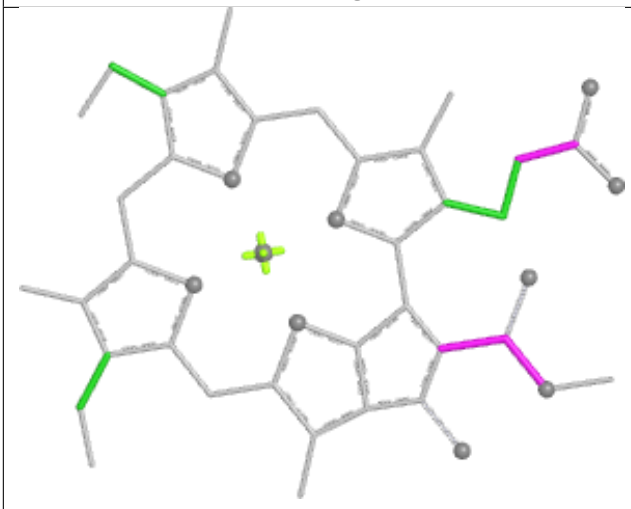
Ligand CLA H 1218



Bond lengths



Bond angles

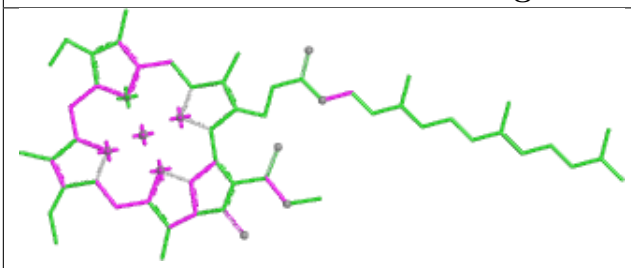


Torsions

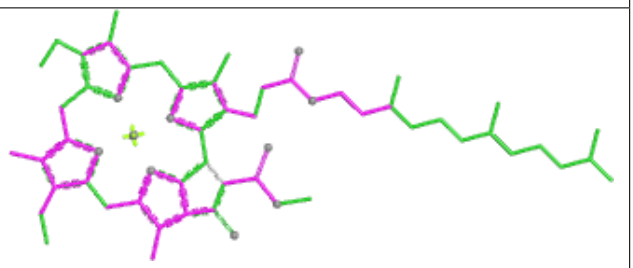


Rings

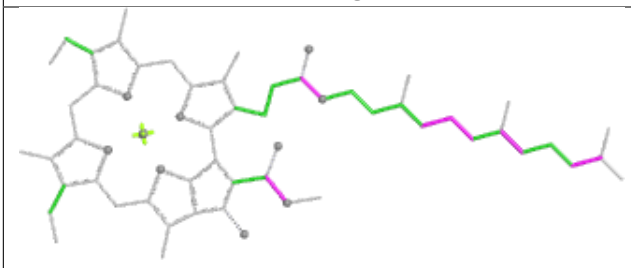
Ligand CLA G 1133



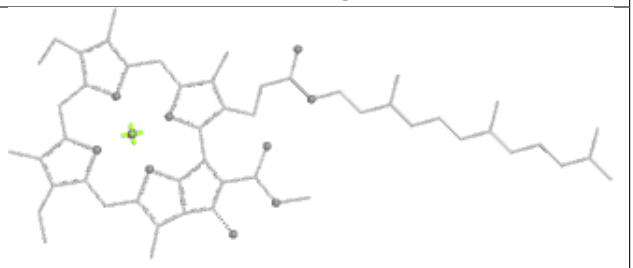
Bond lengths



Bond angles

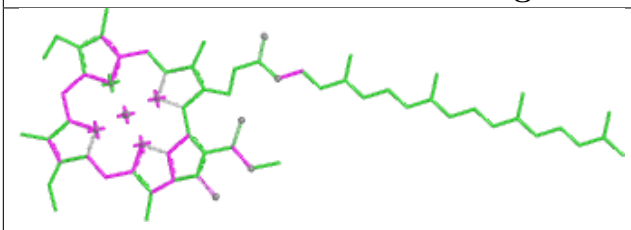


Torsions

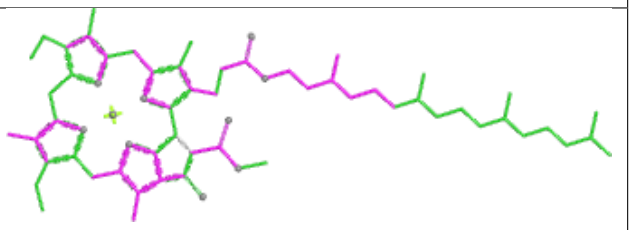


Rings

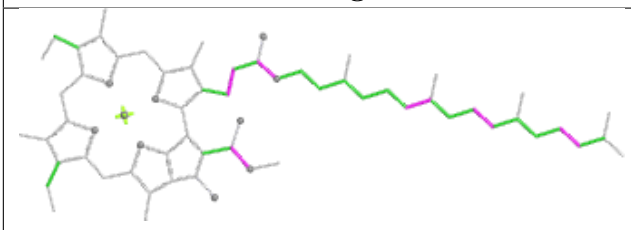
Ligand CLA G 1104



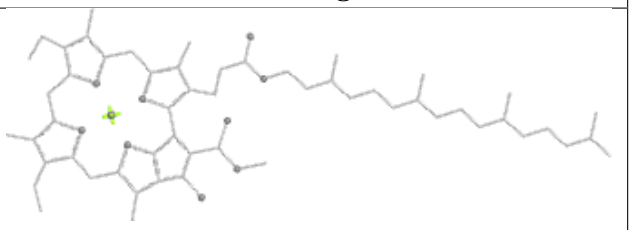
Bond lengths



Bond angles

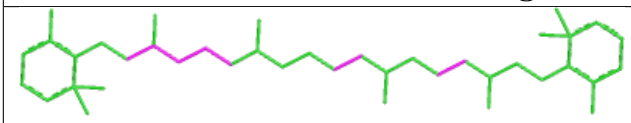


Torsions

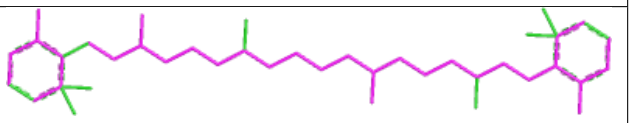


Rings

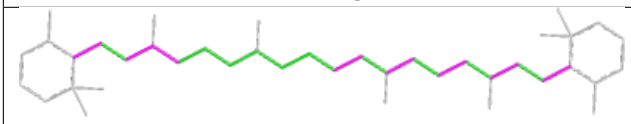
Ligand BCR a 4001



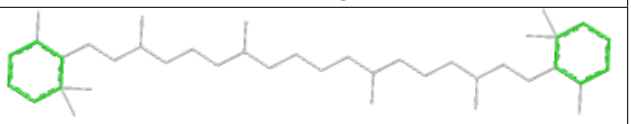
Bond lengths



Bond angles

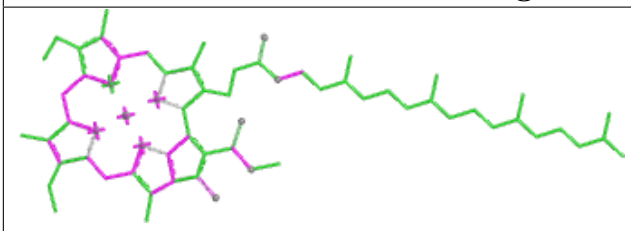


Torsions

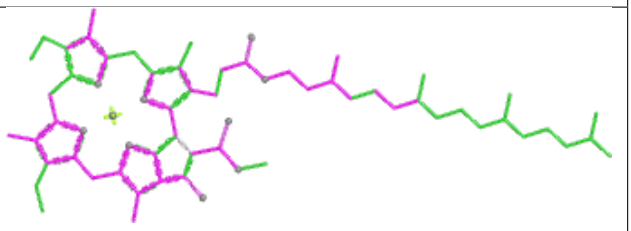


Rings

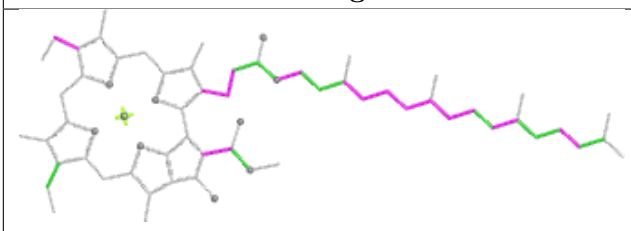
Ligand CLA B 1022



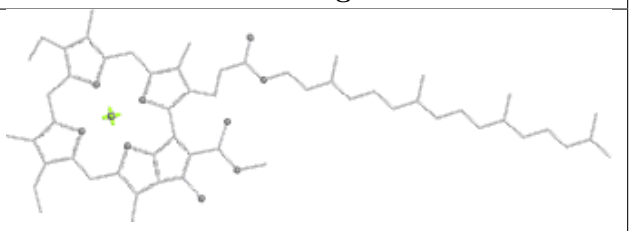
Bond lengths



Bond angles

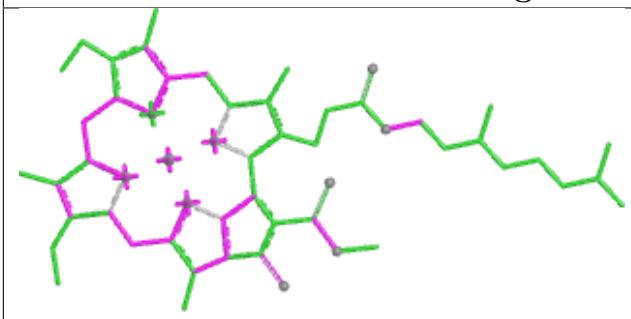


Torsions

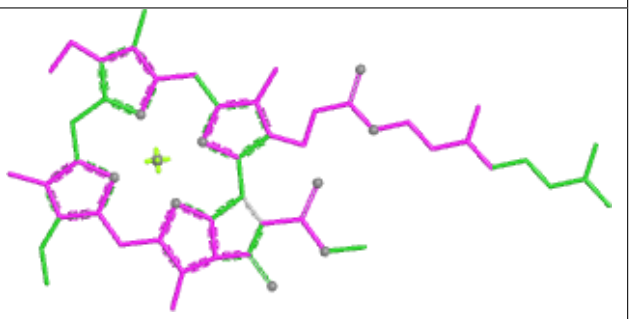


Rings

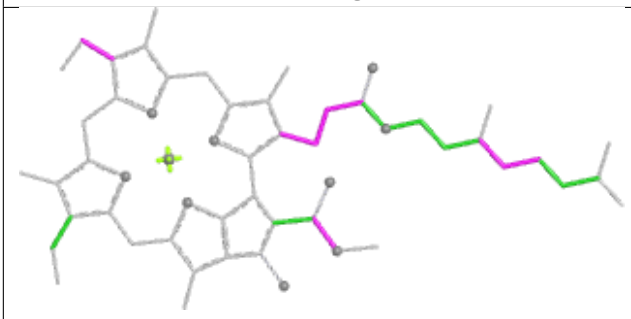
Ligand CLA A 1116



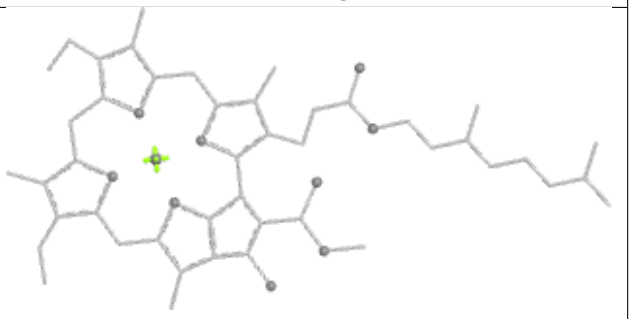
Bond lengths



Bond angles

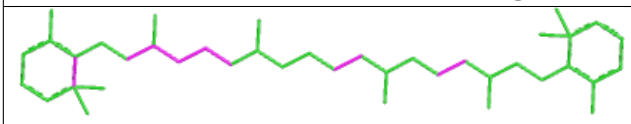


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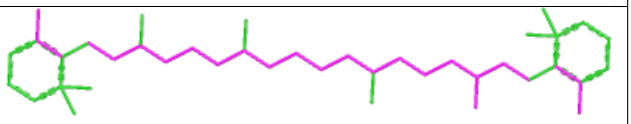


Rings

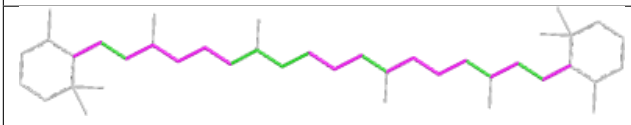
Ligand BCR M 4021



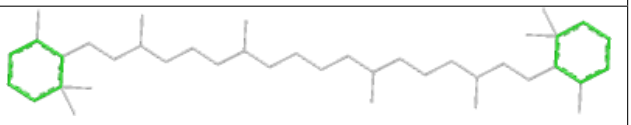
Bond lengths



Bond angles

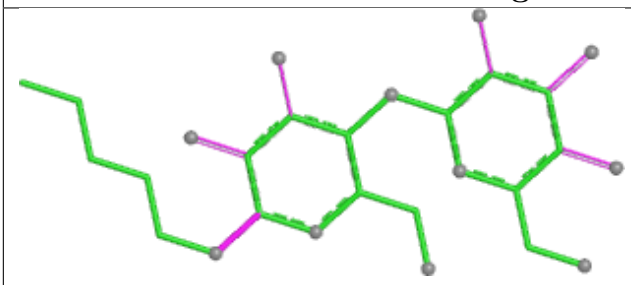


Torsions

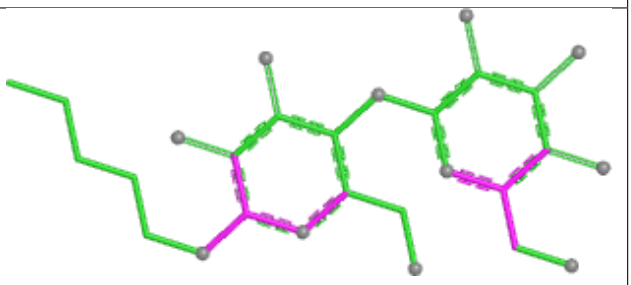


Rings

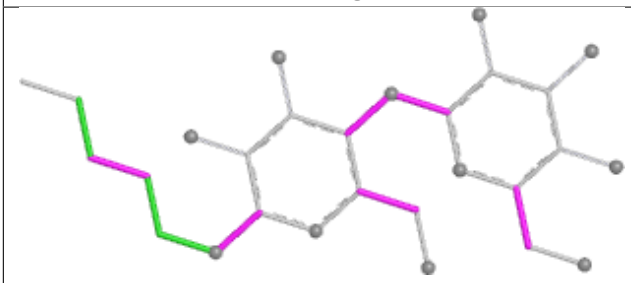
Ligand LMT A 6002



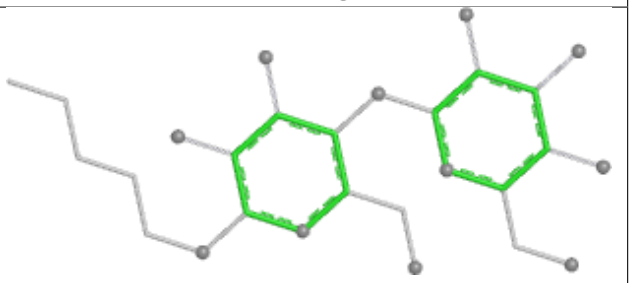
Bond lengths



Bond angles

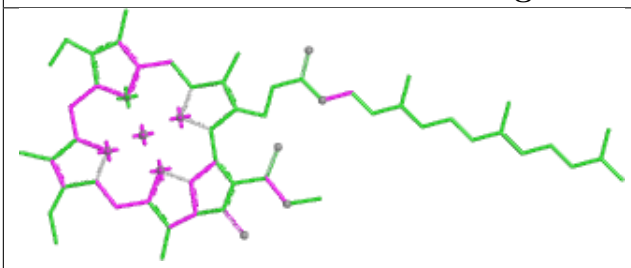


Torsions

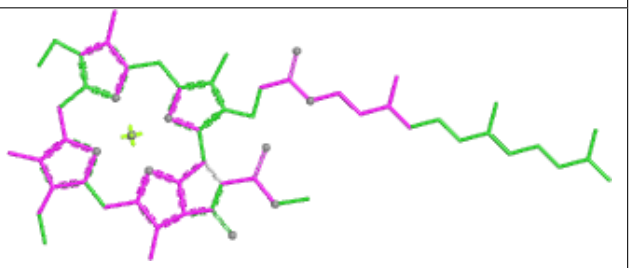


Rings

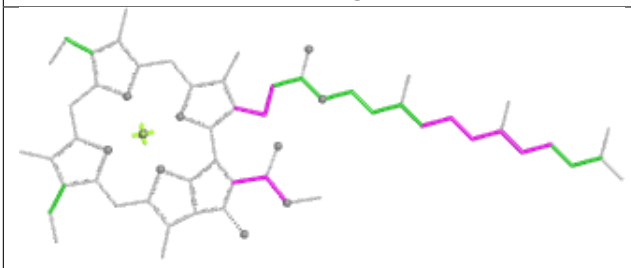
Ligand CLA A 1135



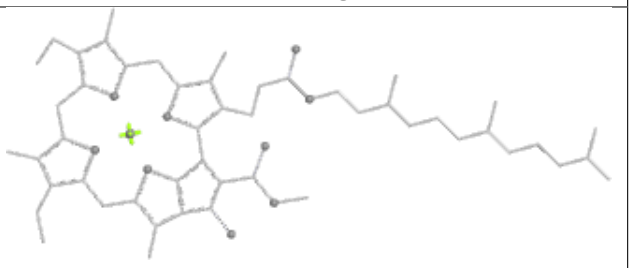
Bond lengths



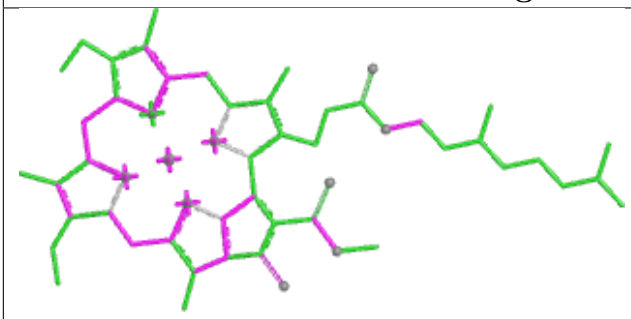
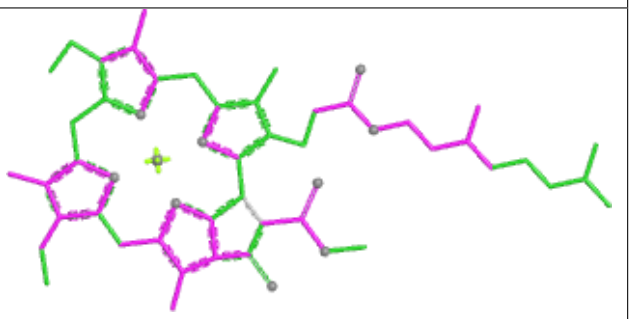
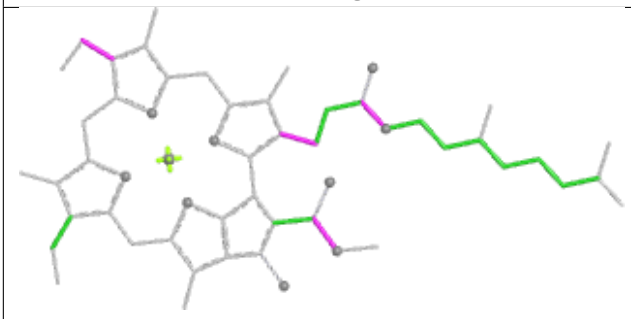
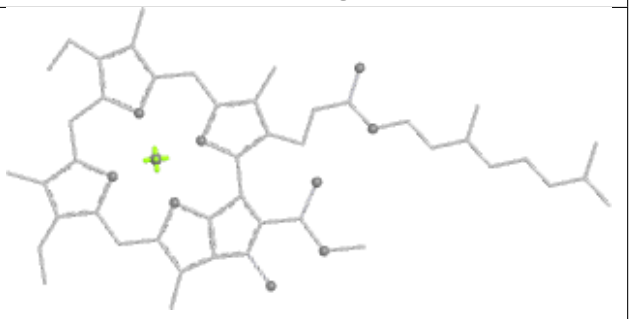
Bond angles

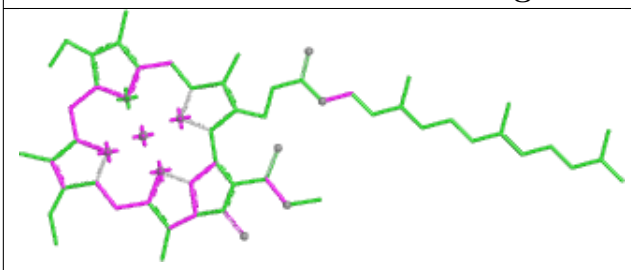
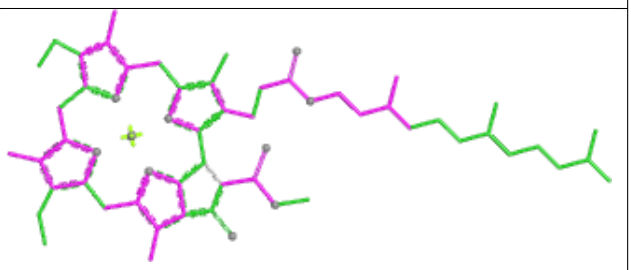
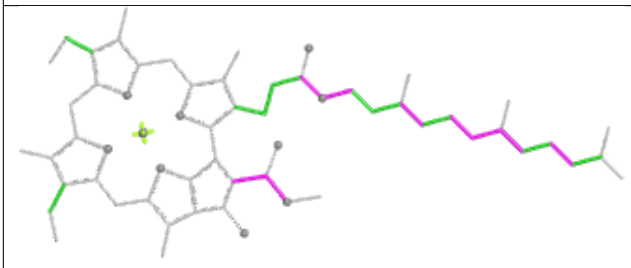
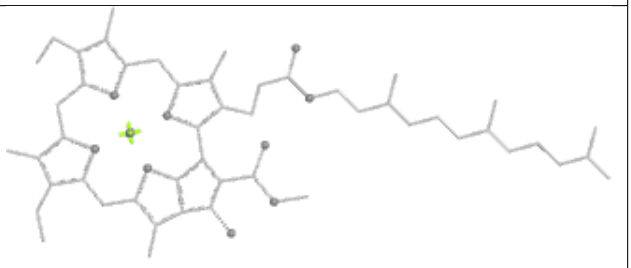


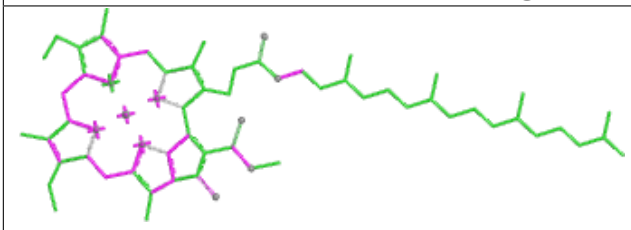
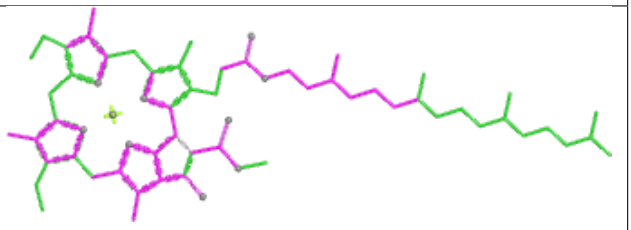
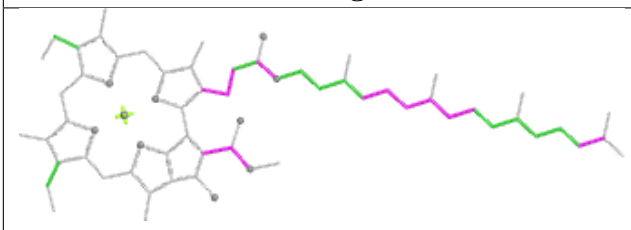
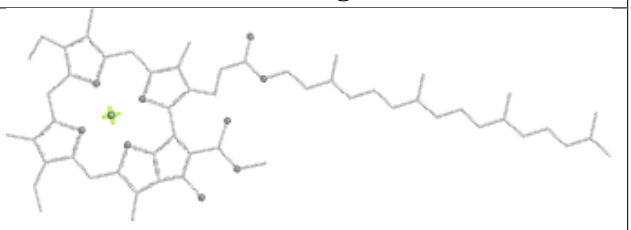
Torsions

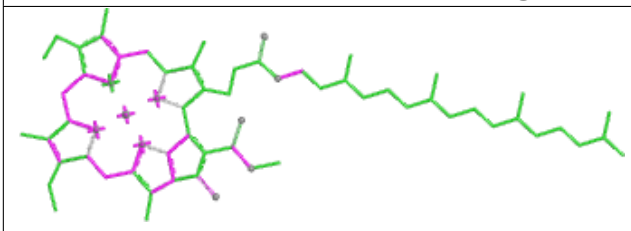
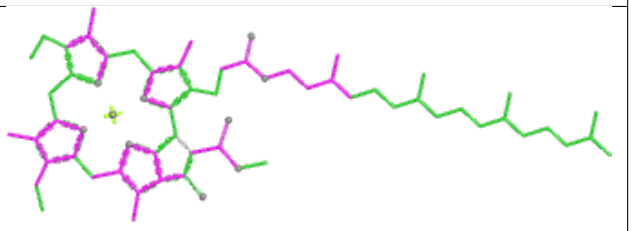
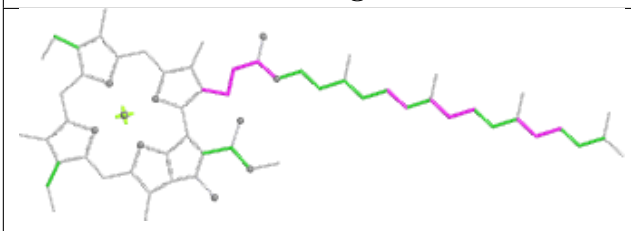
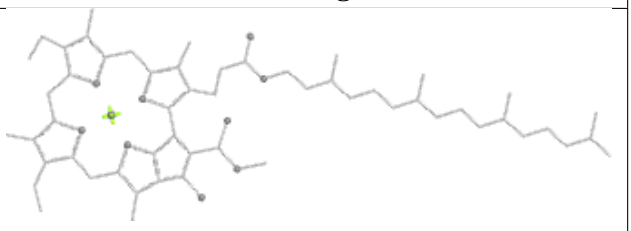


Rings

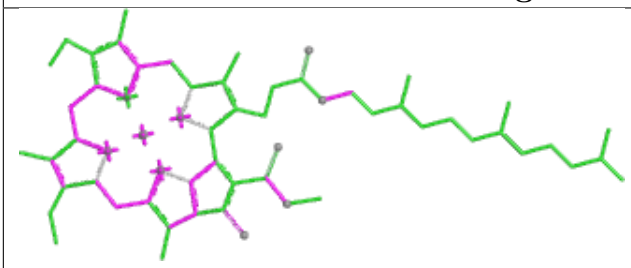
Ligand CLA B 1231	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 1128	
 Bond lengths	 Bond angles
 Torsions	 Rings

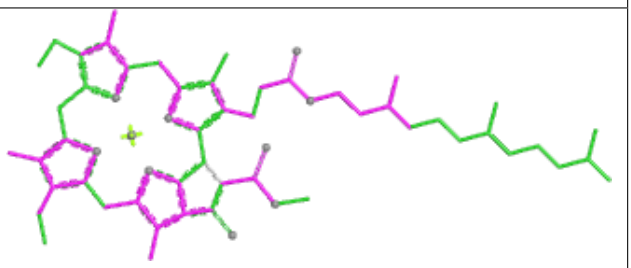
Ligand CLA b 1223	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1127	
	
Bond lengths	Bond angles
	
Torsions	Rings

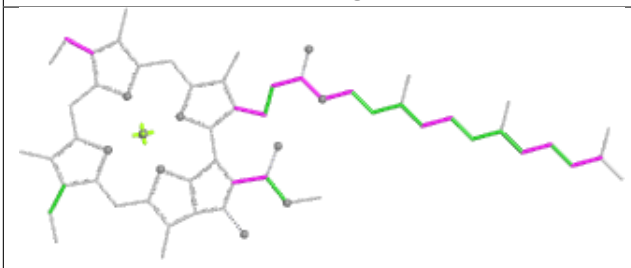
Ligand CLA B 1202



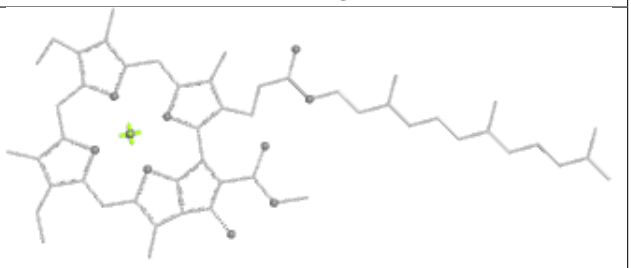
Bond lengths



Bond angles

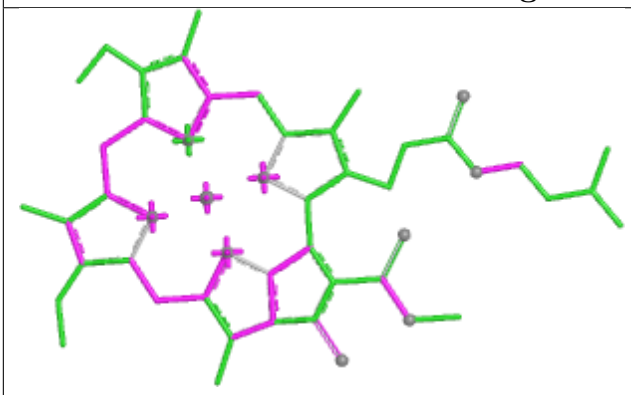


Torsions

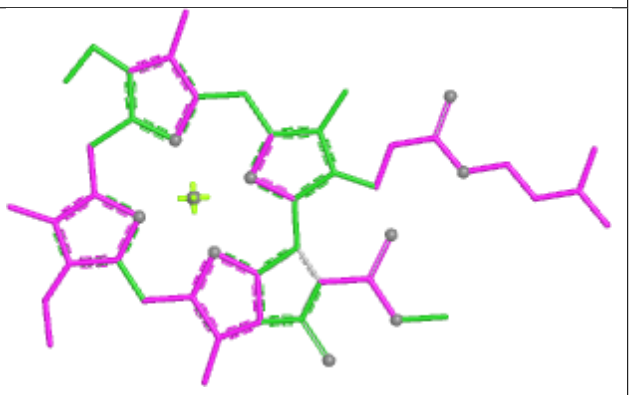


Rings

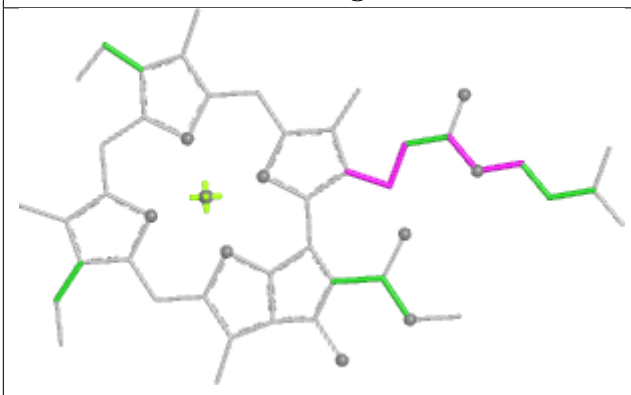
Ligand CLA a 1137



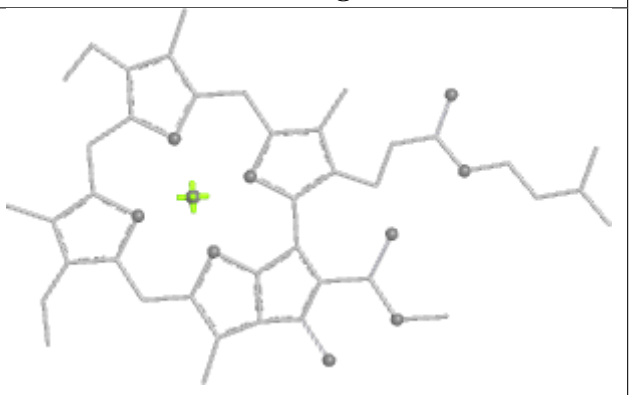
Bond lengths



Bond angles

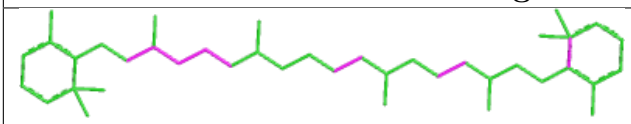


Torsions

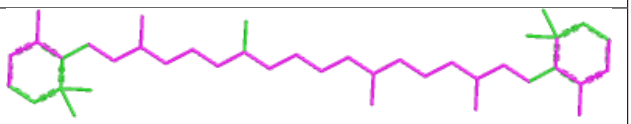


Rings

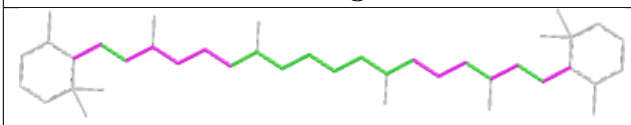
Ligand BCR A 4003



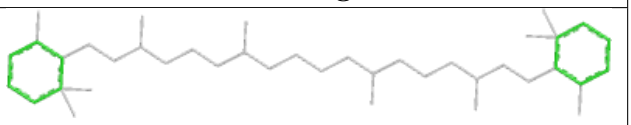
Bond lengths



Bond angles

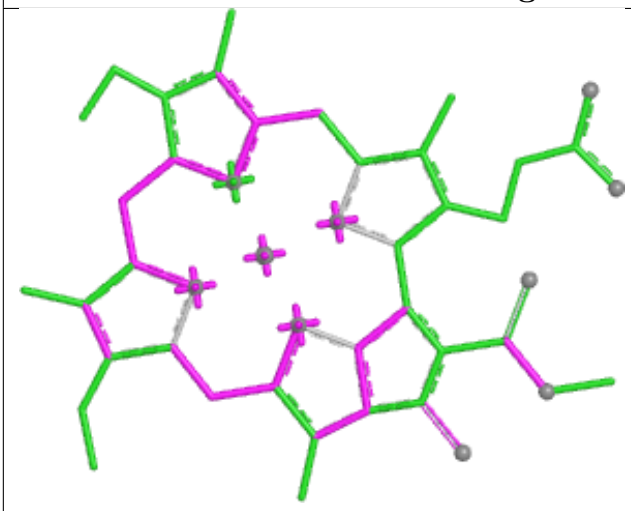


Torsions

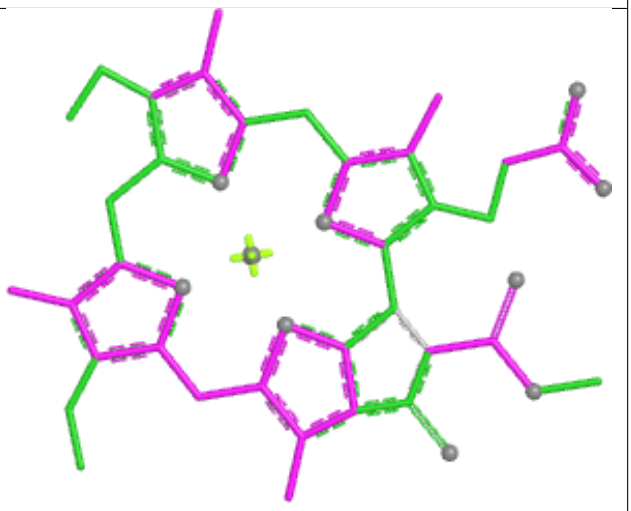


Rings

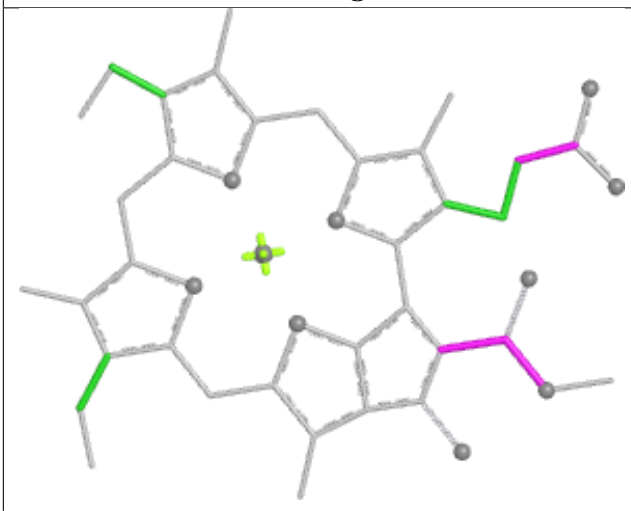
Ligand CLA b 1218



Bond lengths



Bond angles

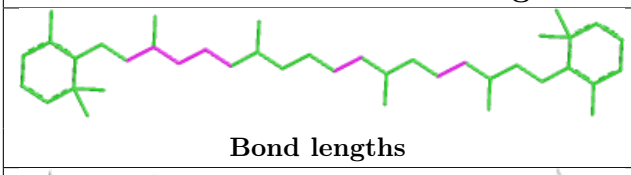


Torsions

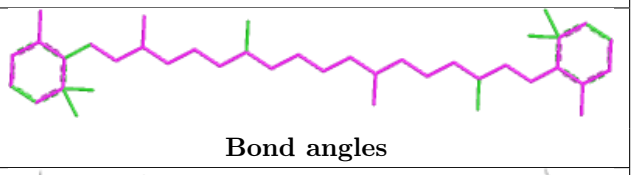


Rings

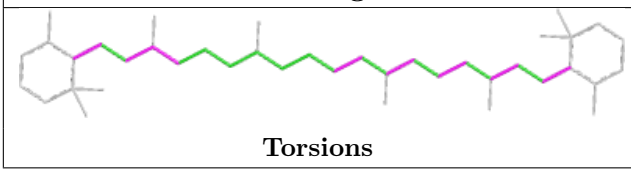
Ligand BCR G 4001



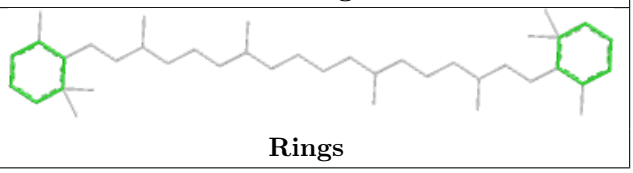
Bond lengths



Bond angles

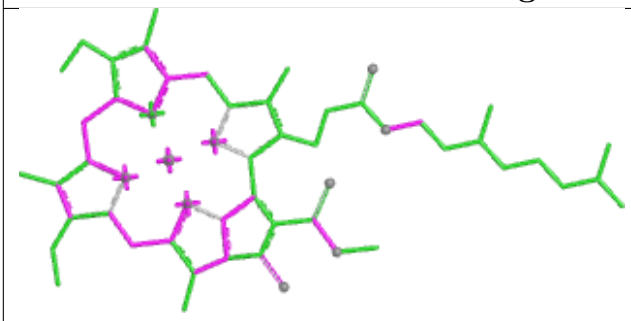


Torsions

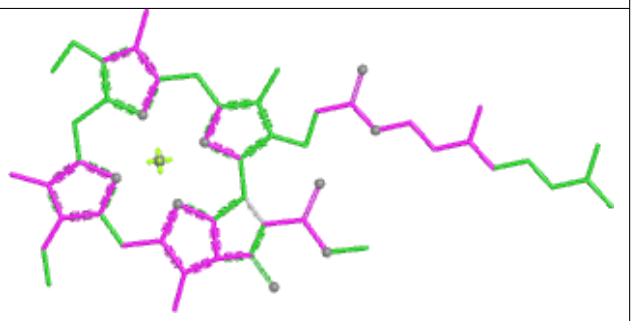


Rings

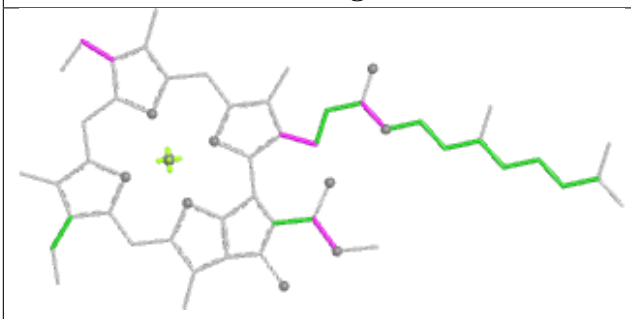
Ligand CLA b 1231



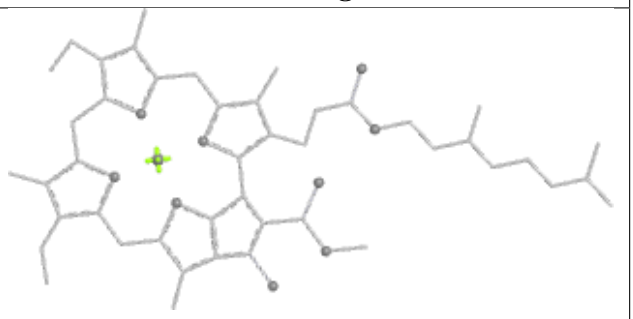
Bond lengths



Bond angles

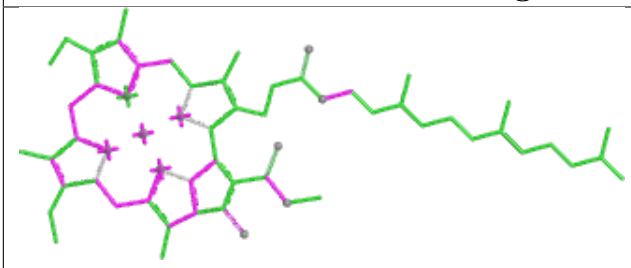


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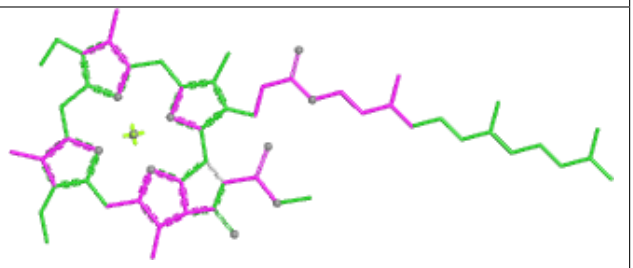


Rings

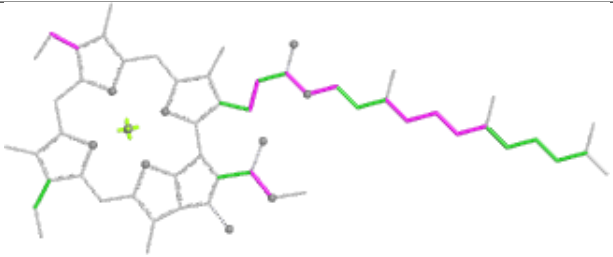
Ligand CLA G 1131



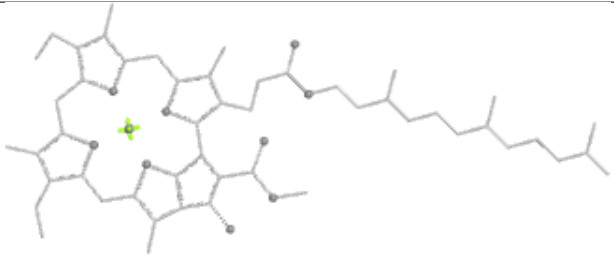
Bond lengths



Bond angles

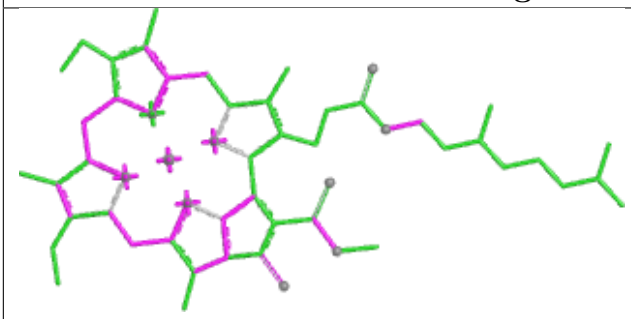


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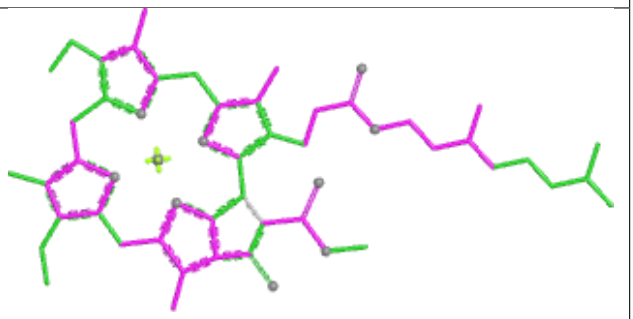


Rings

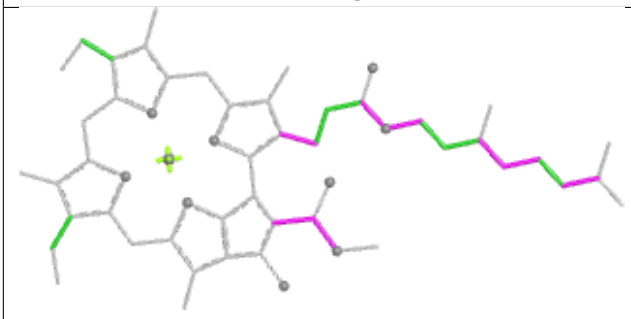
Ligand CLA G 1112



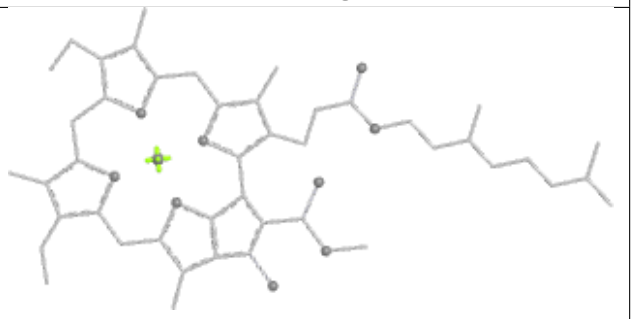
Bond lengths



Bond angles

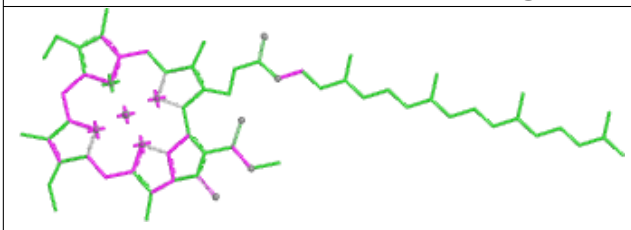


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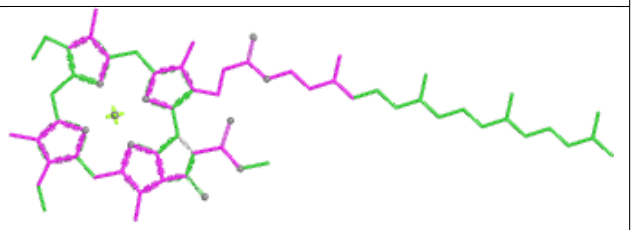


Rings

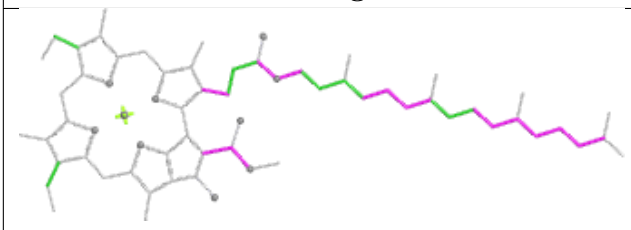
Ligand CLA a 1115



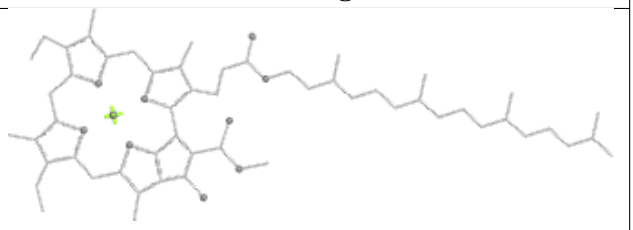
Bond lengths



Bond angles

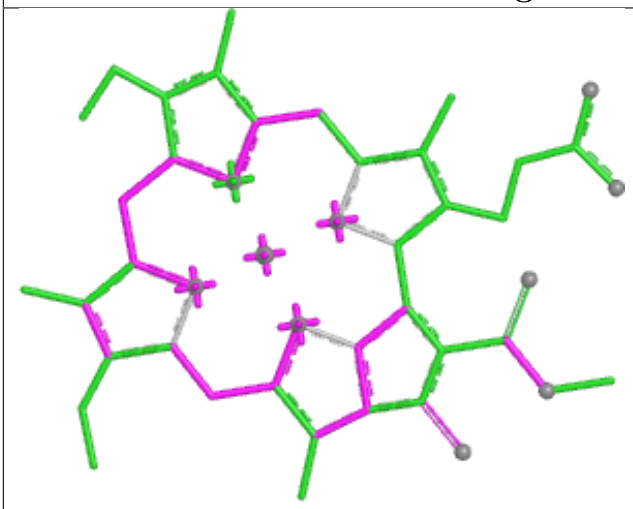


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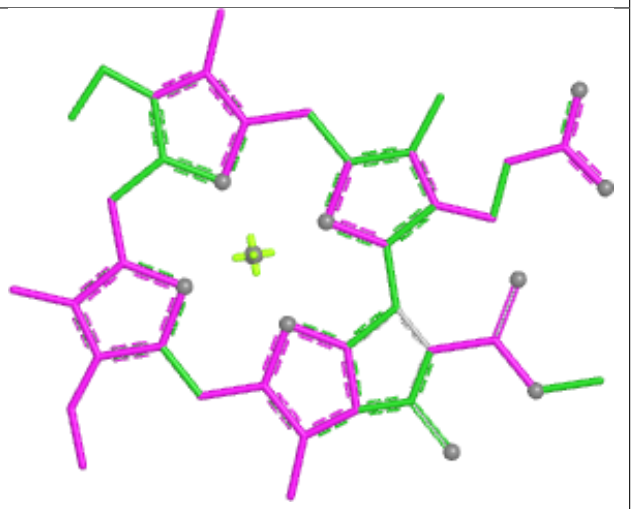


Rings

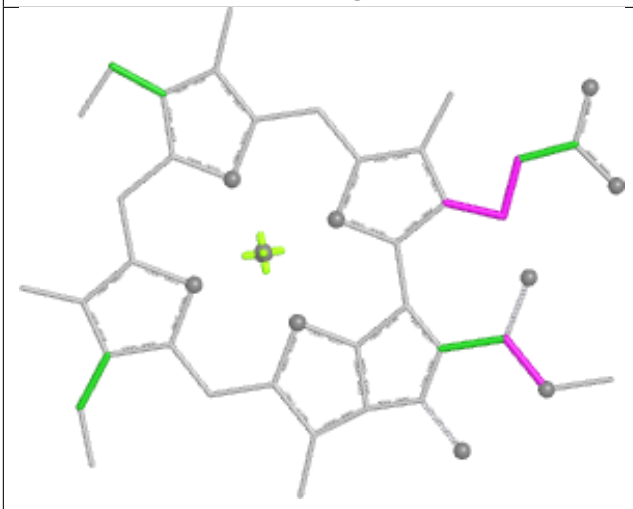
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Bond lengths



Bond angles

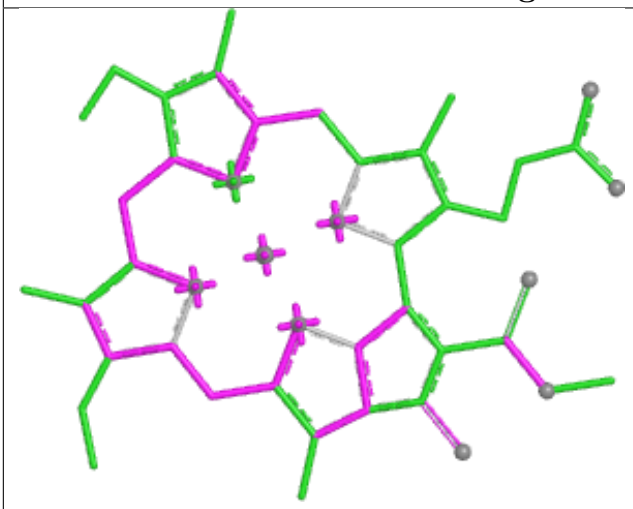


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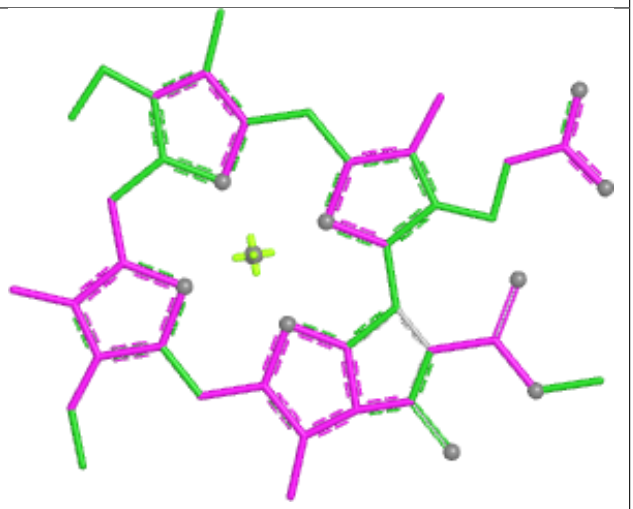


Rings

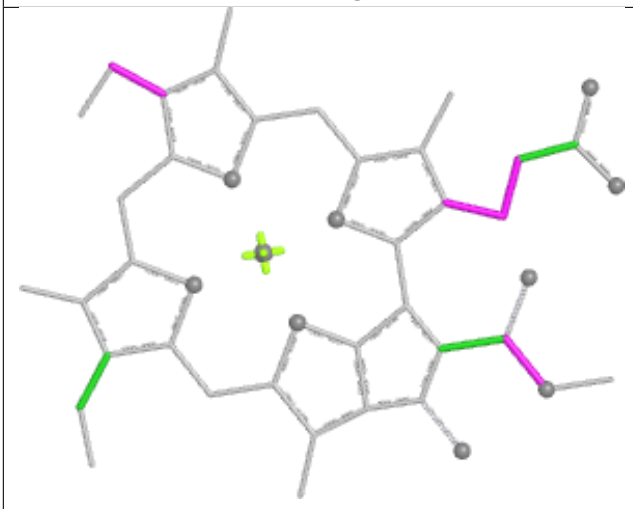
Ligand CLA b 1227



Bond lengths



Bond angles

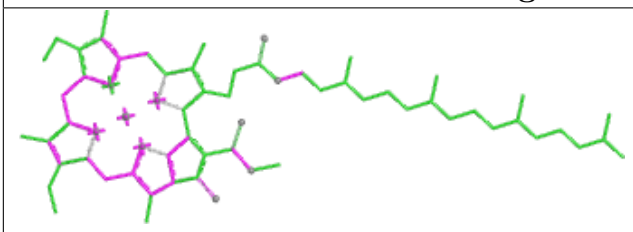


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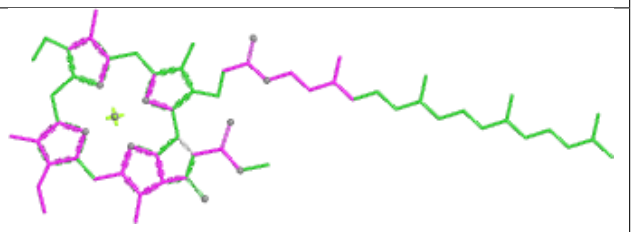


Rings

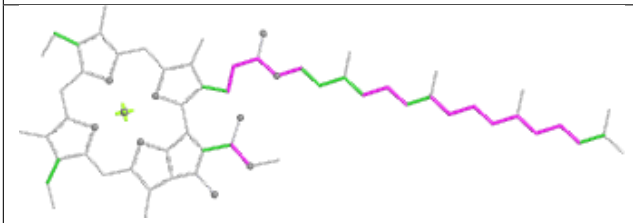
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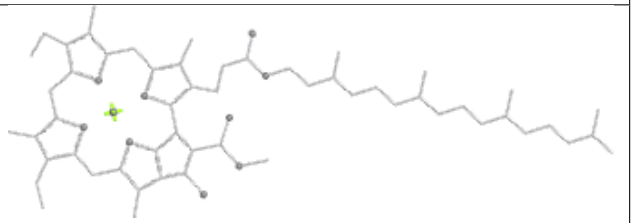
Bond lengths



Bond angles

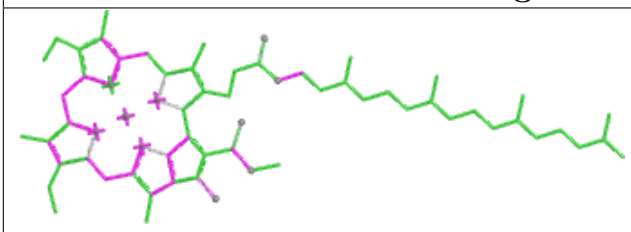


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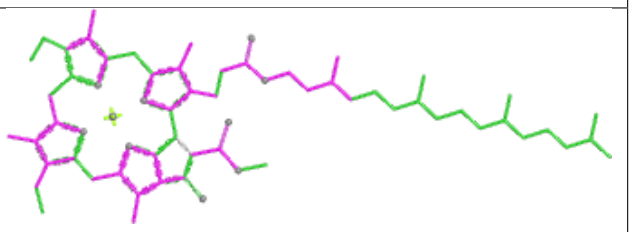


Rings

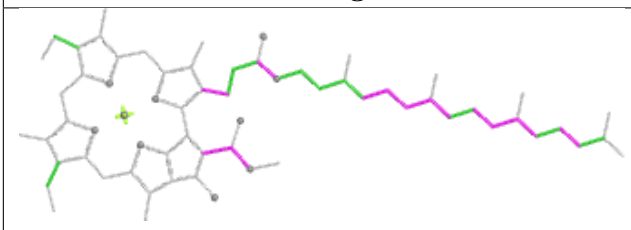
Ligand CLA G 1117



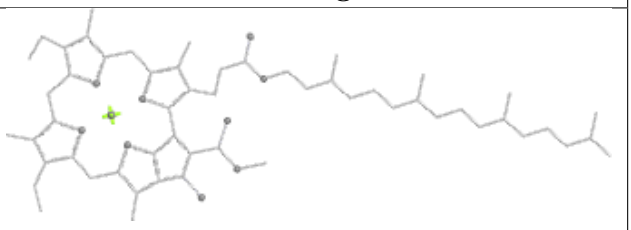
Bond lengths



Bond angles

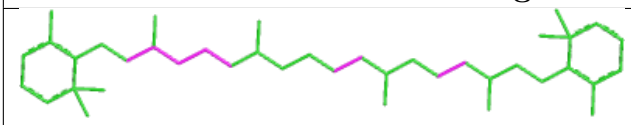


Torsions



Rings

Ligand BCR B 4006



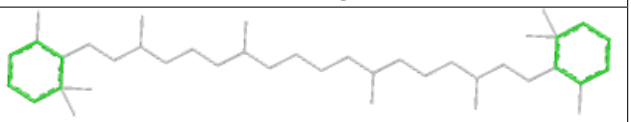
Bond lengths



Bond angles

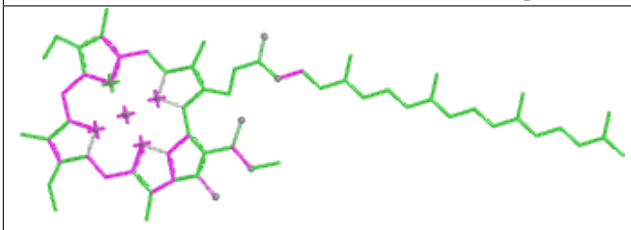


Torsions

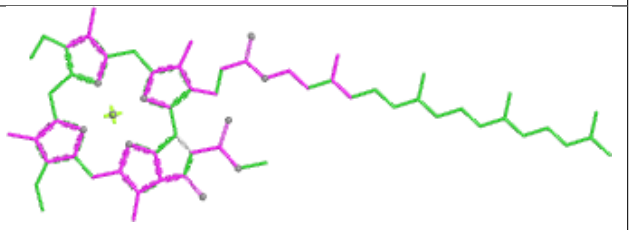


Rings

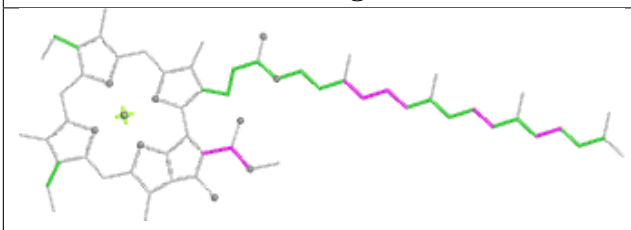
Ligand CLA b 1205



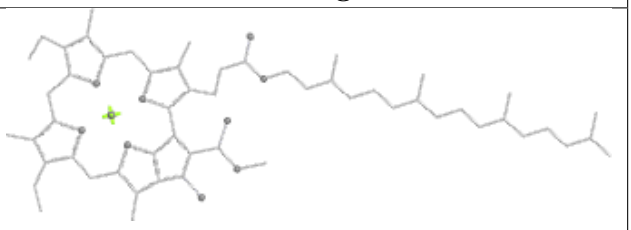
Bond lengths



Bond angles

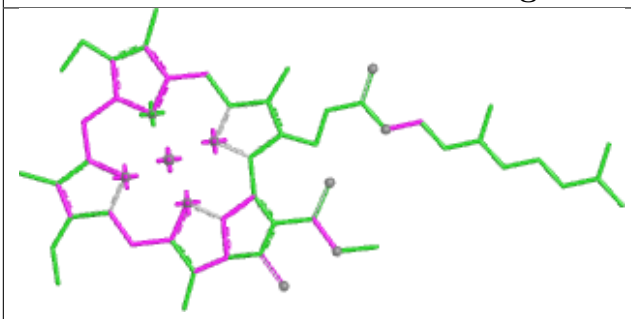


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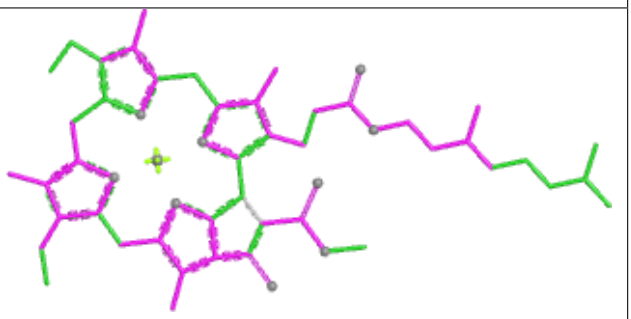


Rings

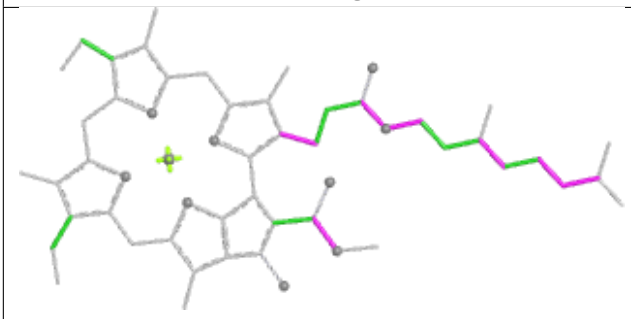
Ligand CLA a 1118



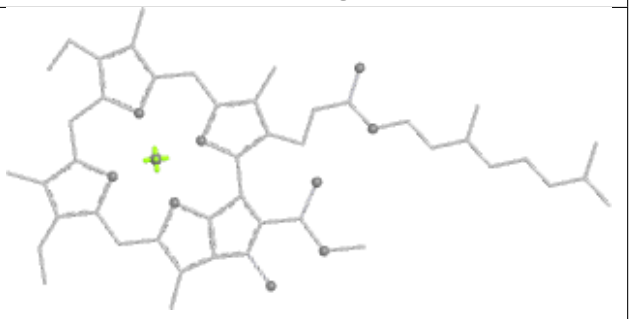
Bond lengths



Bond angles

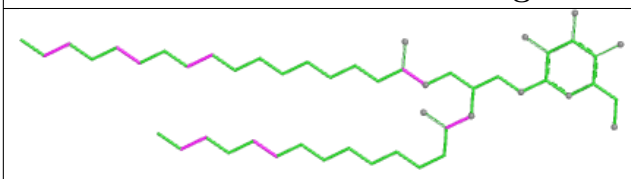


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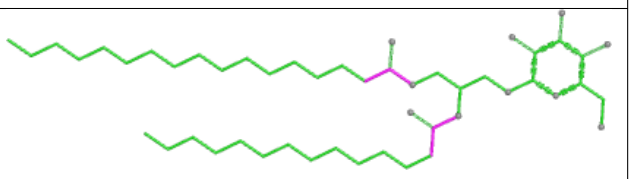


Rings

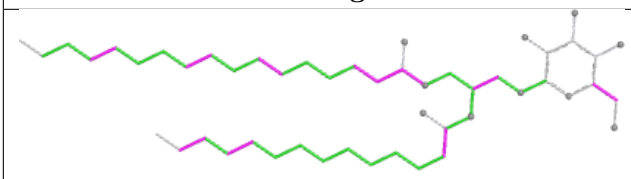
Ligand LMG L 5007



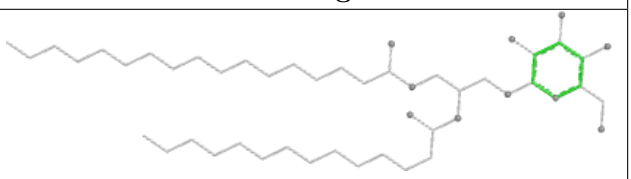
Bond lengths



Bond angles

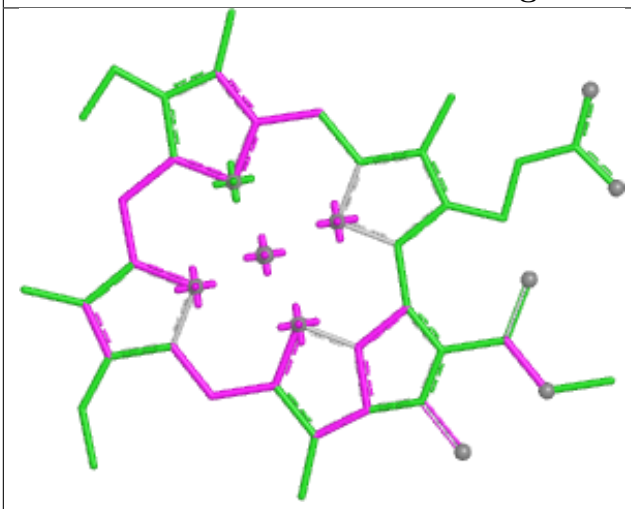


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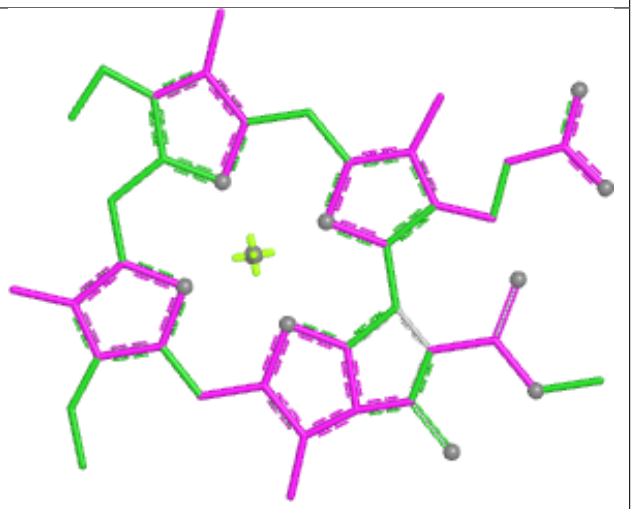


Rings

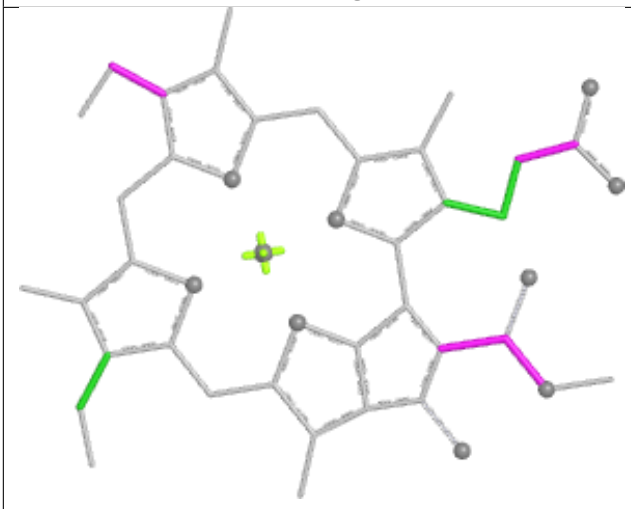
Ligand CLA a 1101



Bond lengths



Bond angles

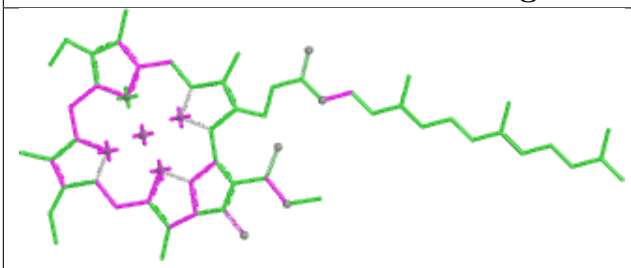


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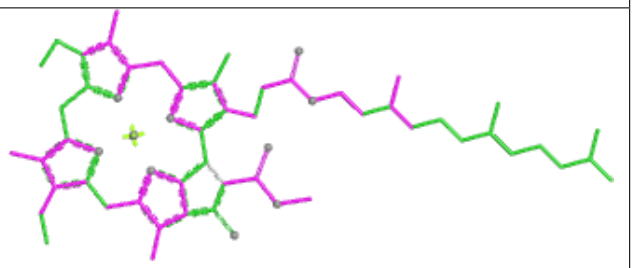


Rings

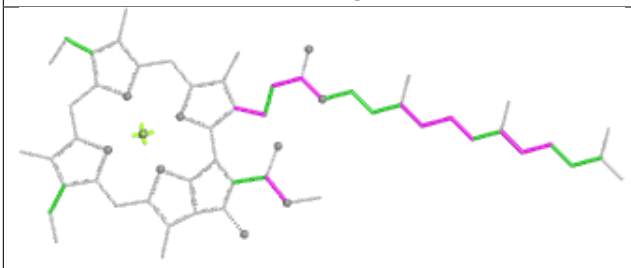
Ligand CLA a 1138



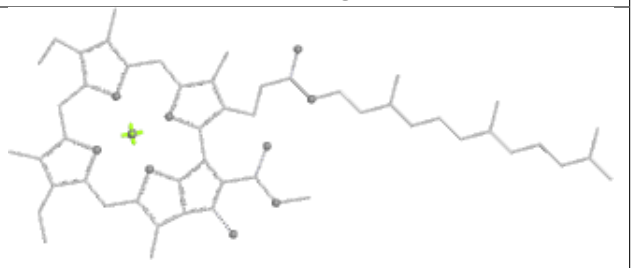
Bond lengths



Bond angles

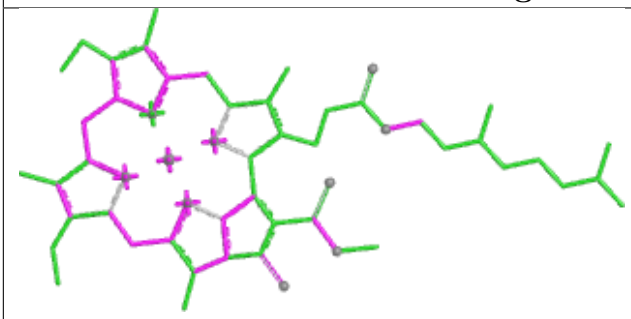


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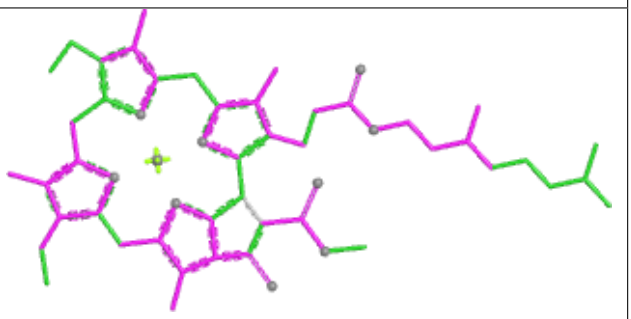


Rings

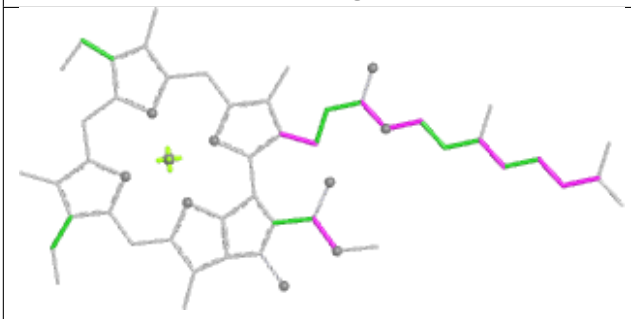
Ligand CLA A 1118



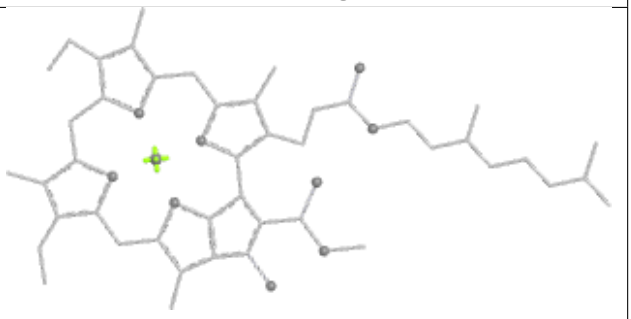
Bond lengths



Bond angles

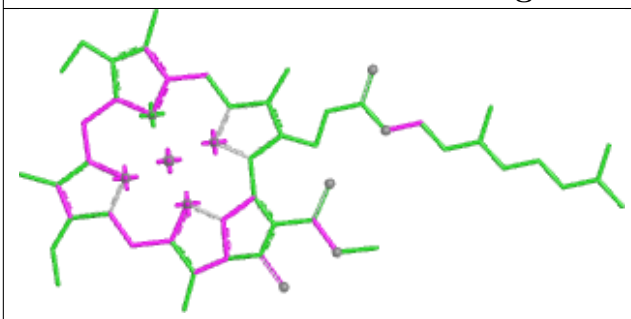


Torsions

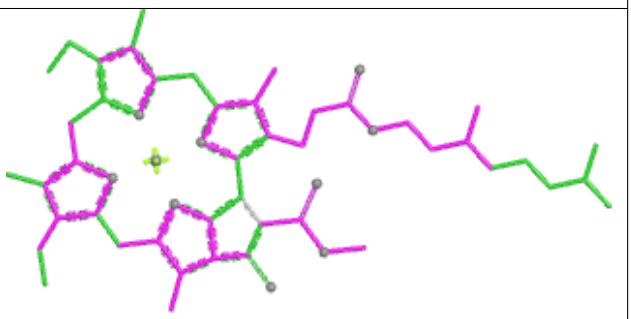


Rings

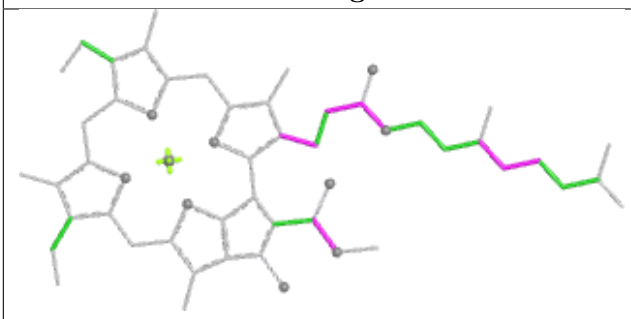
Ligand CLA B 1220



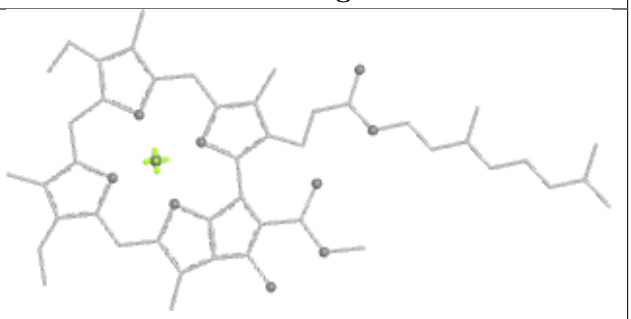
Bond lengths



Bond angles

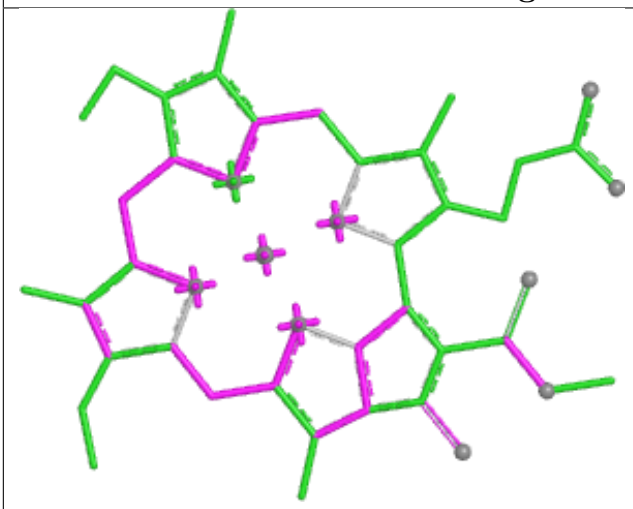


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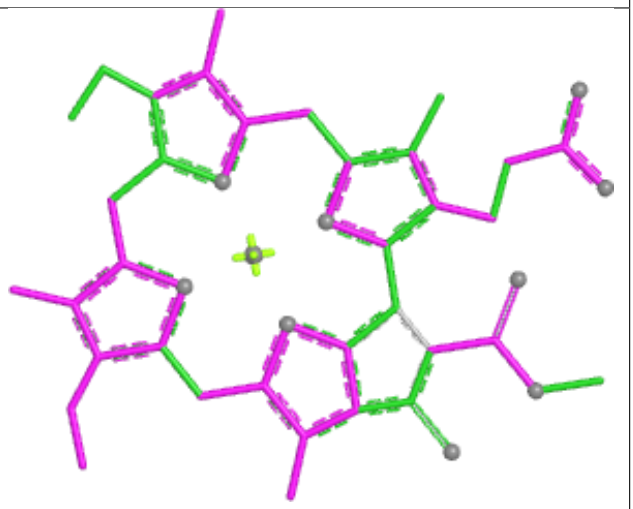


Rings

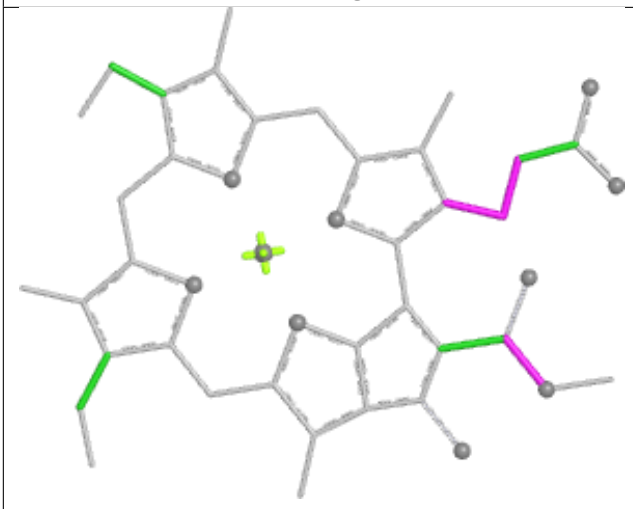
Ligand CLA b 1206



Bond lengths



Bond angles

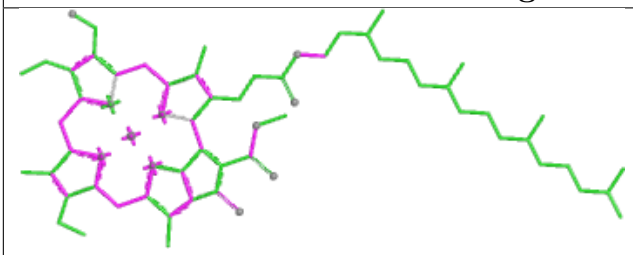


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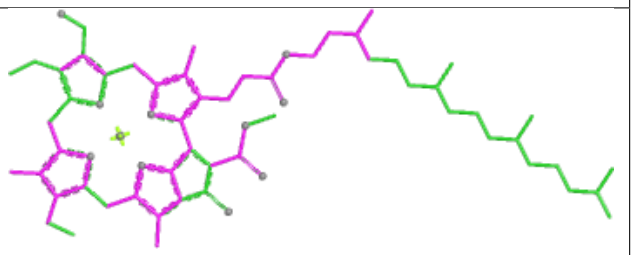


Rings

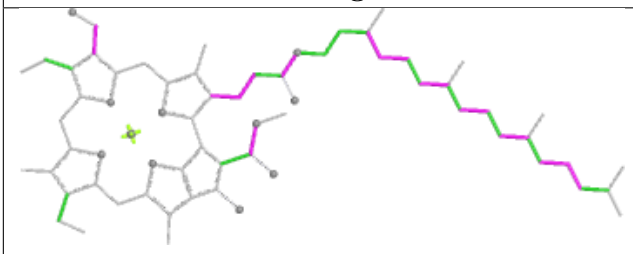
Ligand F6C H 1237



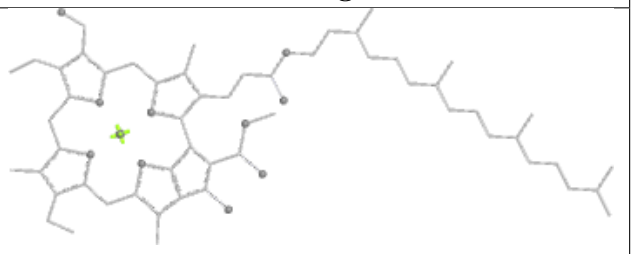
Bond lengths



Bond angles

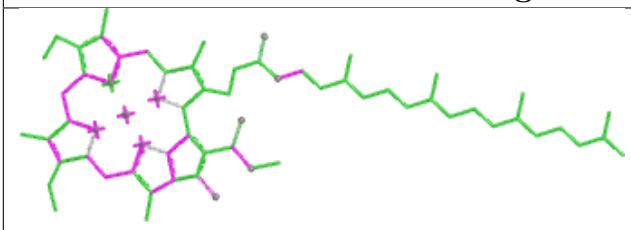


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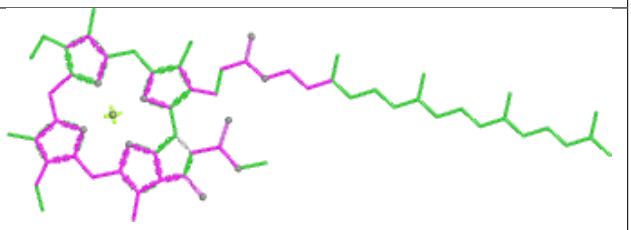


Rings

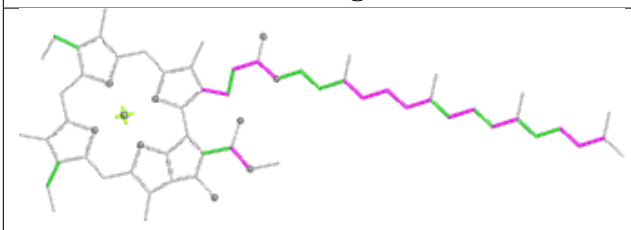
Ligand CLA A 1125



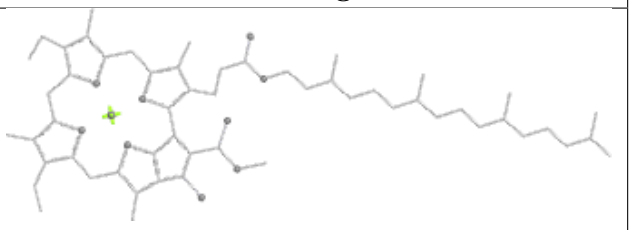
Bond lengths



Bond angles

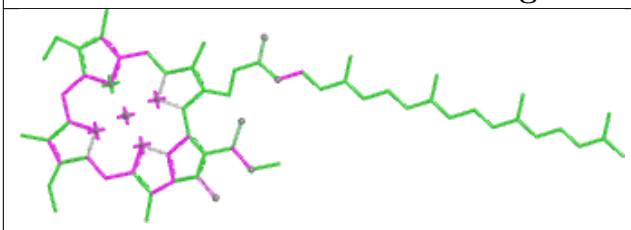


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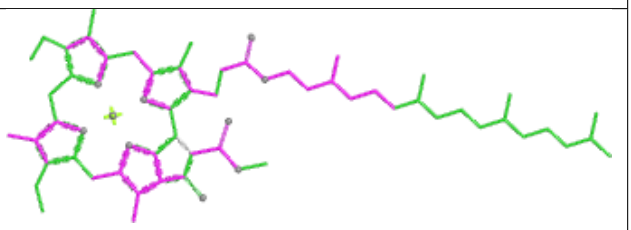


Rings

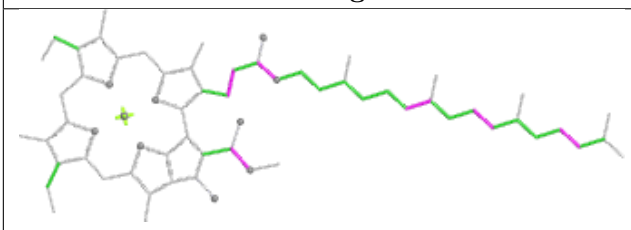
Ligand CLA a 1104



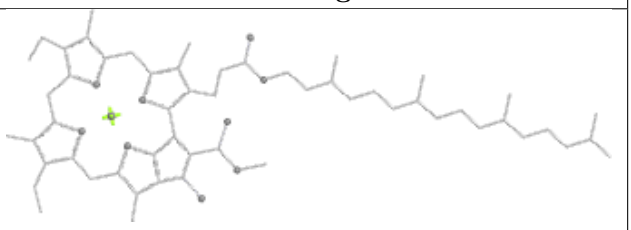
Bond lengths



Bond angles

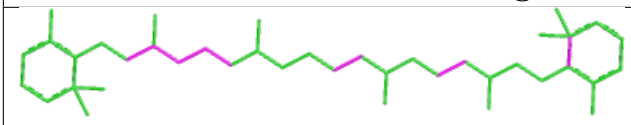


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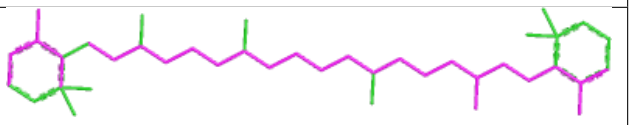


Rings

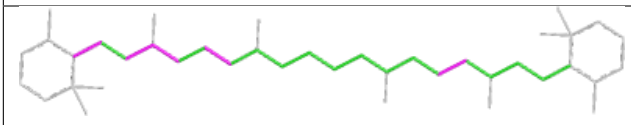
Ligand BCR B 4009



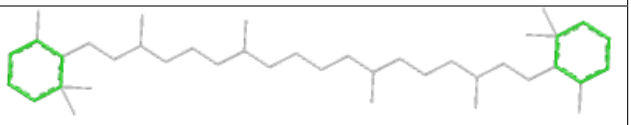
Bond lengths



Bond angles

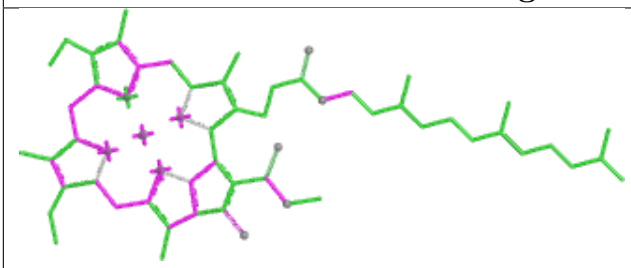


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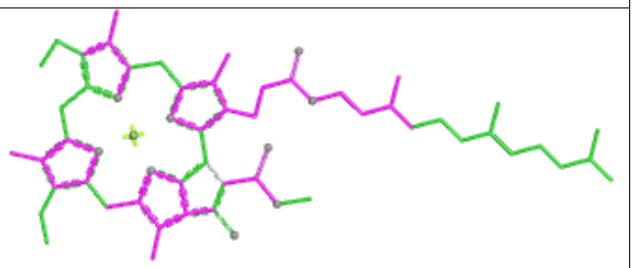


Rings

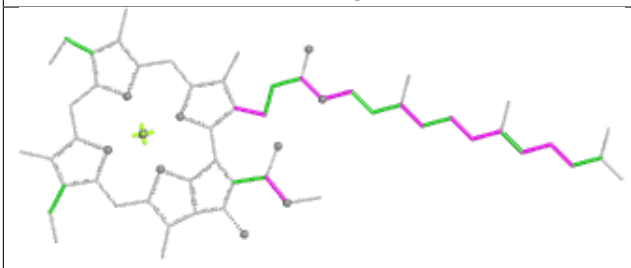
Ligand CLA b 1229



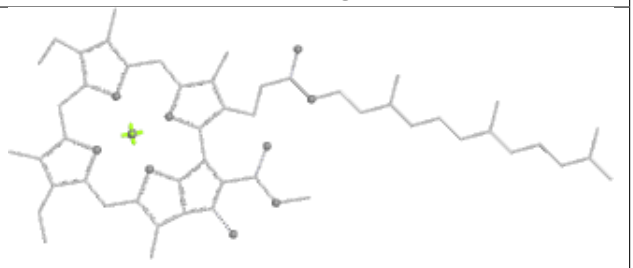
Bond lengths



Bond angles

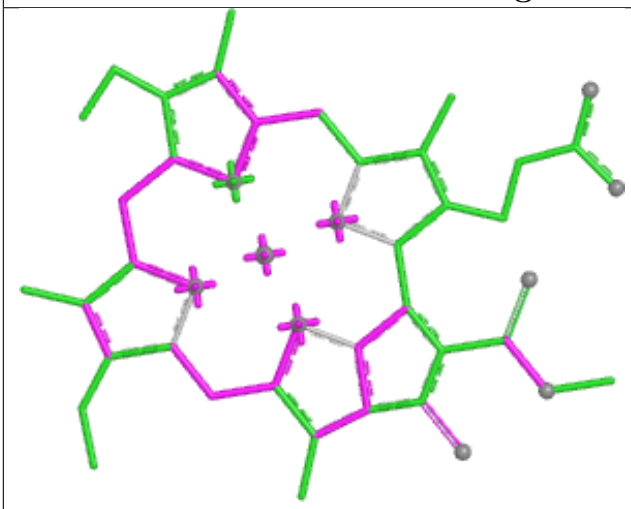


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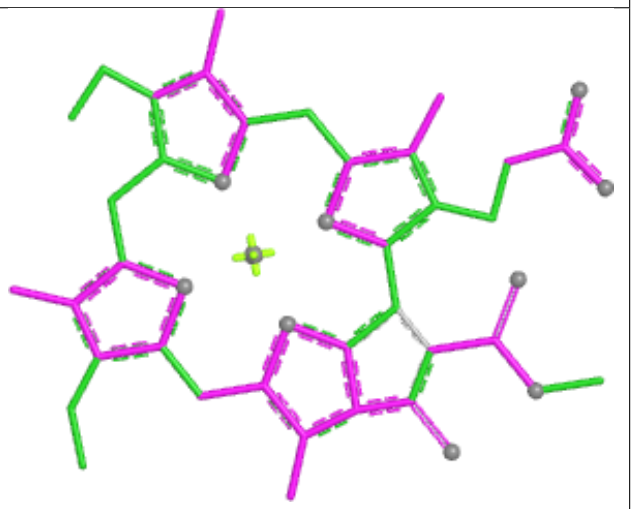


Rings

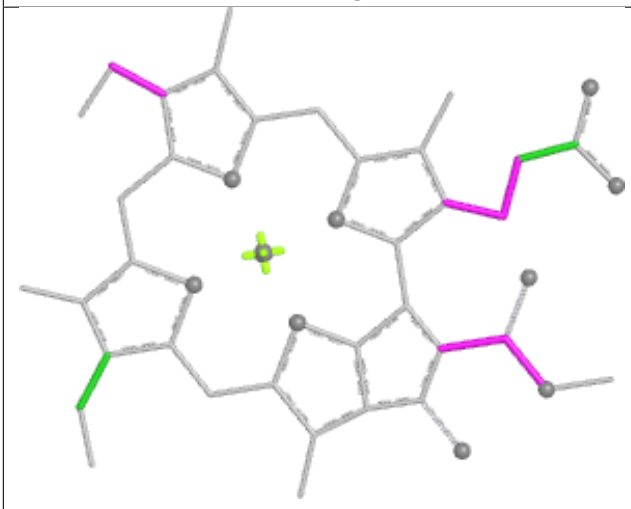
Ligand CLA A 1120



Bond lengths



Bond angles

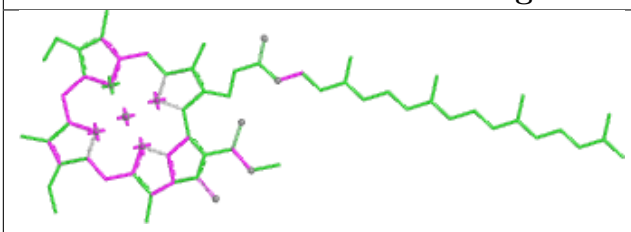


Torsions

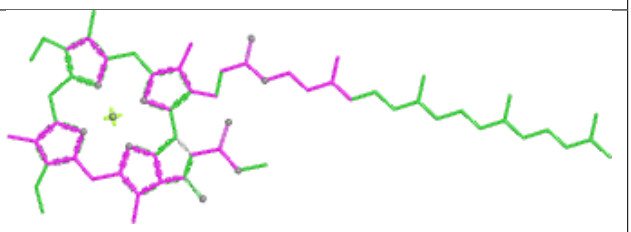


Rings

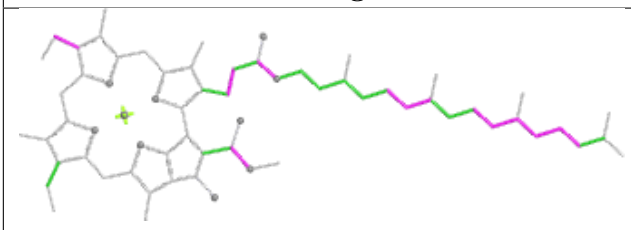
Ligand CLA B 1224



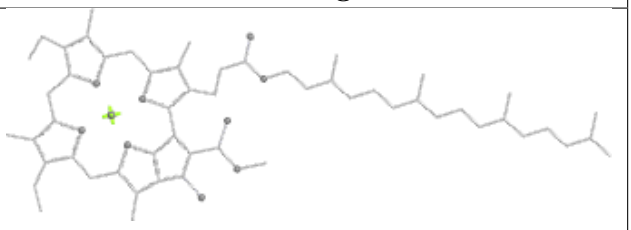
Bond lengths



Bond angles

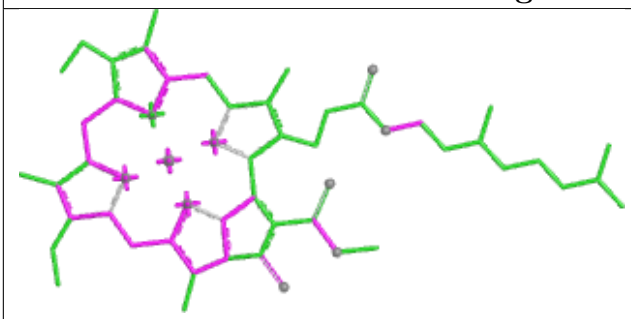


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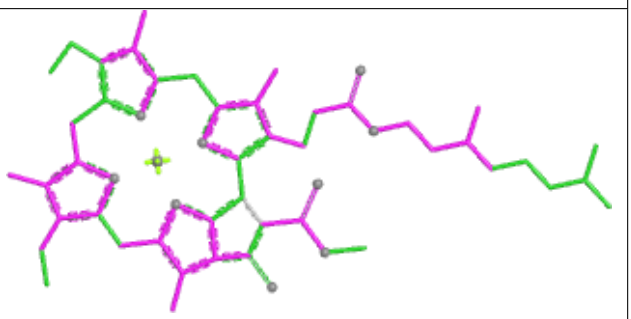


Rings

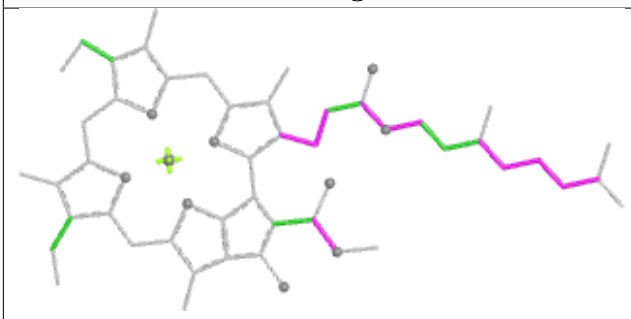
Ligand CLA B 1228



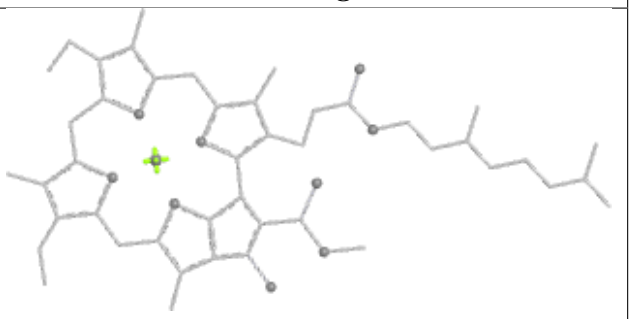
Bond lengths



Bond angles

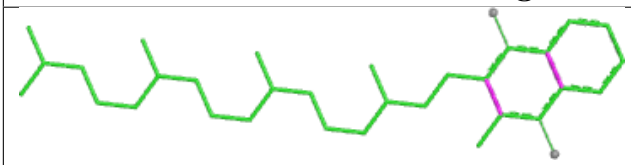


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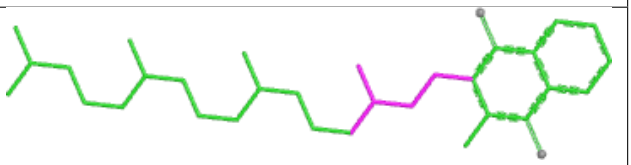


Rings

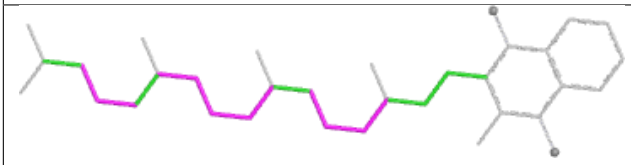
Ligand PQN b 2002



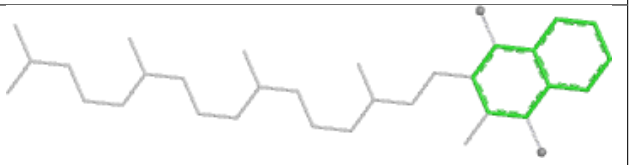
Bond lengths



Bond angles

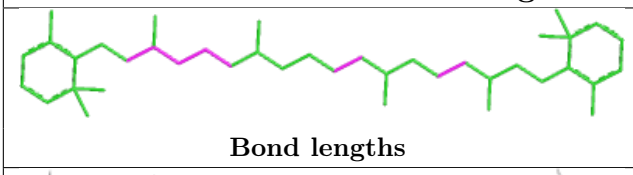


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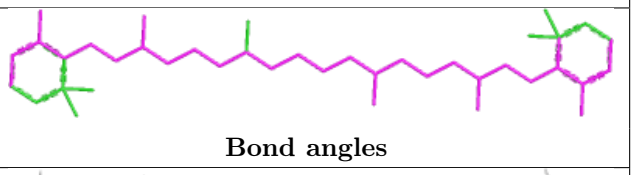


Rings

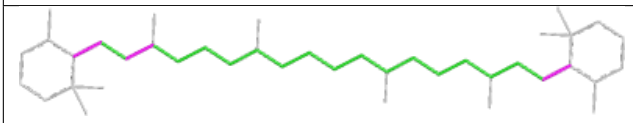
Ligand BCR a 4002



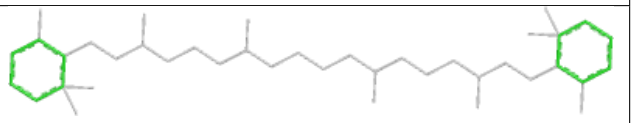
Bond lengths



Bond angles

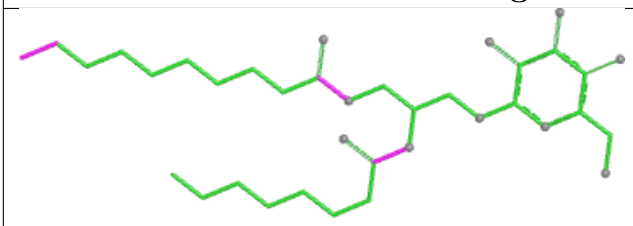


Torsions

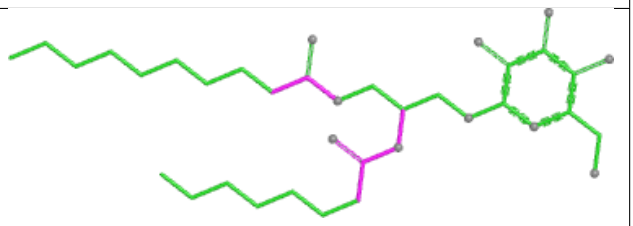


Rings

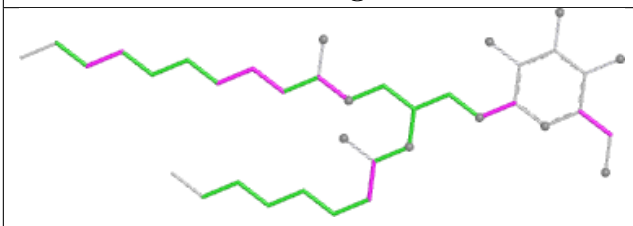
Ligand LMG R 5006



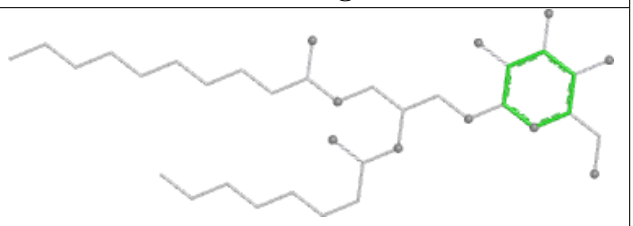
Bond lengths



Bond angles

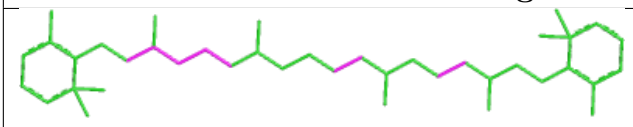


Torsions



Rings

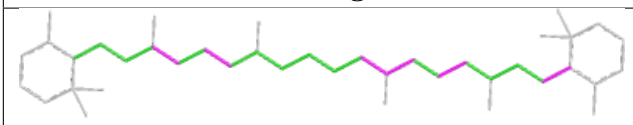
Ligand BCR b 4010



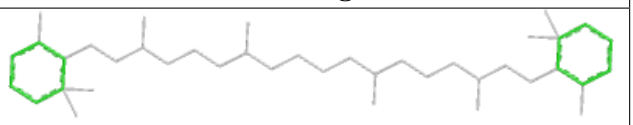
Bond lengths



Bond angles

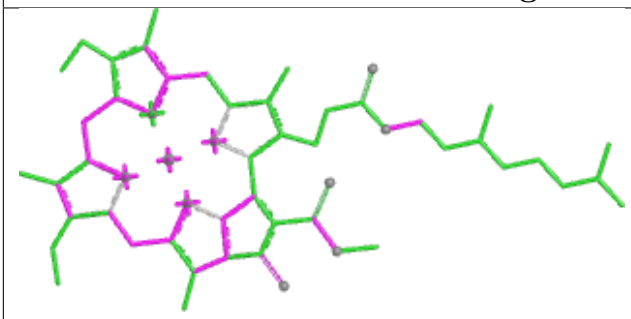


Torsions

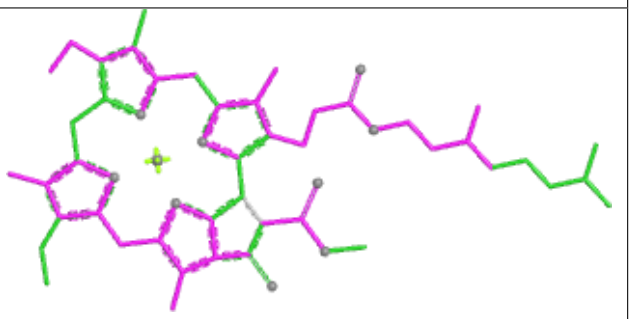


Rings

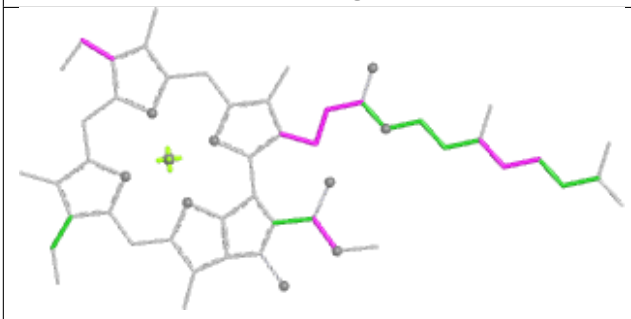
Ligand CLA a 1116



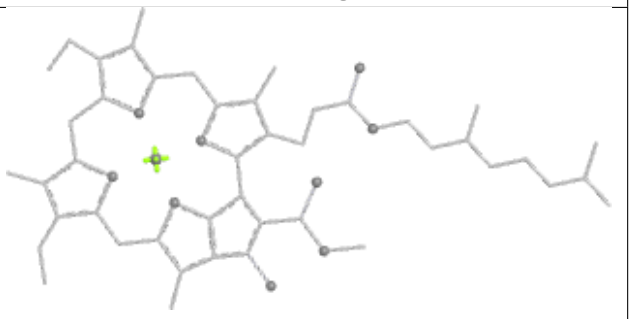
Bond lengths



Bond angles

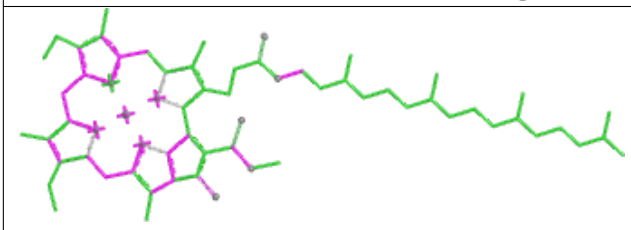


Torsions

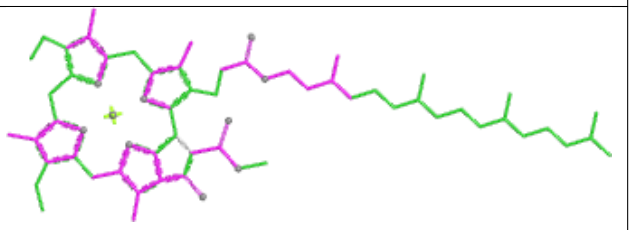


Rings

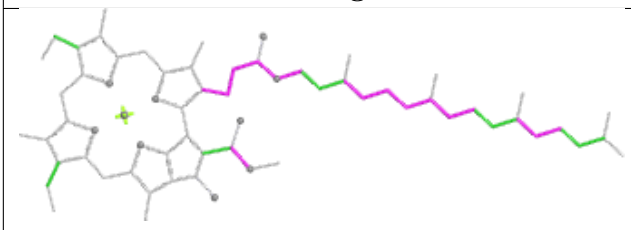
Ligand CLA G 1140



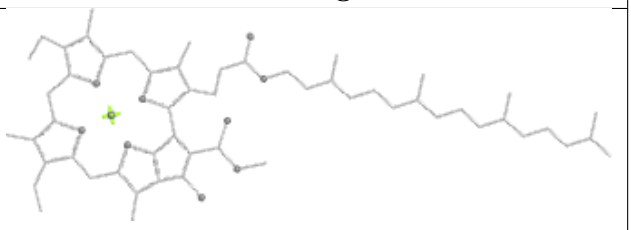
Bond lengths



Bond angles

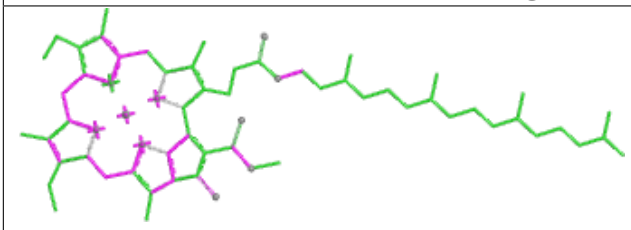


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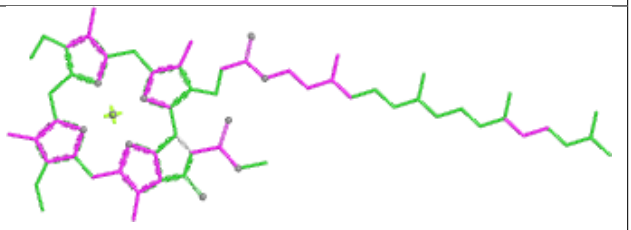


Rings

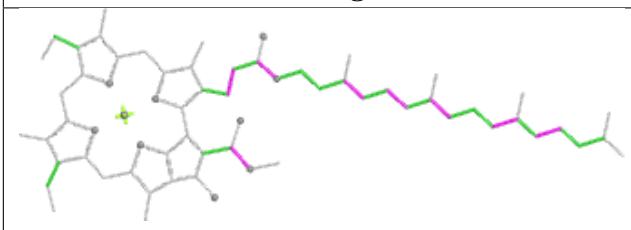
Ligand CLA l 1501



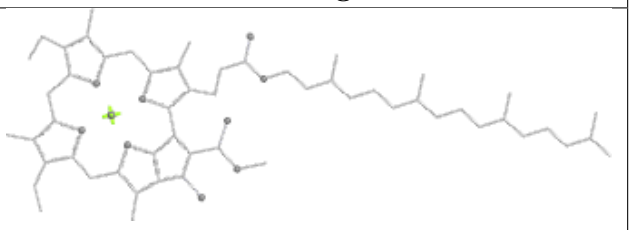
Bond lengths



Bond angles

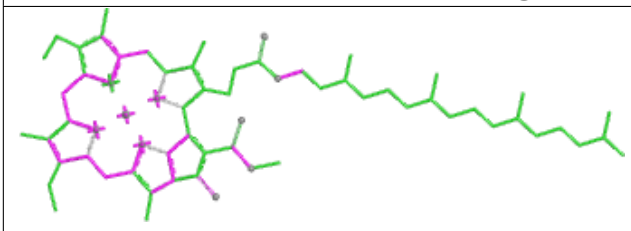


Torsions

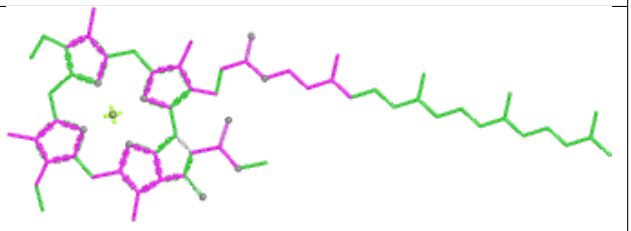


Rings

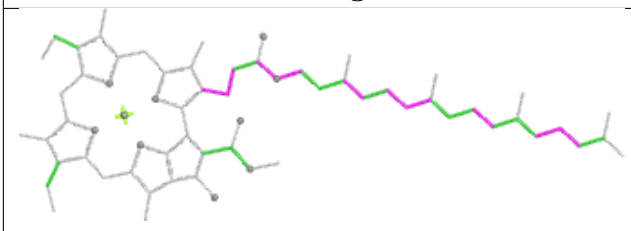
Ligand CLA B 1210



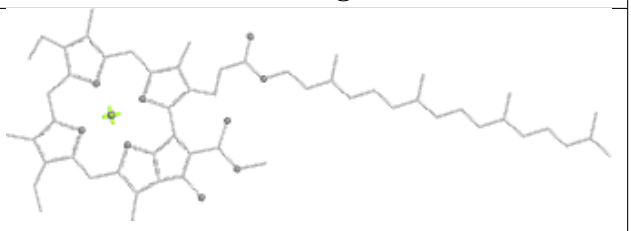
Bond lengths



Bond angles

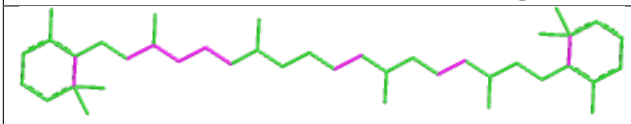


Torsions

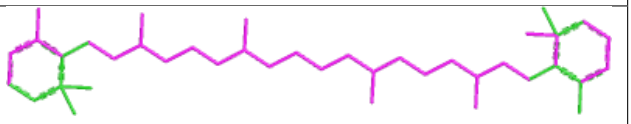


Rings

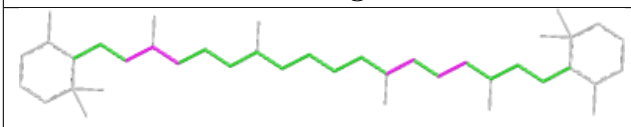
Ligand BCR B 4014



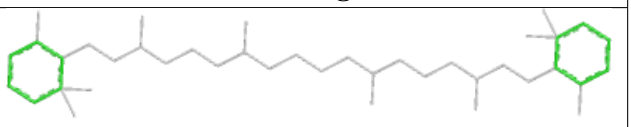
Bond lengths



Bond angles

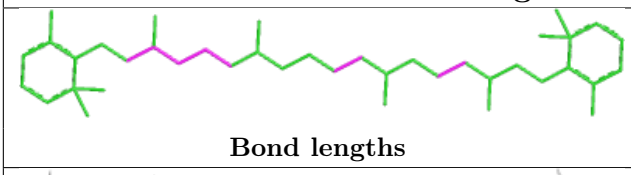


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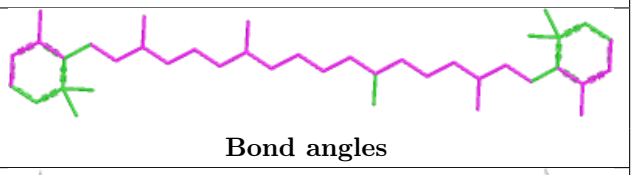


Rings

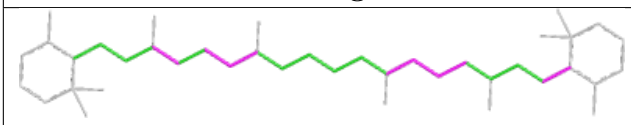
Ligand BCR B 4013



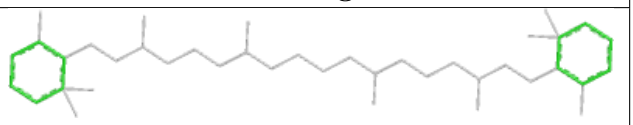
Bond lengths



Bond angles

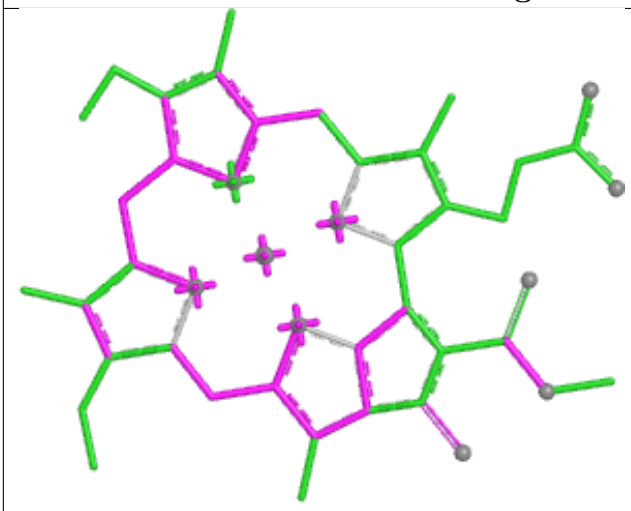


Torsions

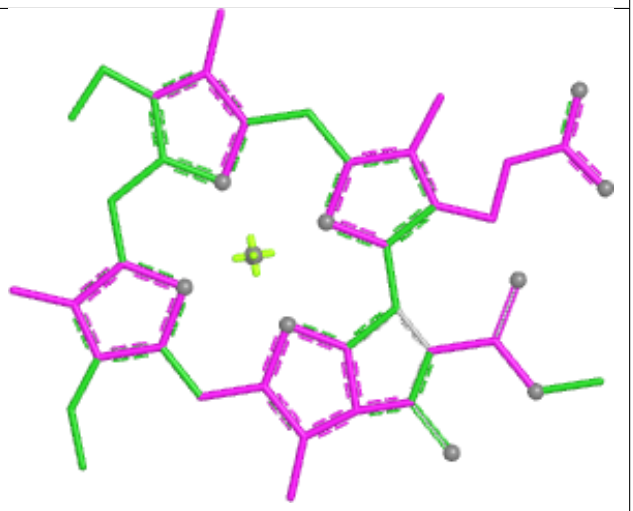


Rings

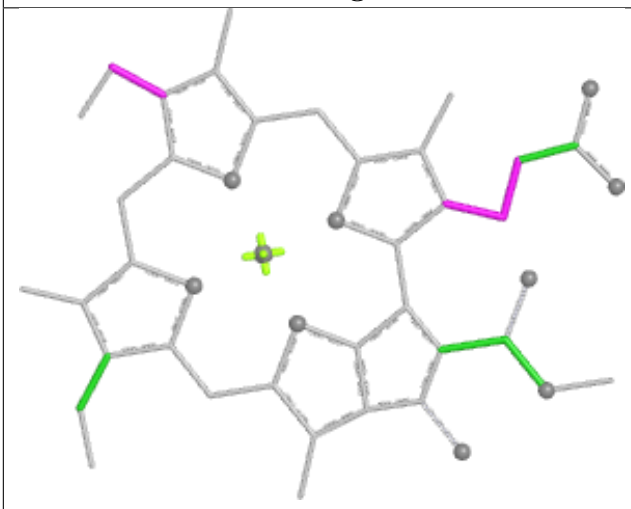
Ligand CLA H 1209



Bond lengths



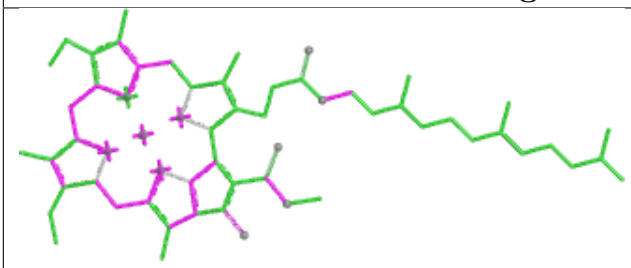
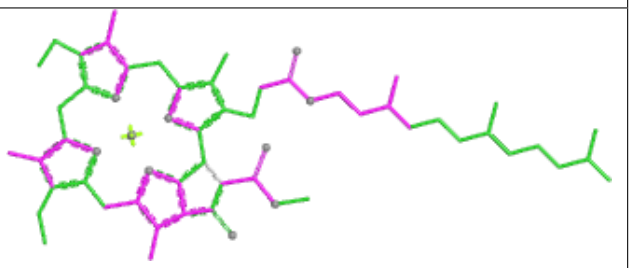
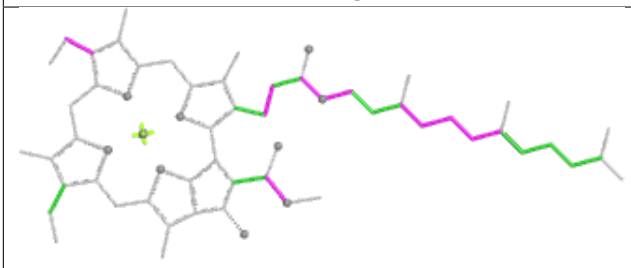
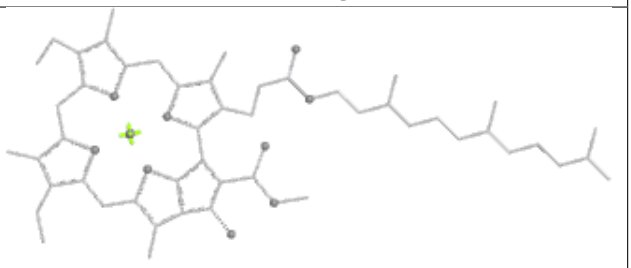
Bond angles

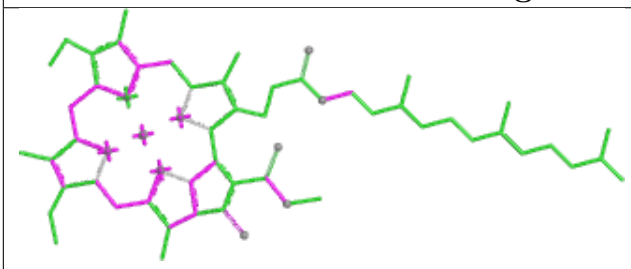
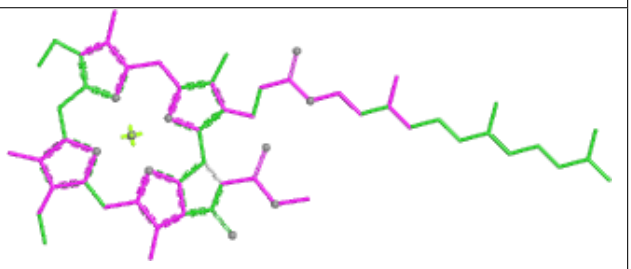
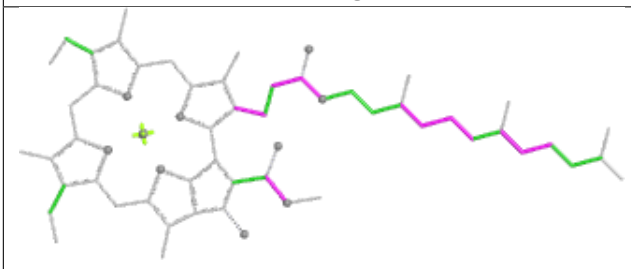
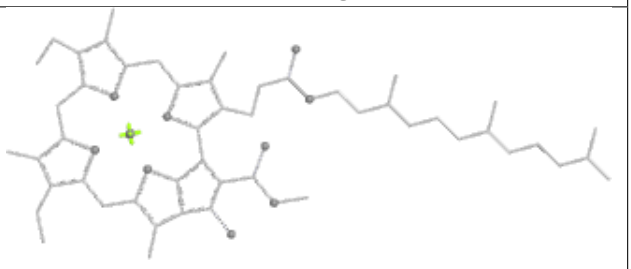


Torsions

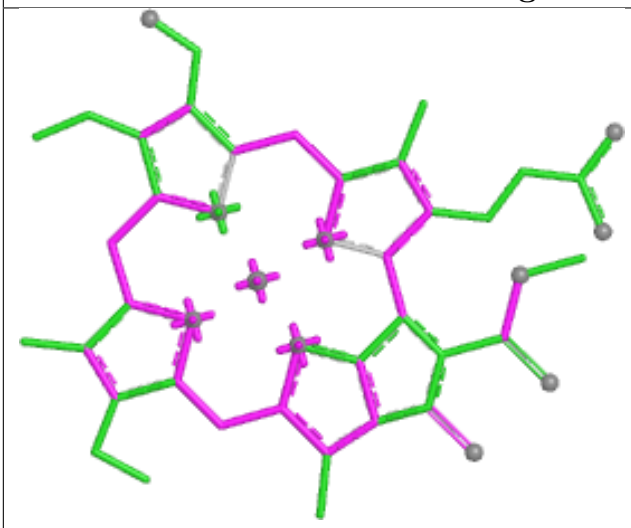


Rings

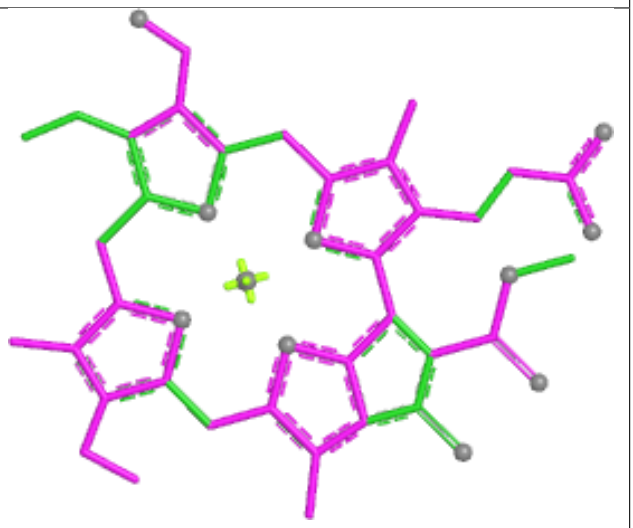
Ligand CLA a 1131	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 1138	
	
Bond lengths	Bond angles
	
Torsions	Rings

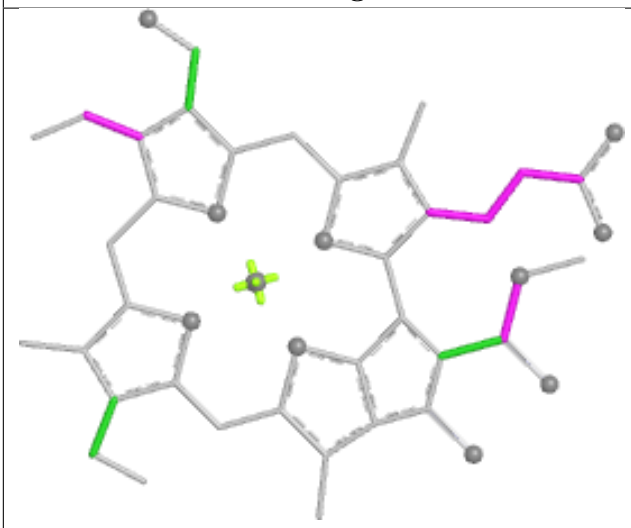
Ligand F6C A 1121



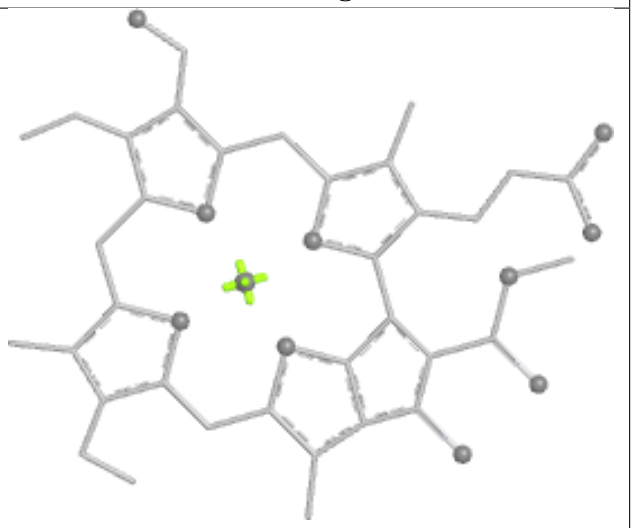
Bond lengths



Bond angles

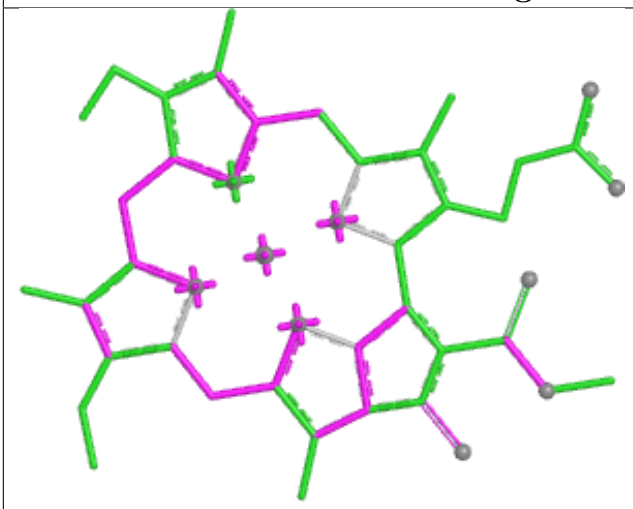


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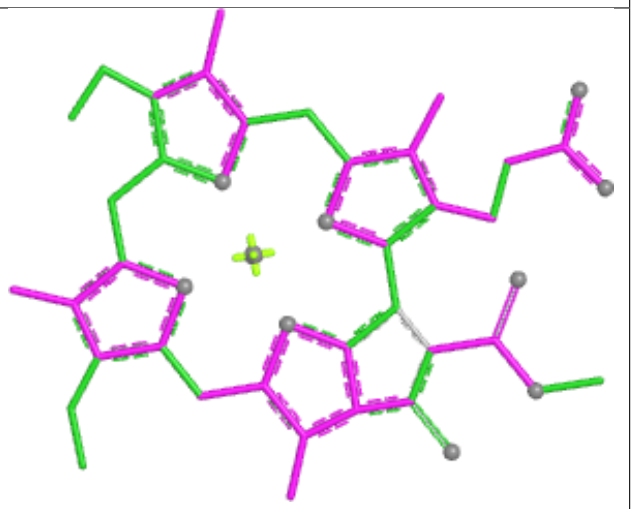


Rings

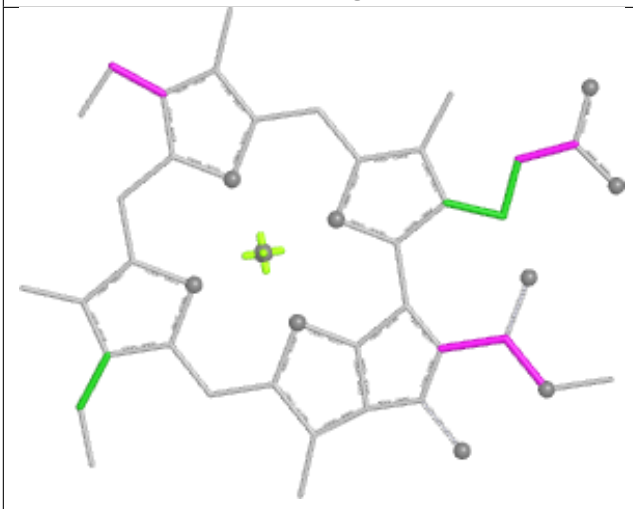
Ligand CLA A 1101



Bond lengths



Bond angles

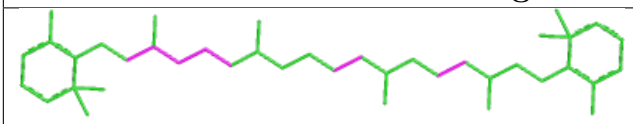


Torsions

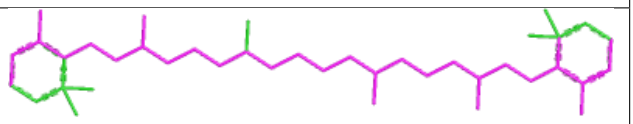


Rings

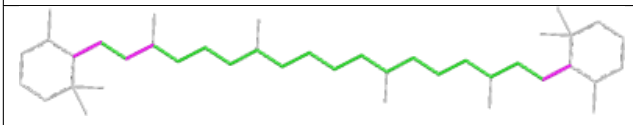
Ligand BCR G 4002



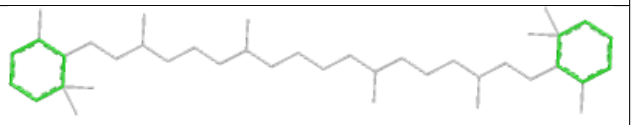
Bond lengths



Bond angles

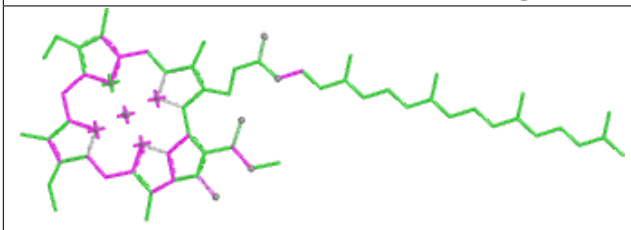


Torsions

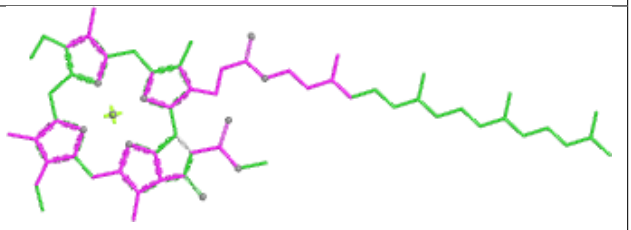


Rings

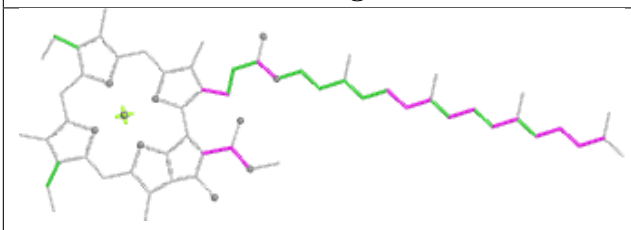
Ligand CLA B 1222



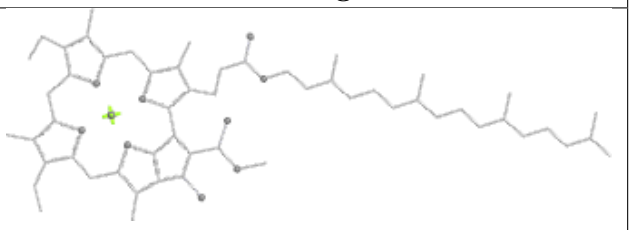
Bond lengths



Bond angles

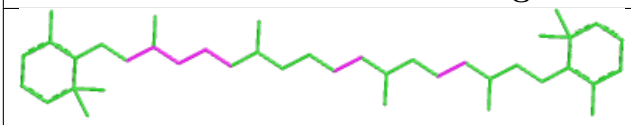


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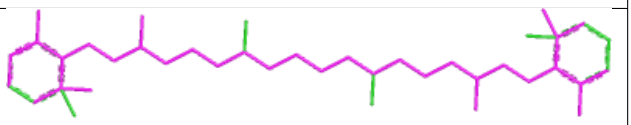


Rings

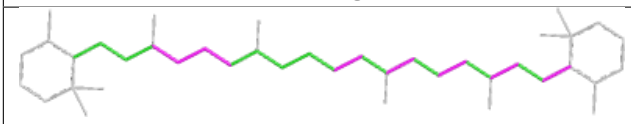
Ligand BCR U 4019



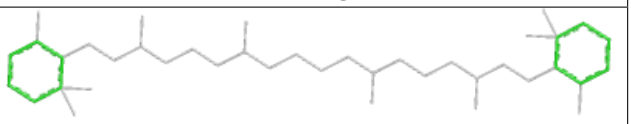
Bond lengths



Bond angles

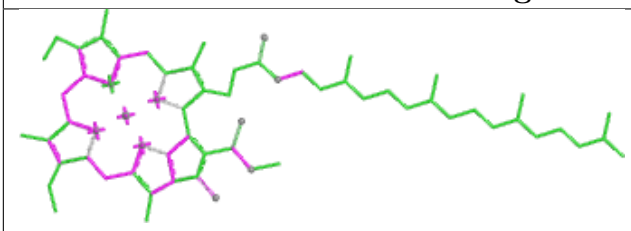


Torsions

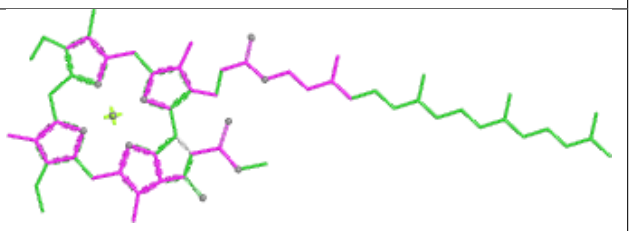


Rings

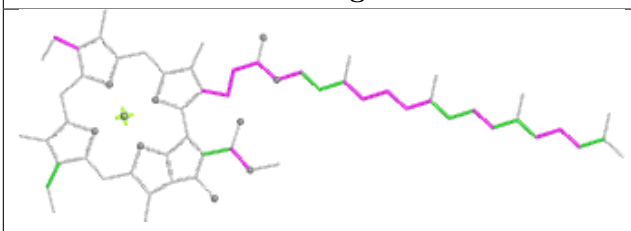
Ligand CLA G 1136



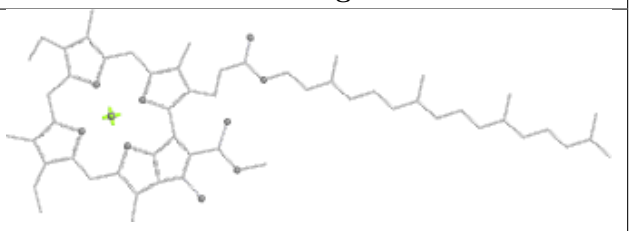
Bond lengths



Bond angles

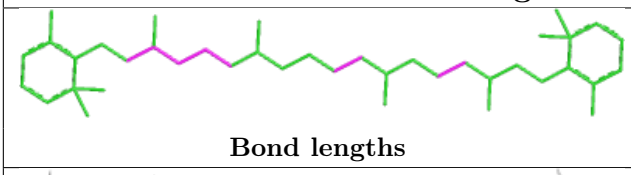


Torsions

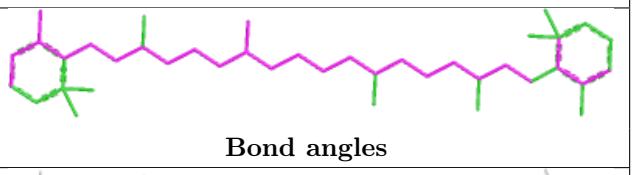


Rings

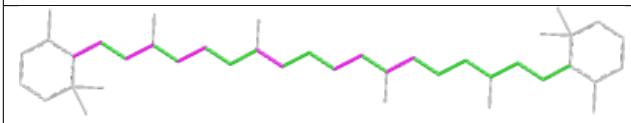
Ligand BCR B 4016



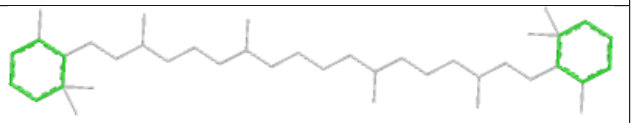
Bond lengths



Bond angles

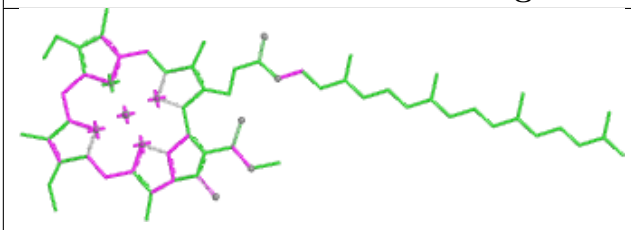


Torsions

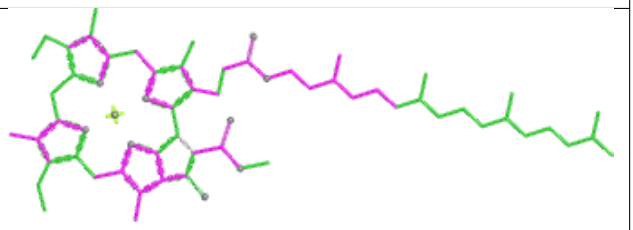


Rings

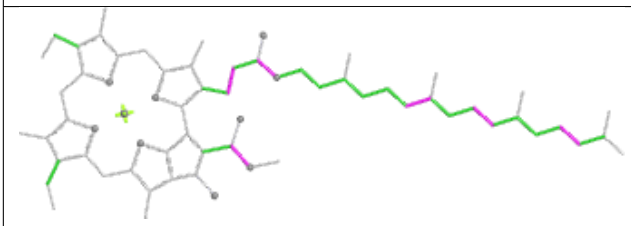
Ligand CLA A 1104



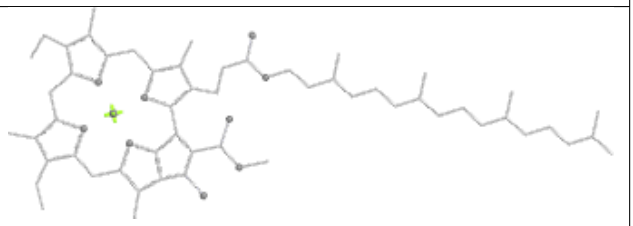
Bond lengths



Bond angles

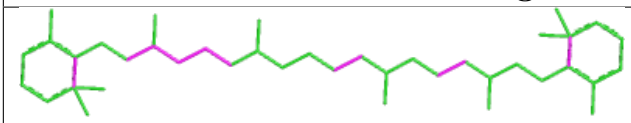


Torsions



Rings

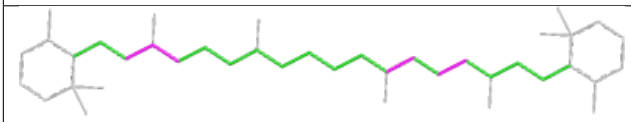
Ligand BCR b 4014



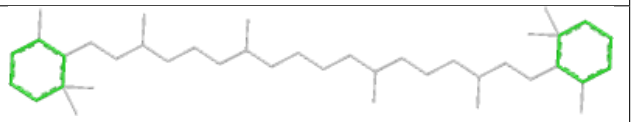
Bond lengths



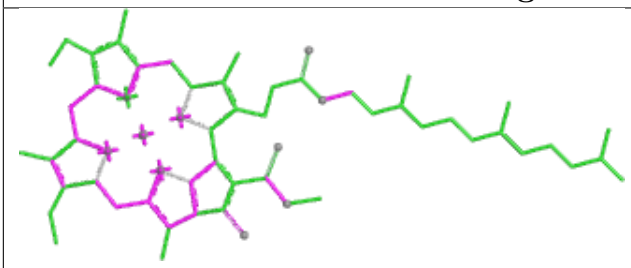
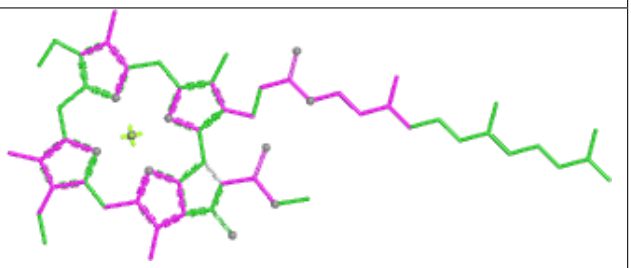
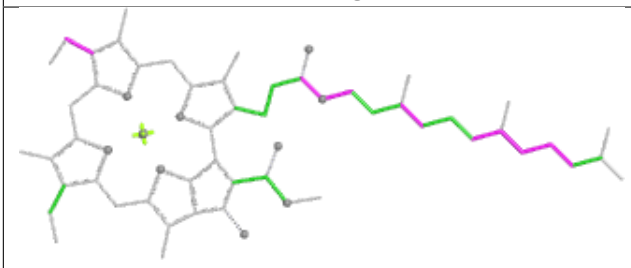
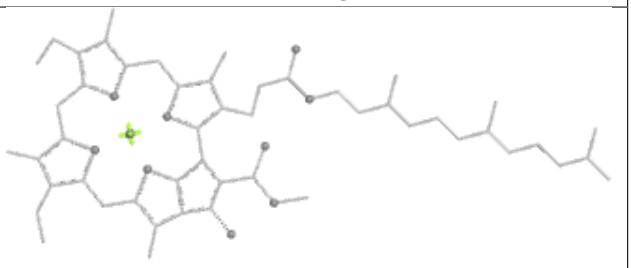
Bond angles

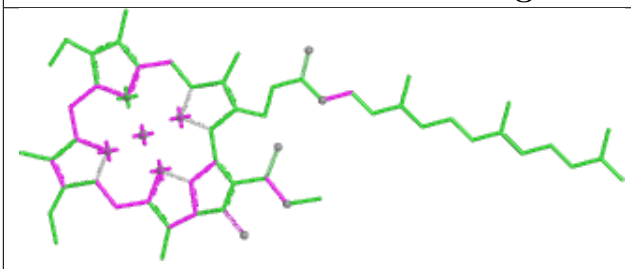
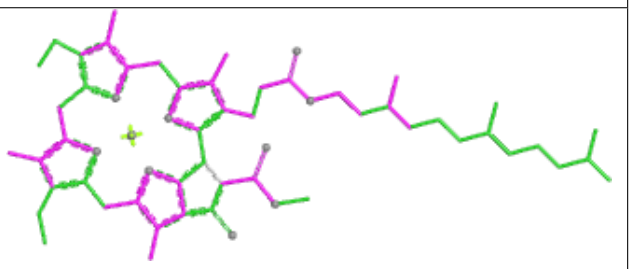
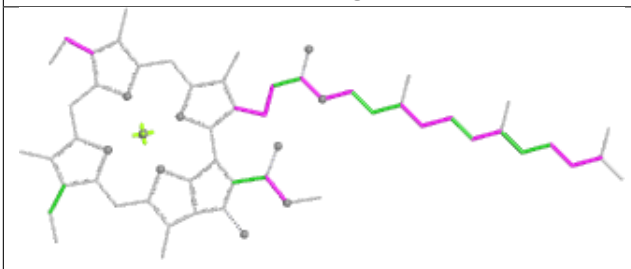
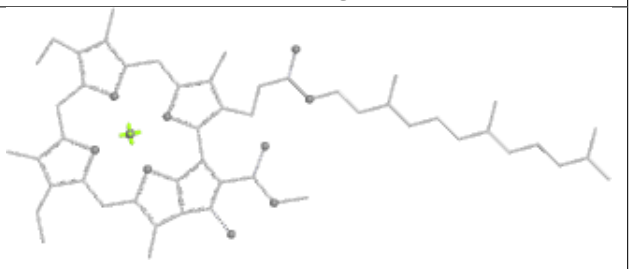


Torsions

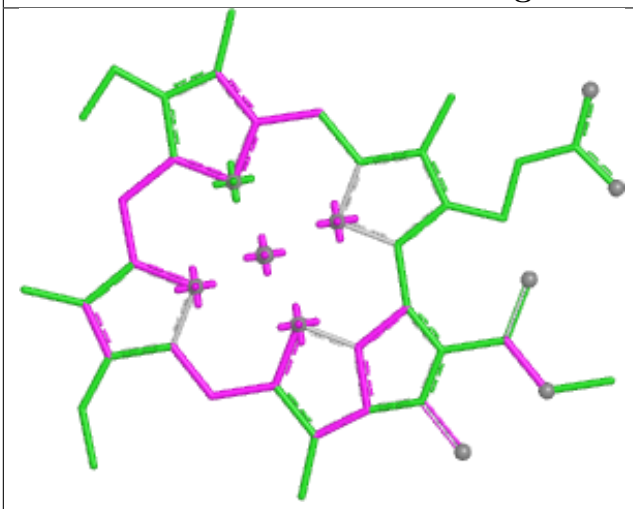


Rings

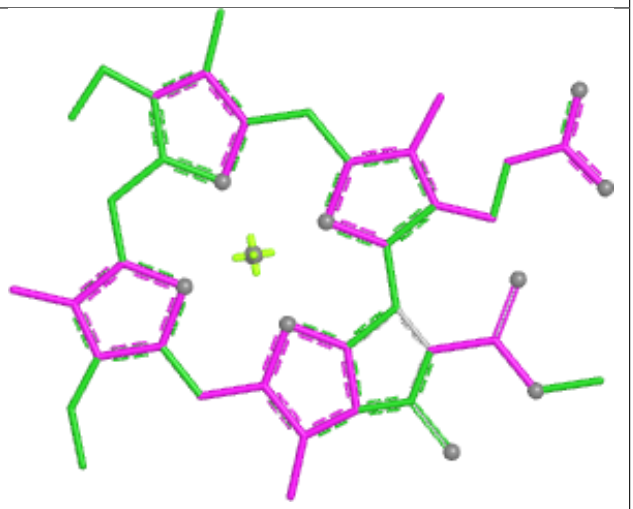
Ligand CLA L 1502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1215	
	
Bond lengths	Bond angles
	
Torsions	Rings

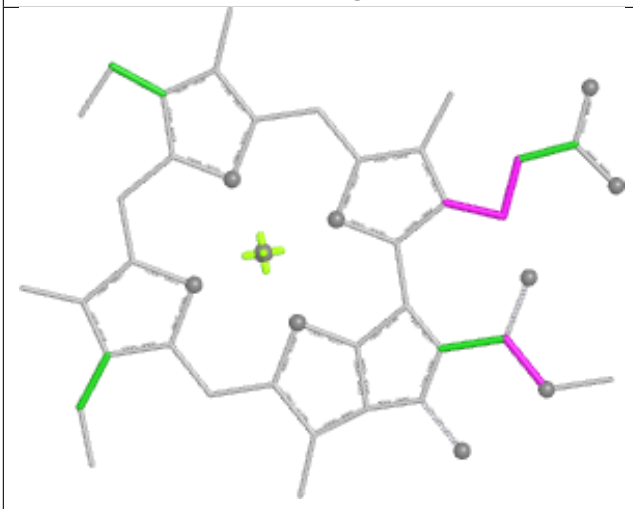
Ligand CLA H 1212



Bond lengths



Bond angles

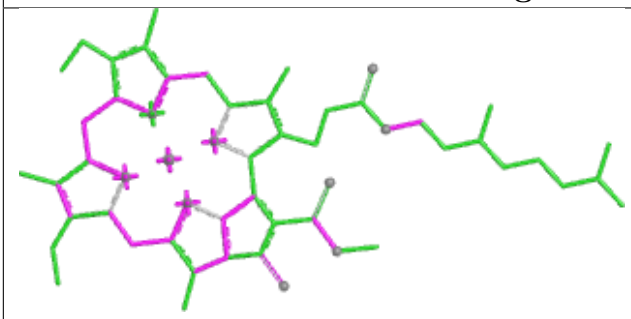


Torsions

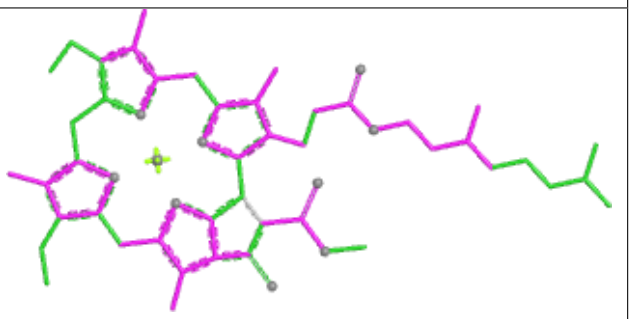


Rings

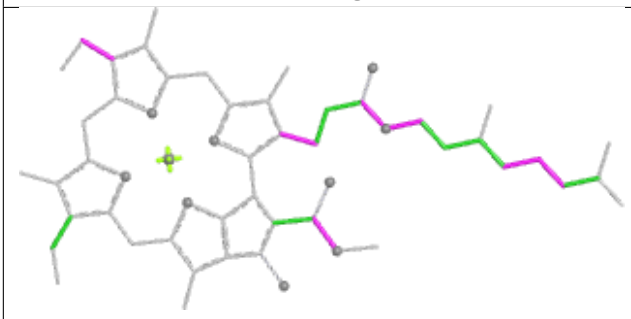
Ligand CLA A 1124



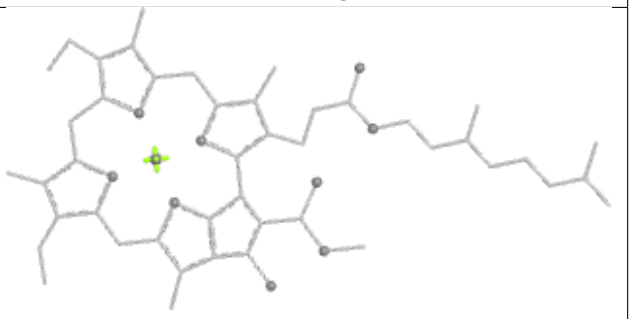
Bond lengths



Bond angles

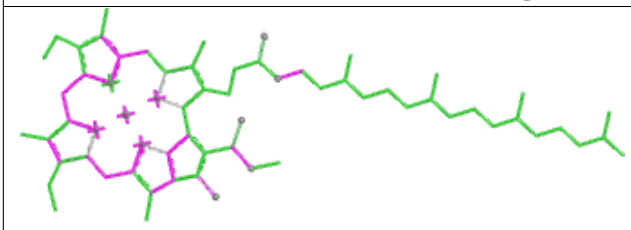


Torsions

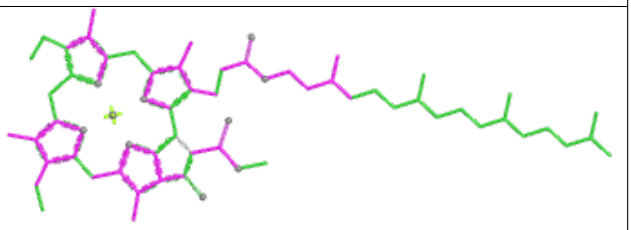


Rings

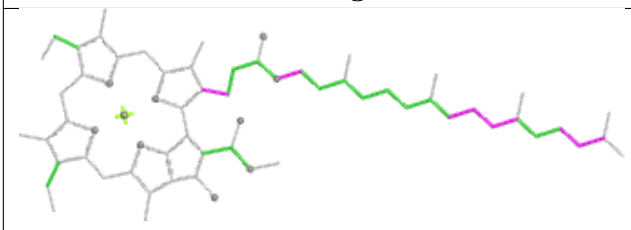
Ligand CLA b 1221



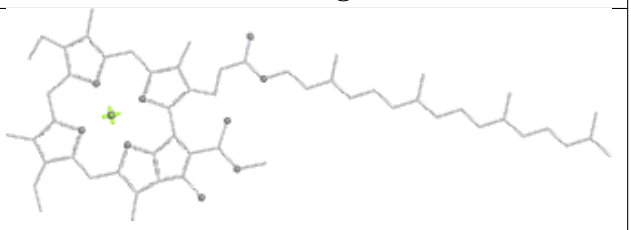
Bond lengths



Bond angles

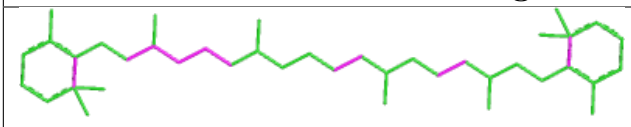


Torsions

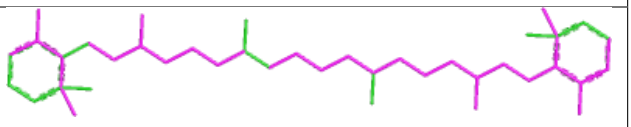


Rings

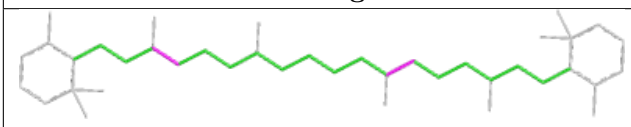
Ligand BCR H 4005



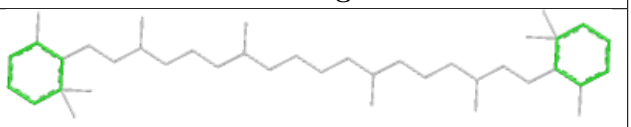
Bond lengths



Bond angles

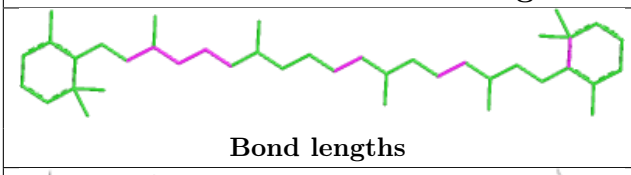


Torsions

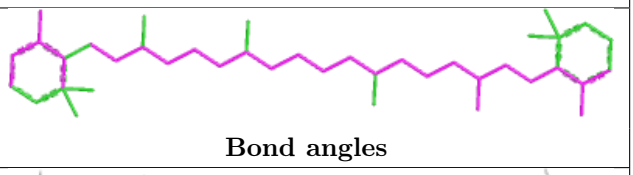


Rings

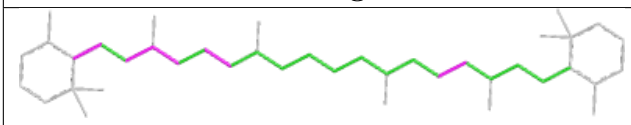
Ligand BCR b 4009



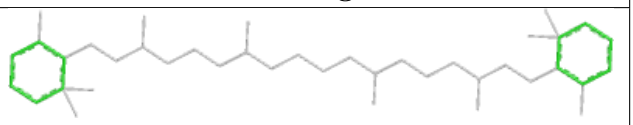
Bond lengths



Bond angles

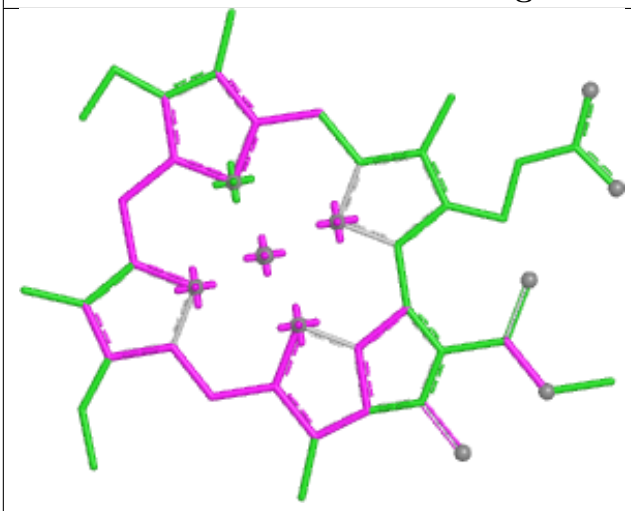


Torsions

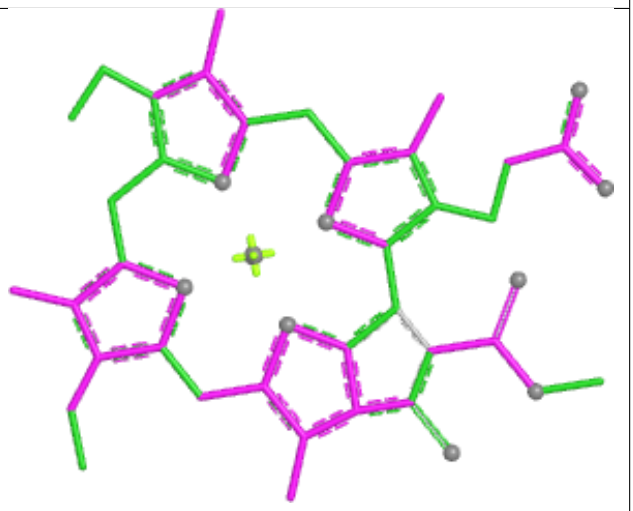


Rings

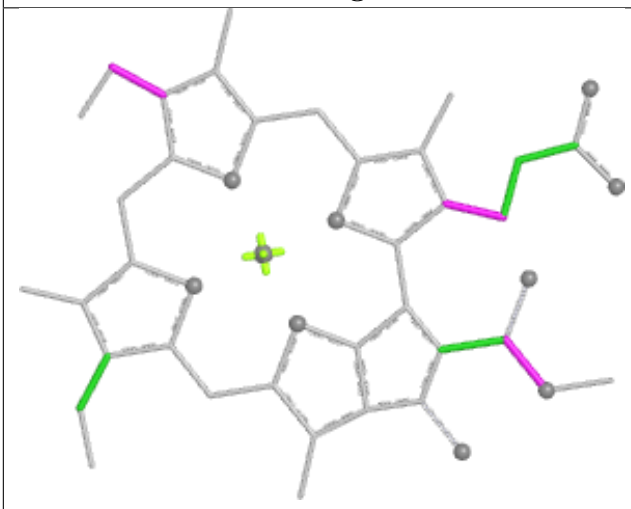
Ligand CLA B 1219



Bond lengths



Bond angles

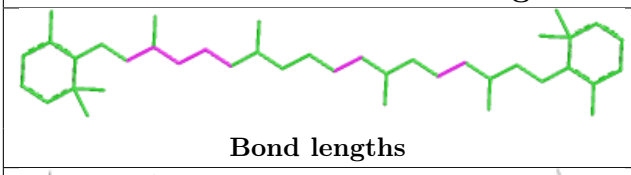


Torsions

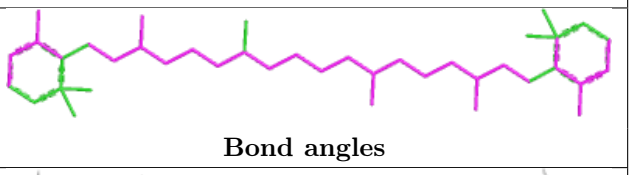


Rings

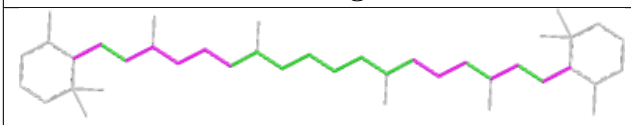
Ligand BCR G 4003



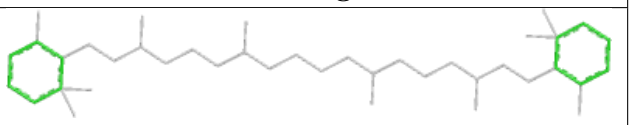
Bond lengths



Bond angles

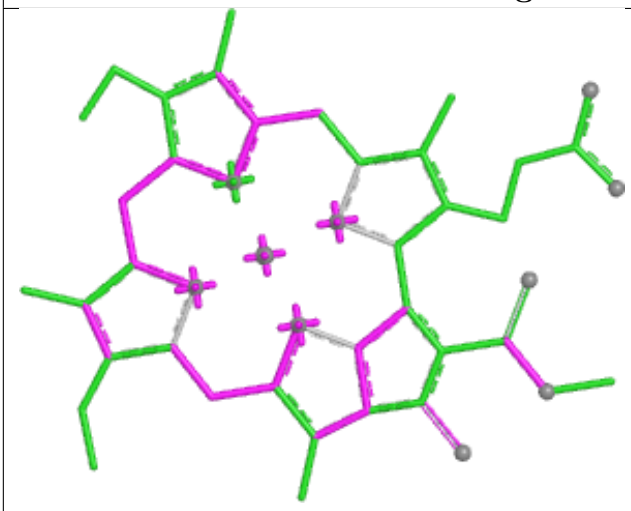


Torsions

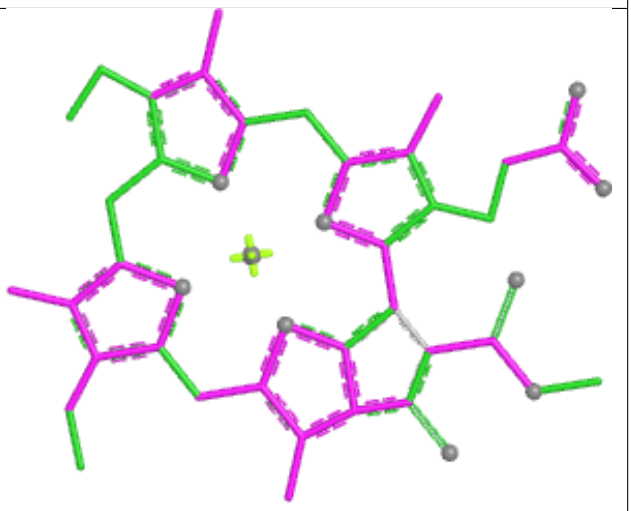


Rings

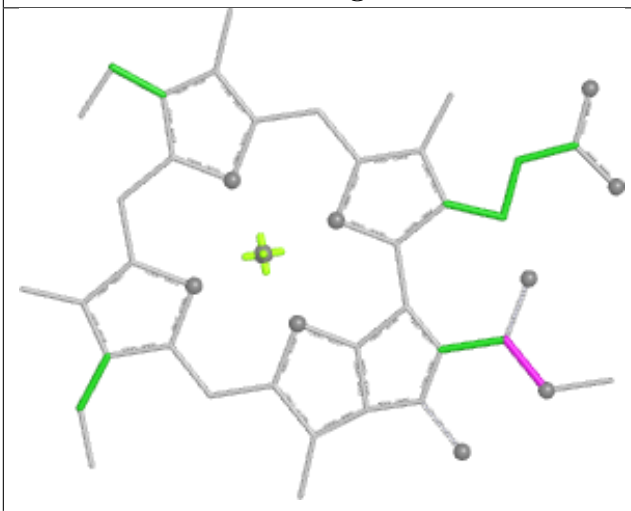
Ligand CLA B 1232



Bond lengths



Bond angles

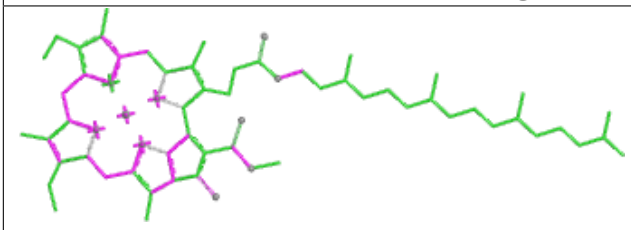


Torsions

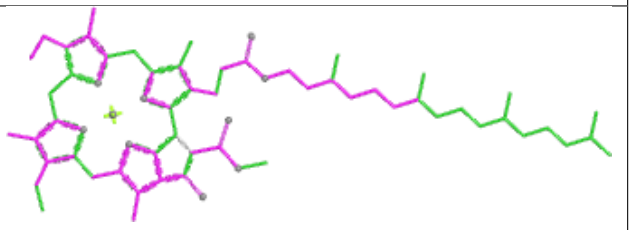


Rings

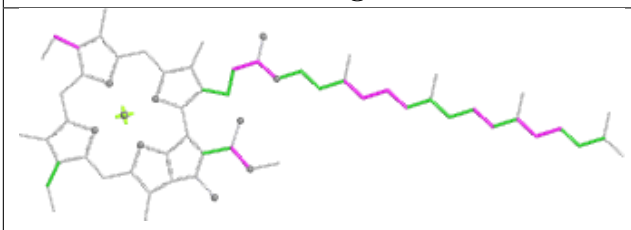
Ligand CLA H 1204



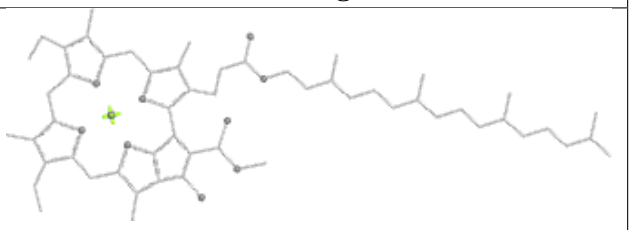
Bond lengths



Bond angles

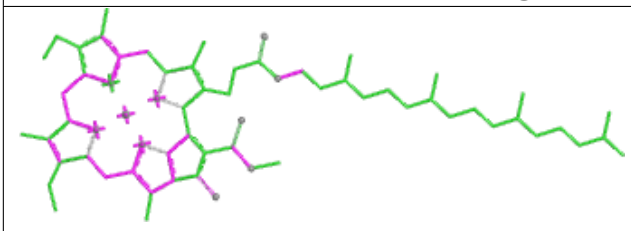


Torsions

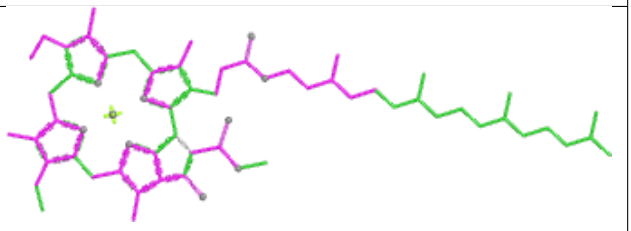


Rings

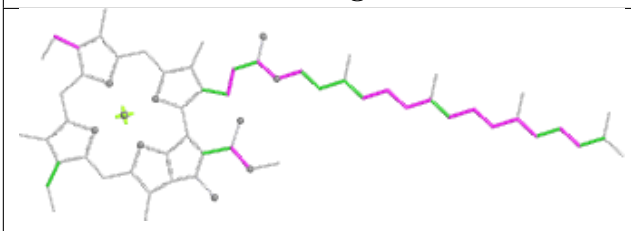
Ligand CLA B 1214



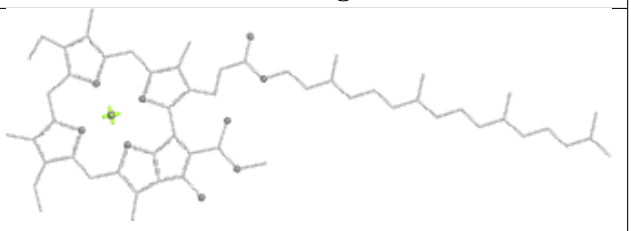
Bond lengths



Bond angles

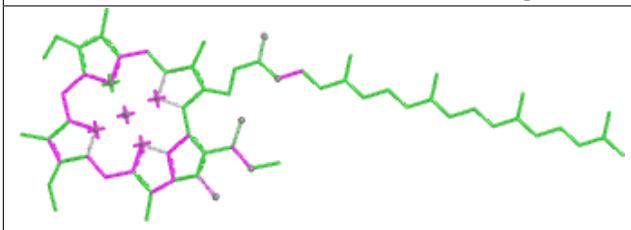


Torsions

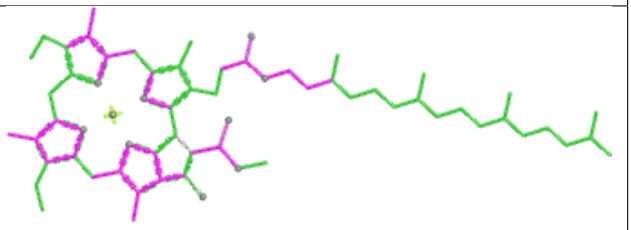


Rings

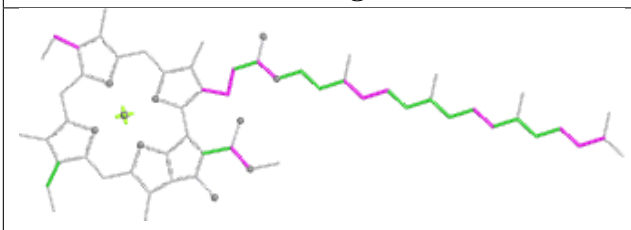
Ligand CLA b 1225



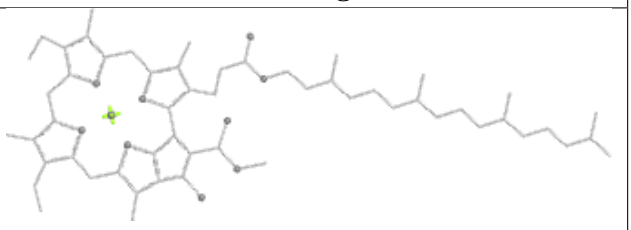
Bond lengths



Bond angles

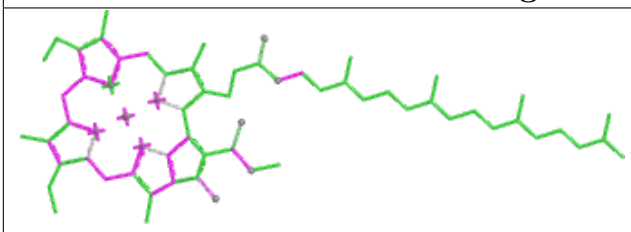


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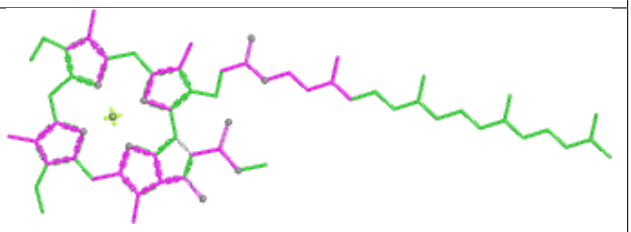


Rings

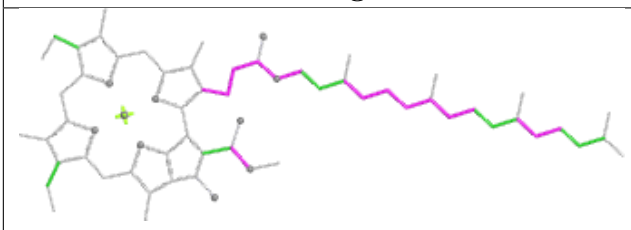
Ligand CLA a 1140



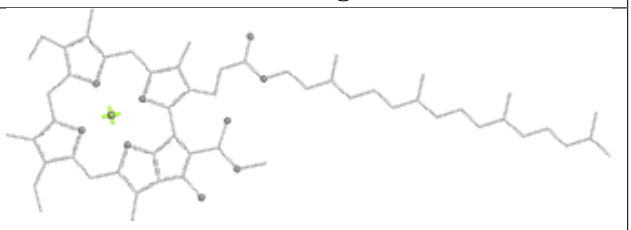
Bond lengths



Bond angles

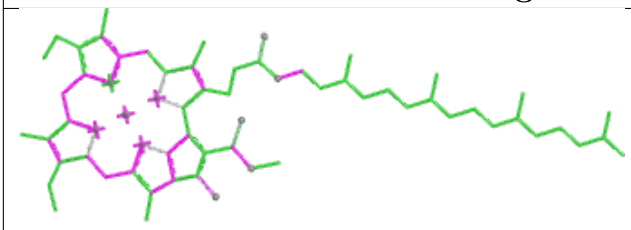


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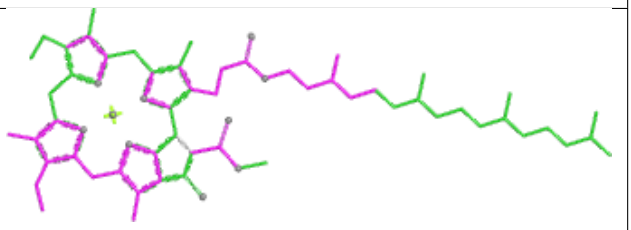


Rings

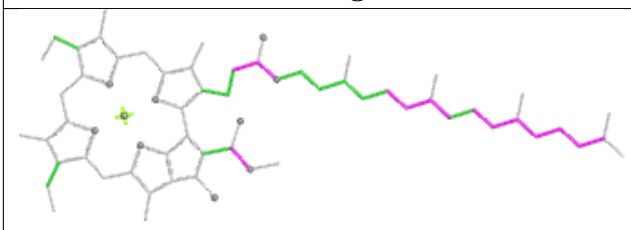
Ligand CLA B 1021



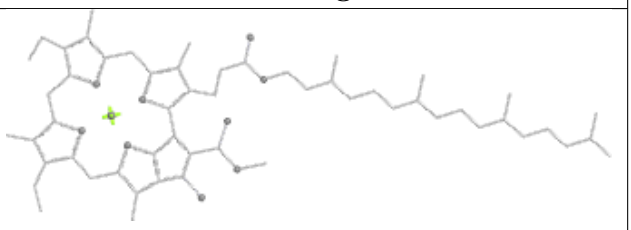
Bond lengths



Bond angles

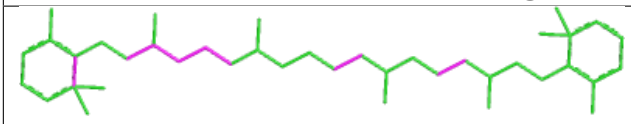


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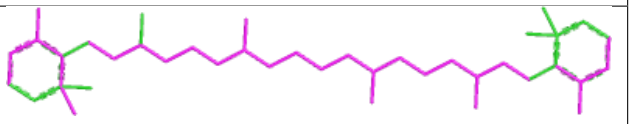


Rings

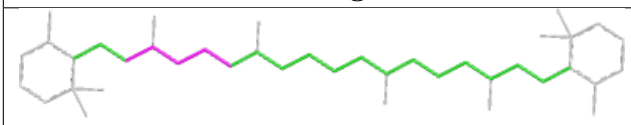
Ligand BCR l 4022



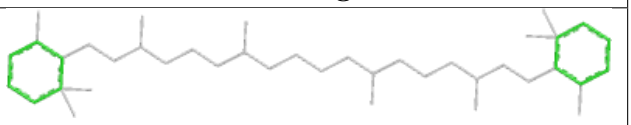
Bond lengths



Bond angles

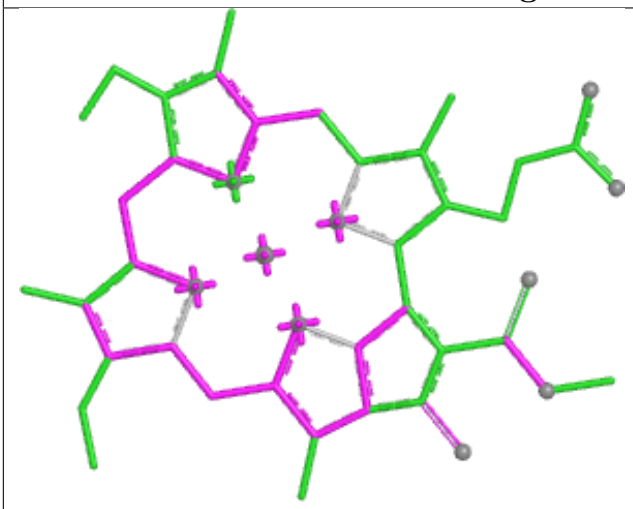


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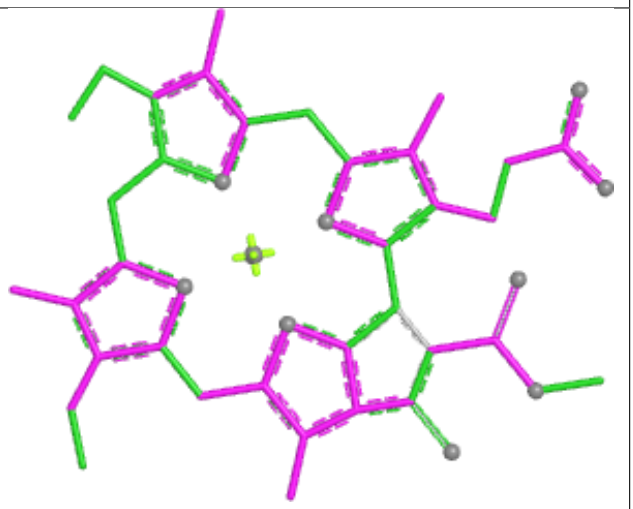


Rings

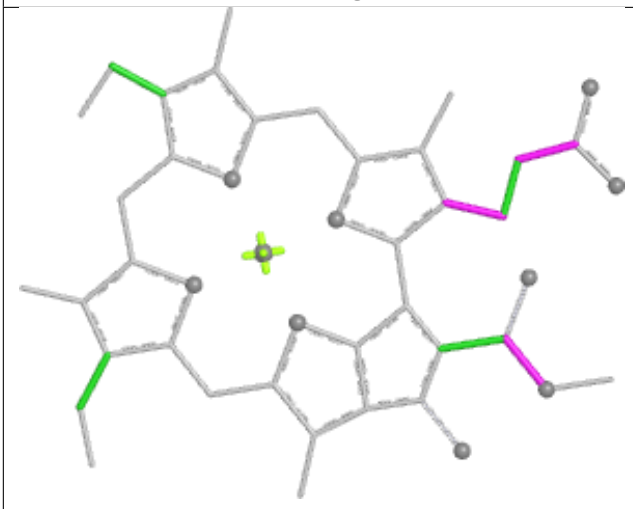
Ligand CLA a 1105



Bond lengths



Bond angles

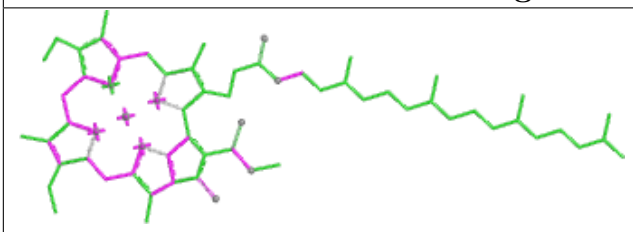


Torsions

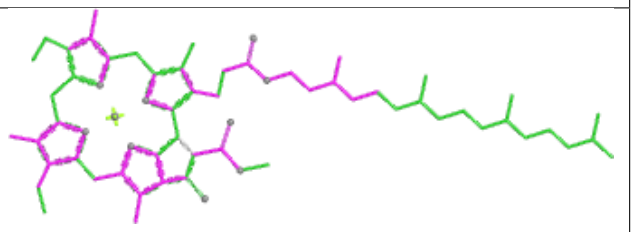


Rings

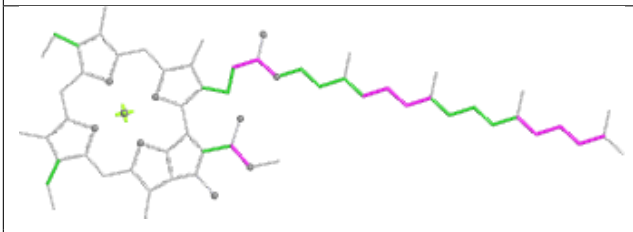
Ligand CLA H 1208



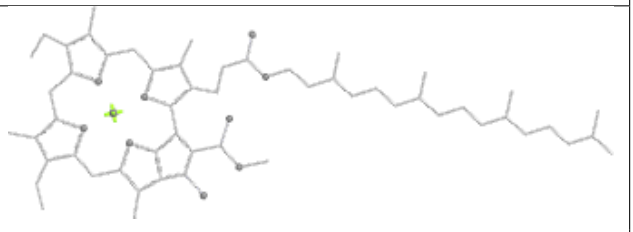
Bond lengths



Bond angles

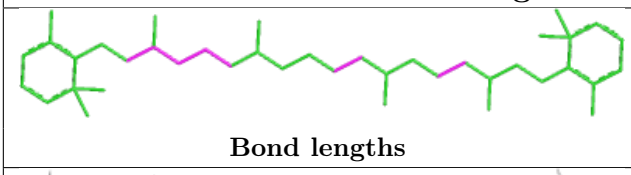


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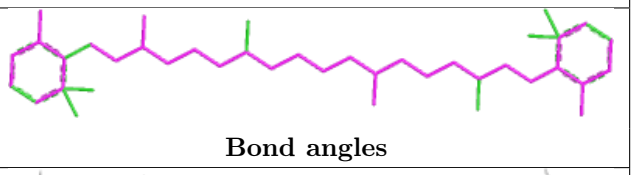


Rings

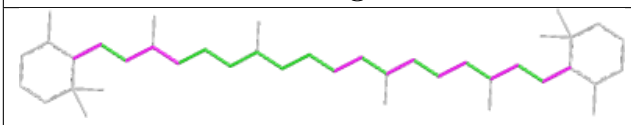
Ligand BCR A 4001



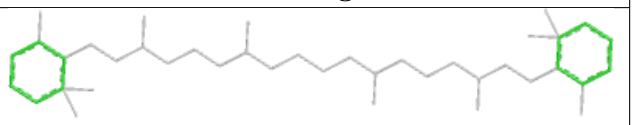
Bond lengths



Bond angles

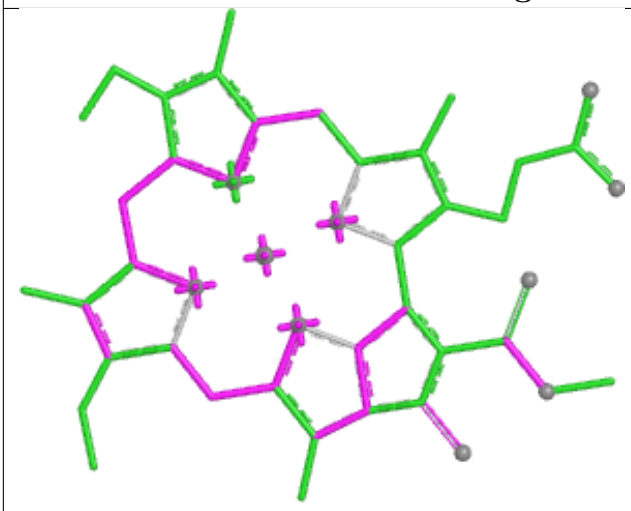


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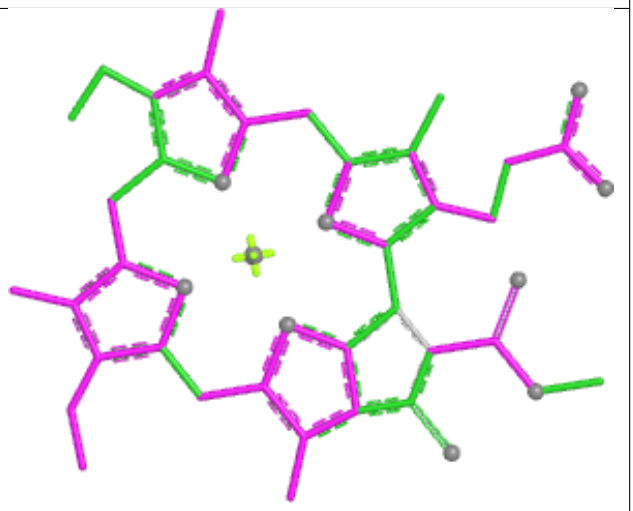


Rings

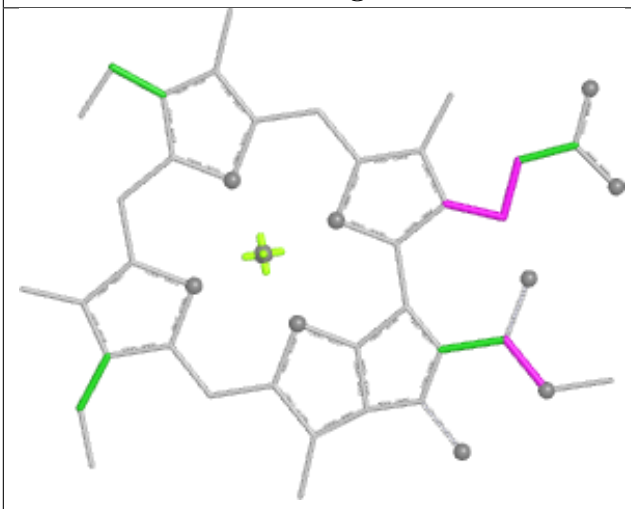
Ligand CLA H 1206



Bond lengths



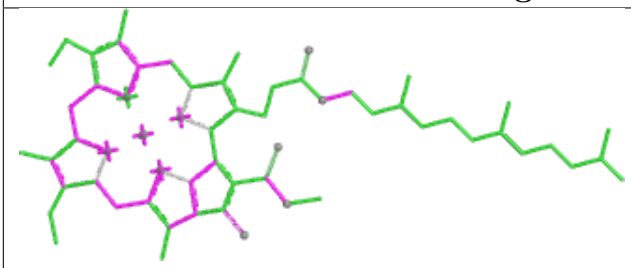
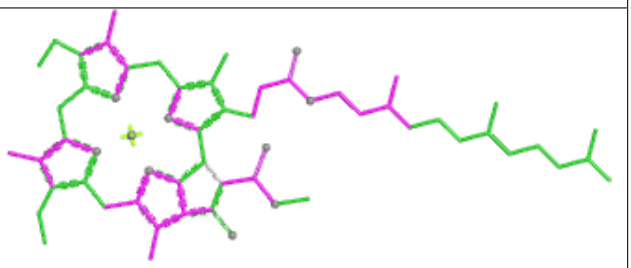
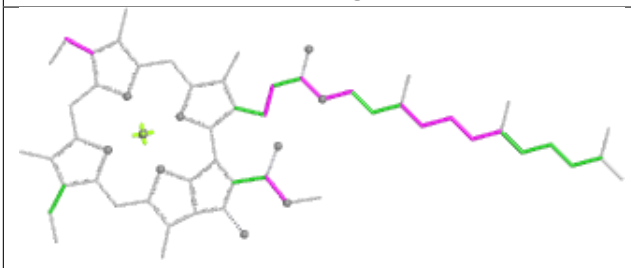
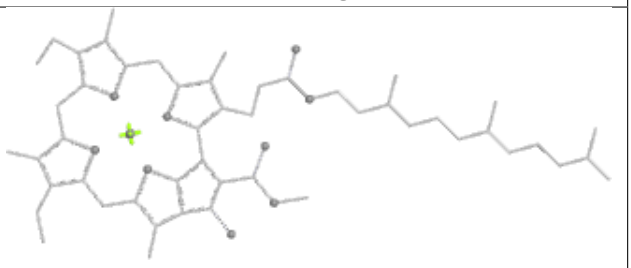
Bond angles

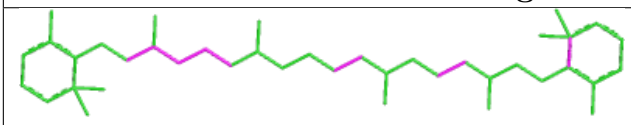
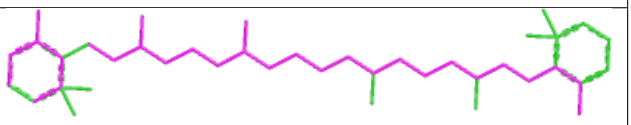
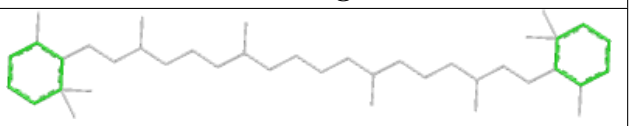


Torsions

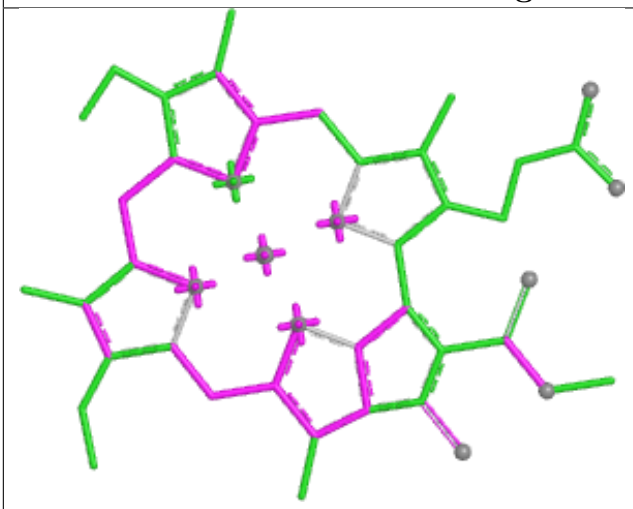


Rings

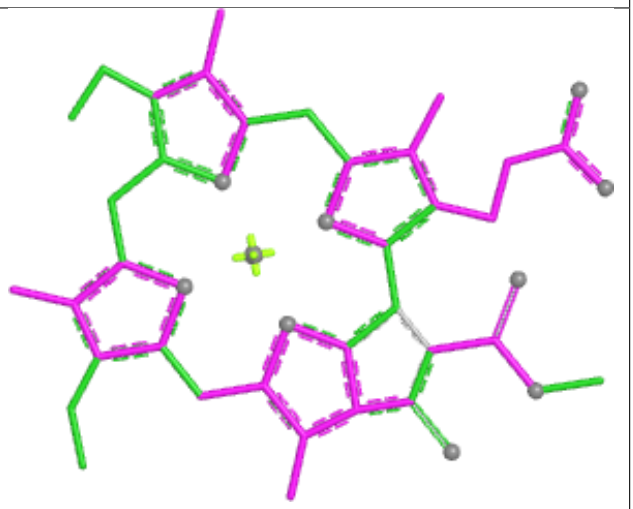
Ligand CLA A 1131	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 4017	
	
Bond lengths	Bond angles
	
Torsions	Rings

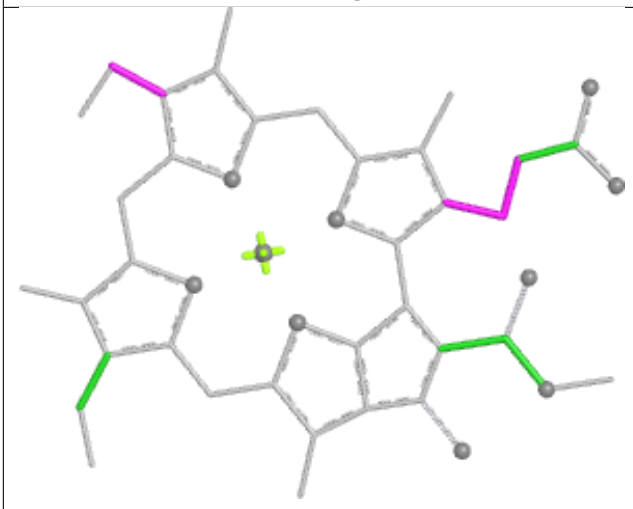
Ligand CLA B 1209



Bond lengths



Bond angles

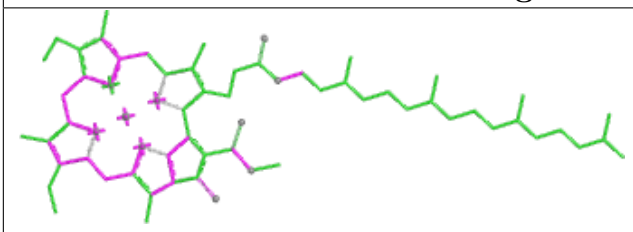


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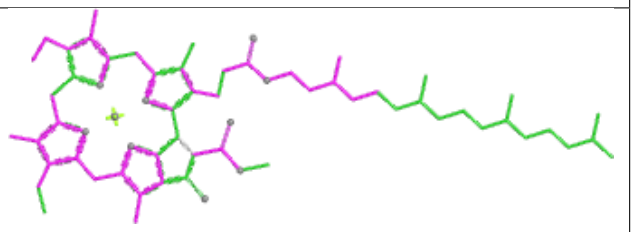


Rings

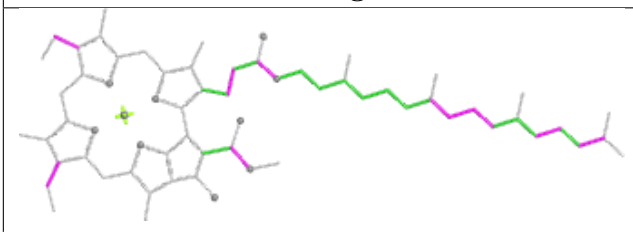
Ligand CLA B 1023



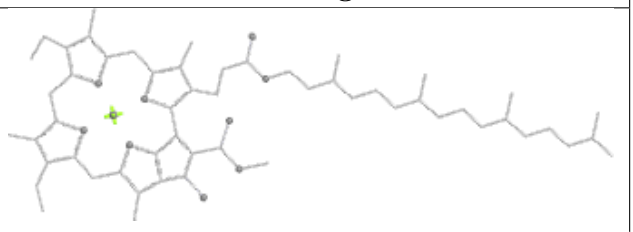
Bond lengths



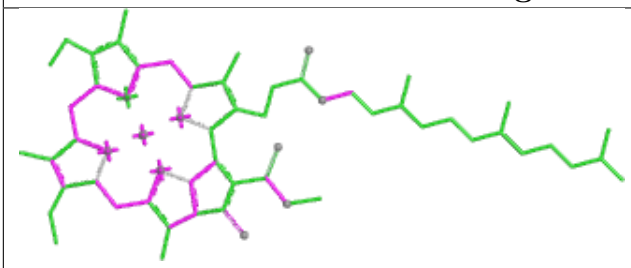
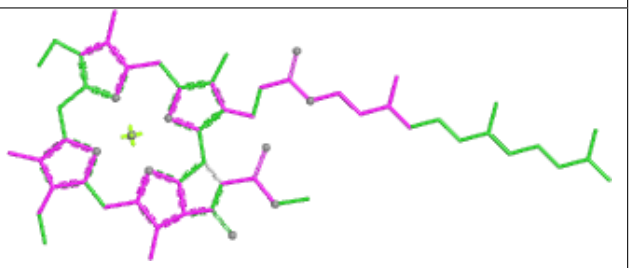
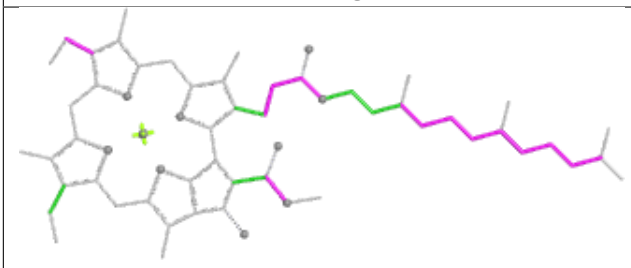
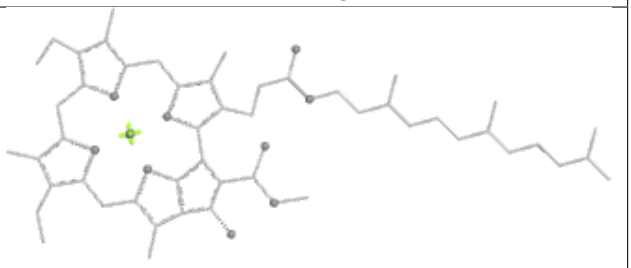
Bond angles

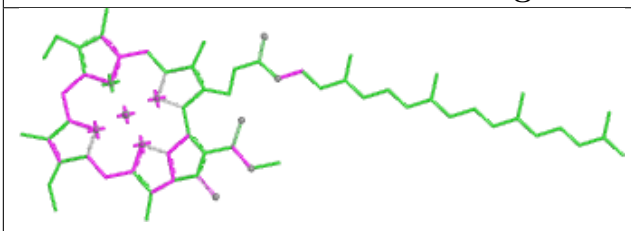
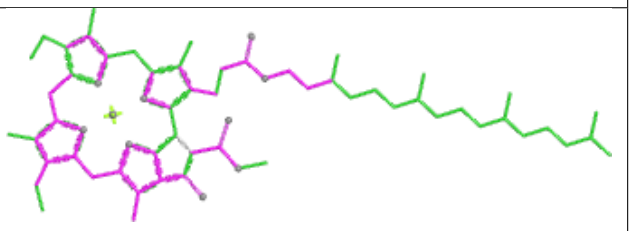
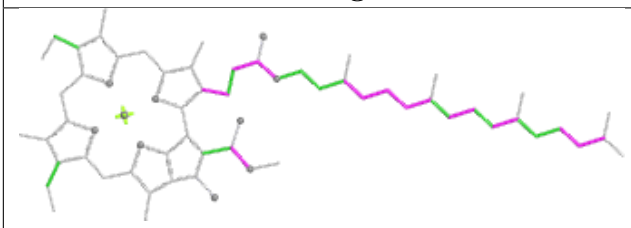
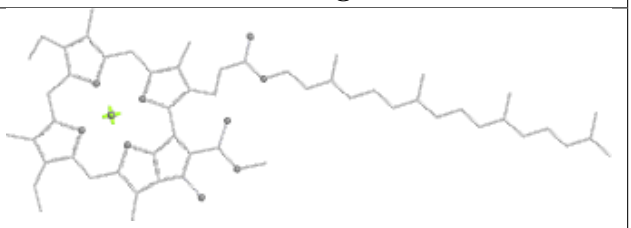


Torsions

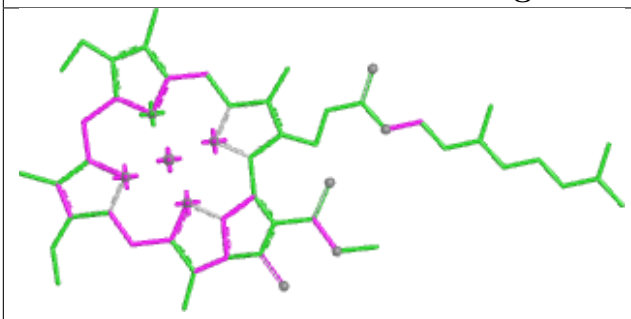


Rings

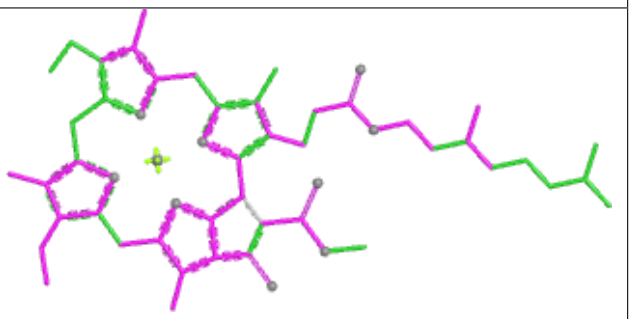
Ligand CLA A 1126	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 1125	
	
Bond lengths	Bond angles
	
Torsions	Rings

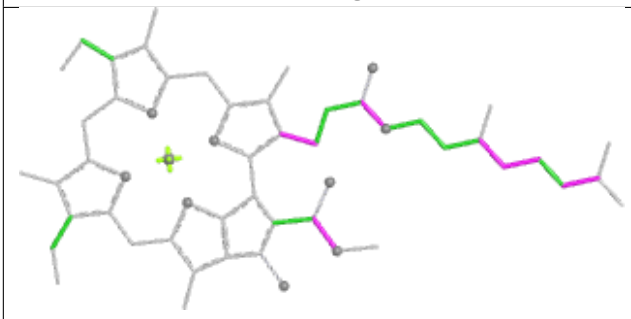
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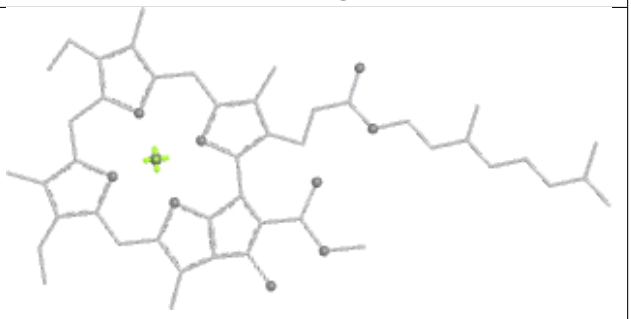
Bond lengths



Bond angles

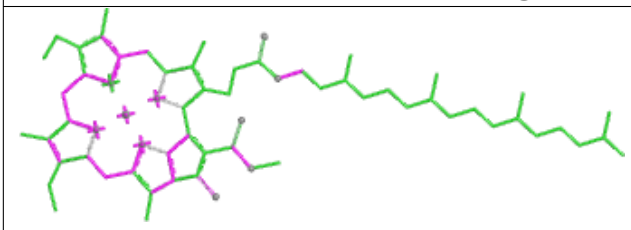


Torsions

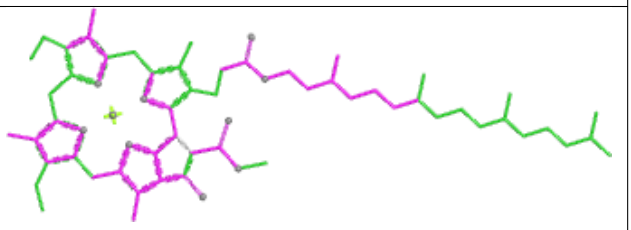


Rings

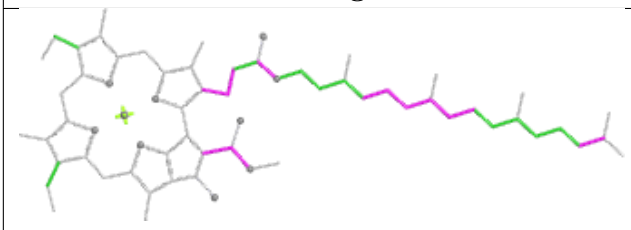
Ligand CLA B 1223



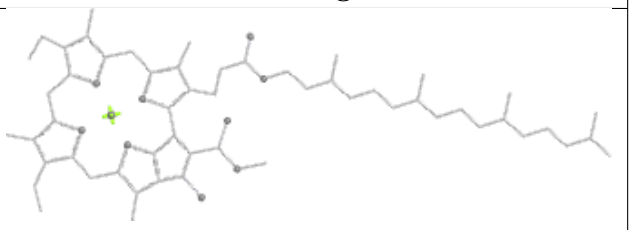
Bond lengths



Bond angles

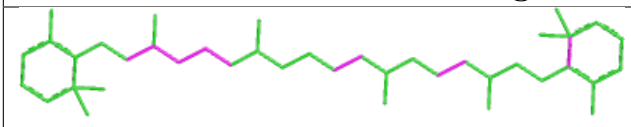


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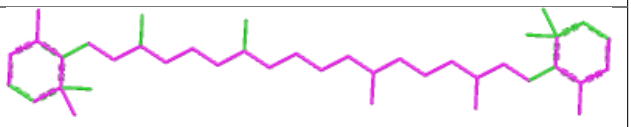


Rings

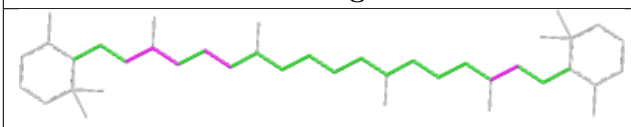
Ligand BCR H 4004



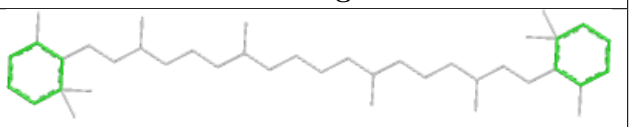
Bond lengths



Bond angles

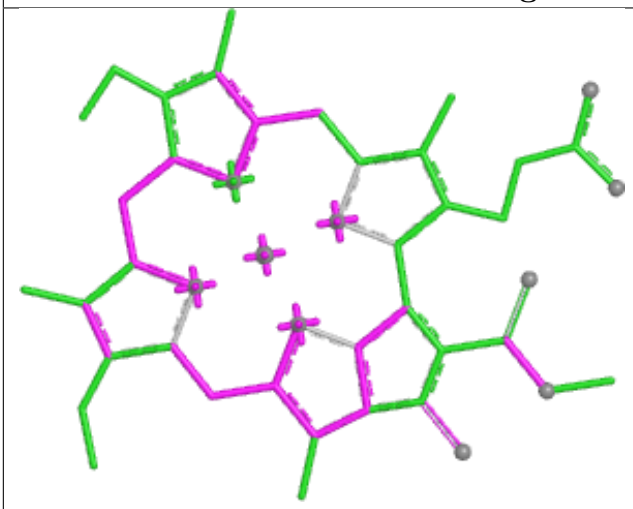


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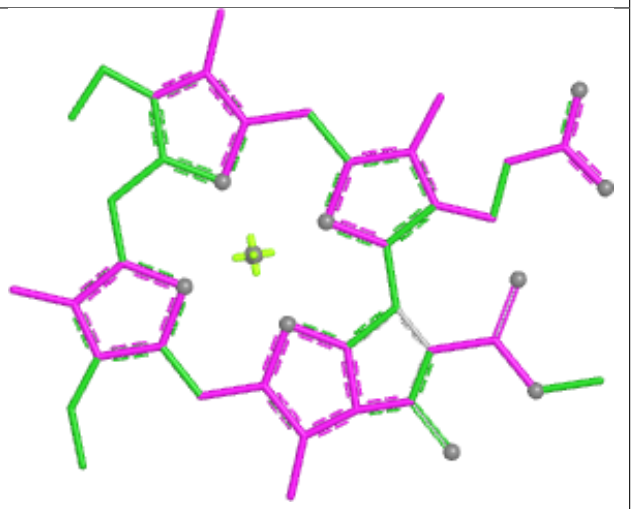


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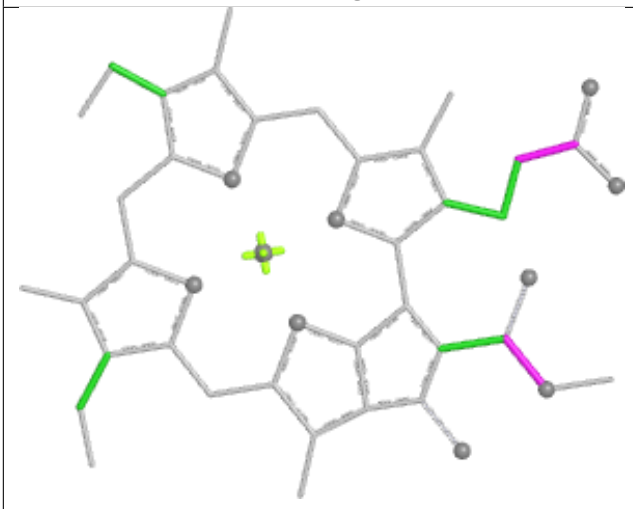
Ligand CLA a 1108



Bond lengths



Bond angles

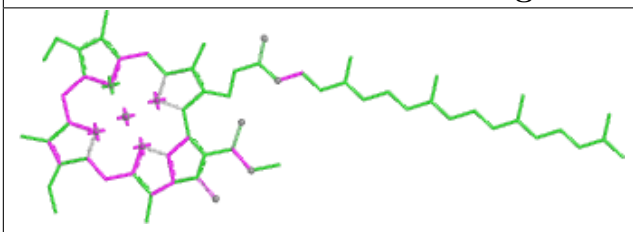


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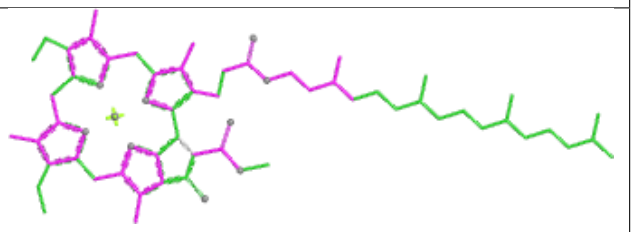


Rings

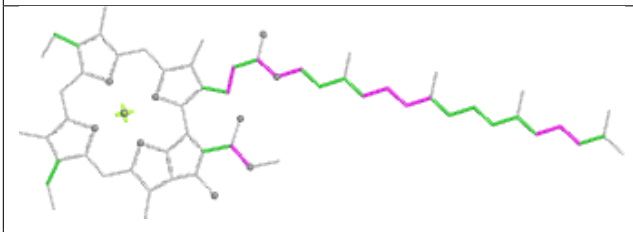
Ligand CLA B 1226



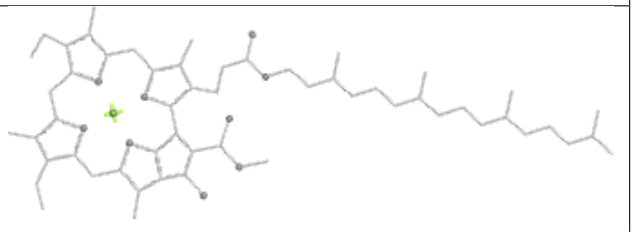
Bond lengths



Bond angles

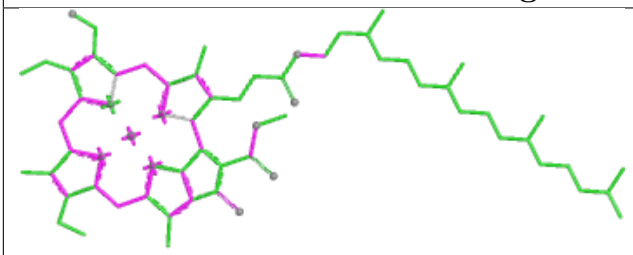


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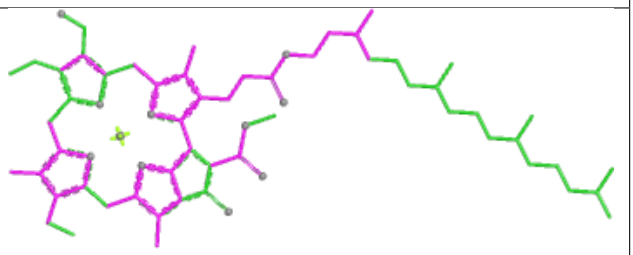


Rings

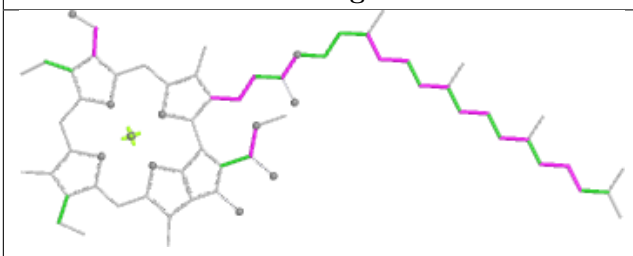
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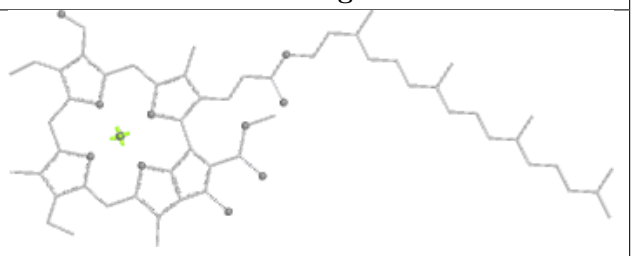
Bond lengths



Bond angles

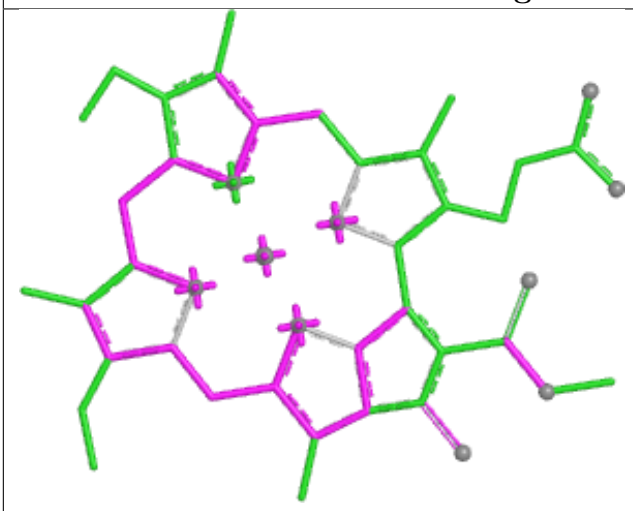


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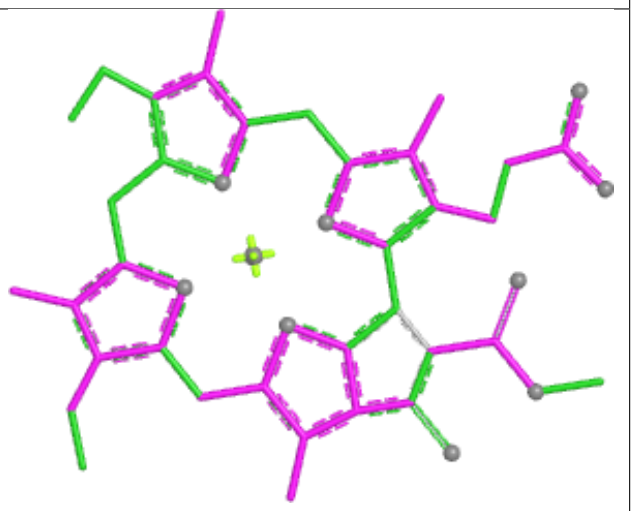


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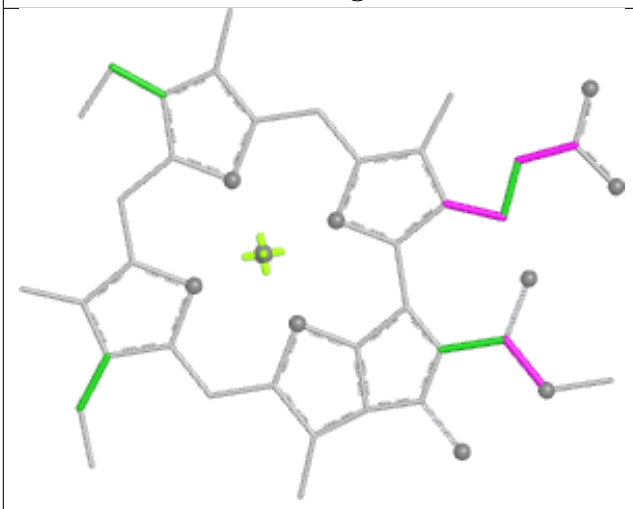
Ligand CLA G 1105



Bond lengths



Bond angles

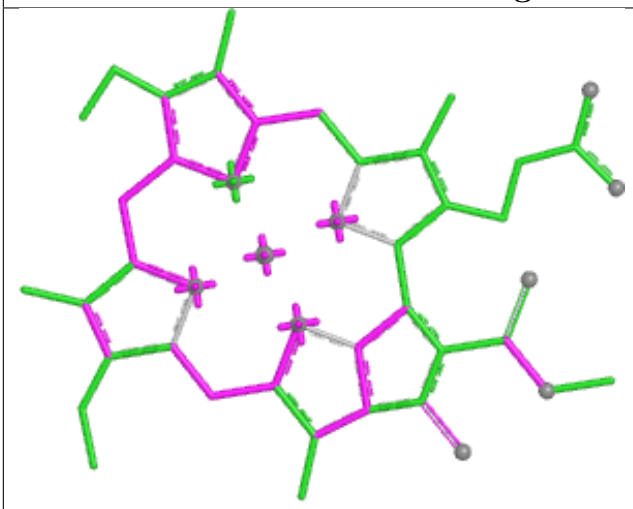


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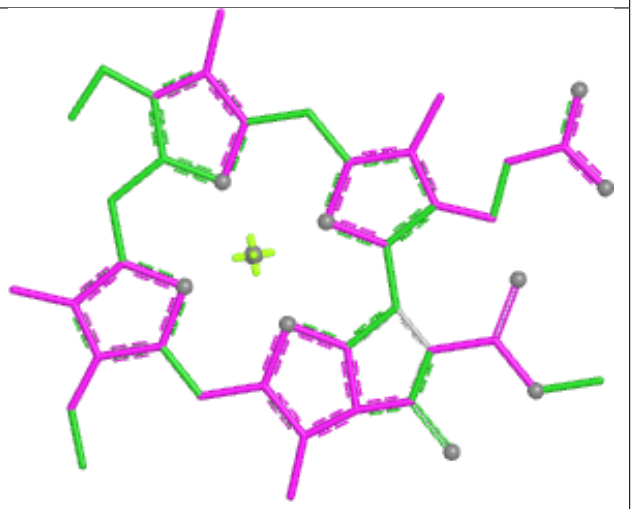


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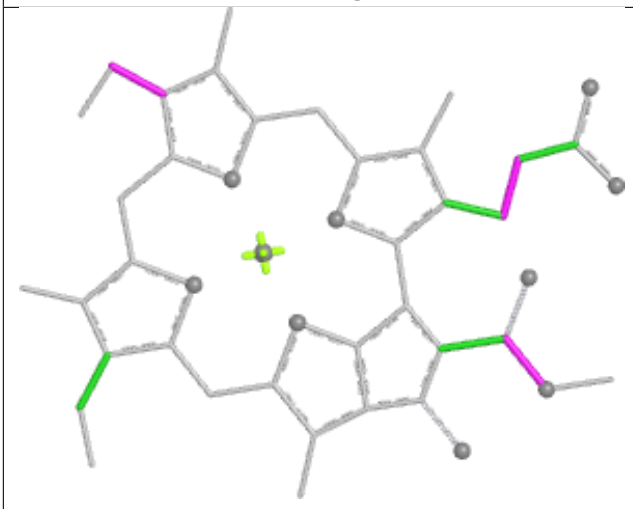
Ligand CLA G 1139



Bond lengths



Bond angles

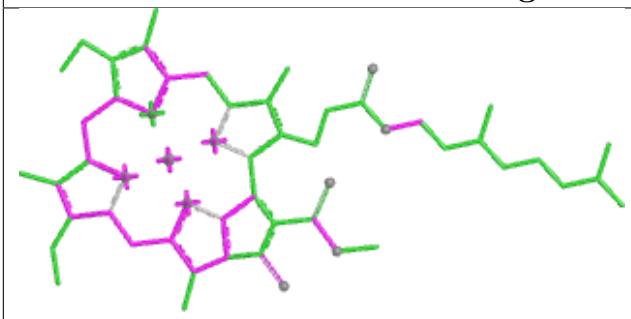


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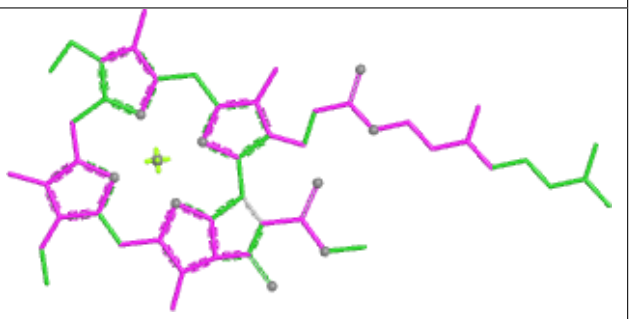


Rings

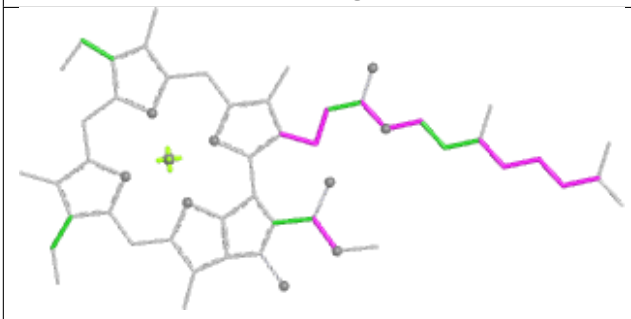
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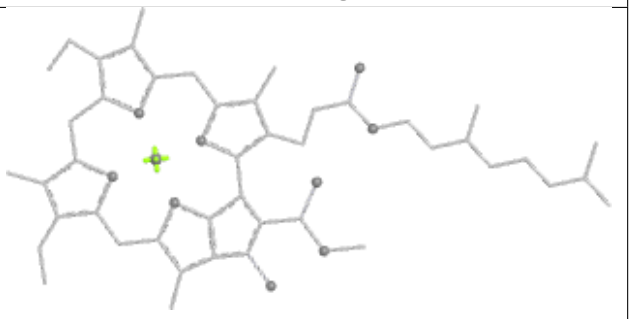
Bond lengths



Bond angles

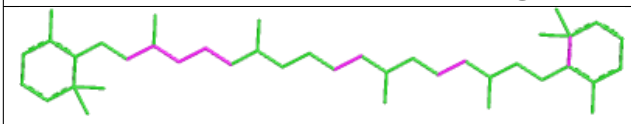


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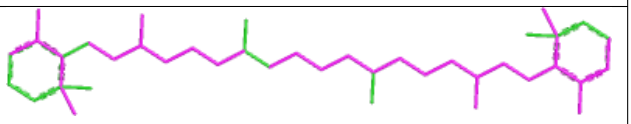


Rings

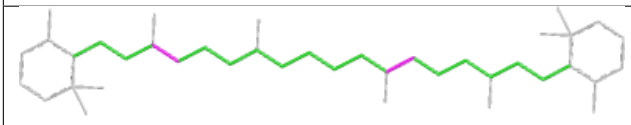
Ligand BCR B 4005



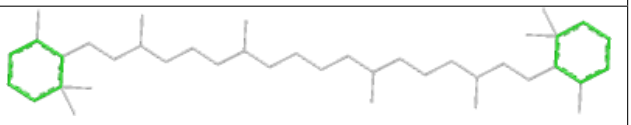
Bond lengths



Bond angles

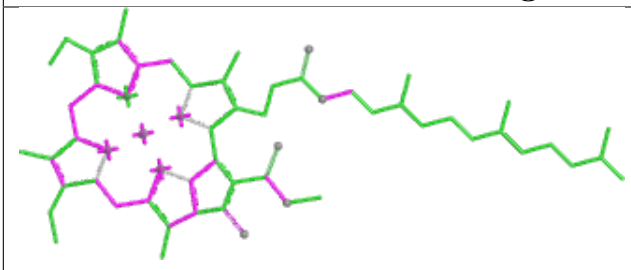


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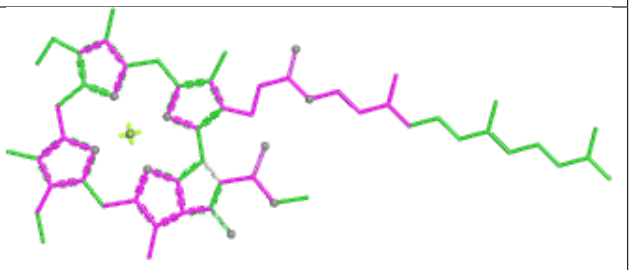


Rings

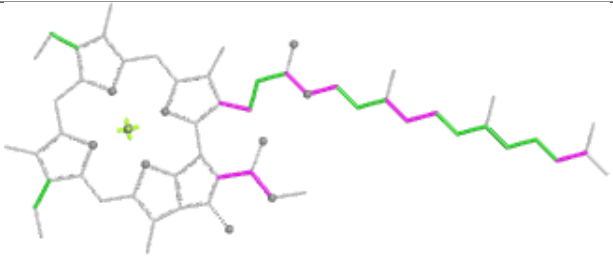
Ligand CLA a 1103



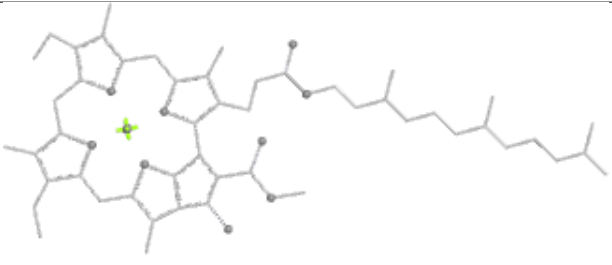
Bond lengths



Bond angles

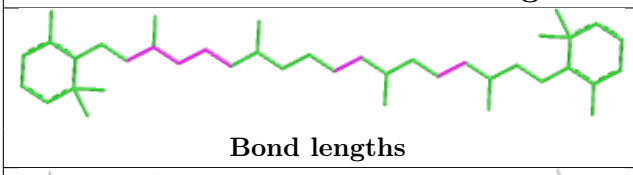


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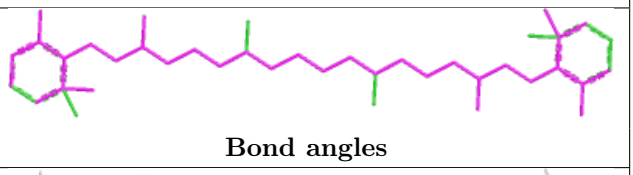


Rings

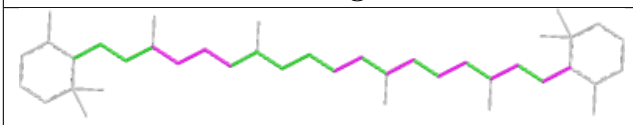
Ligand BCR l 4019



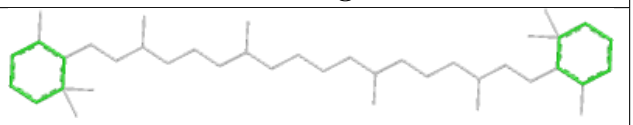
Bond lengths



Bond angles

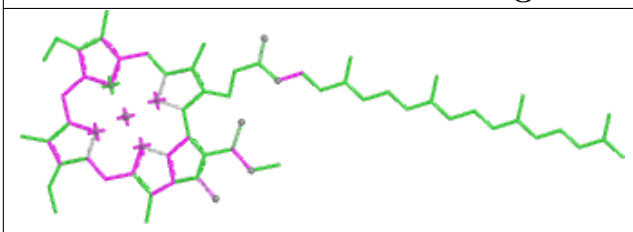


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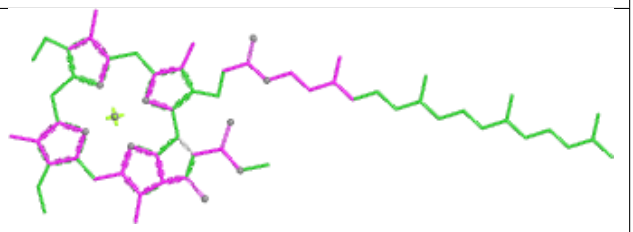


Rings

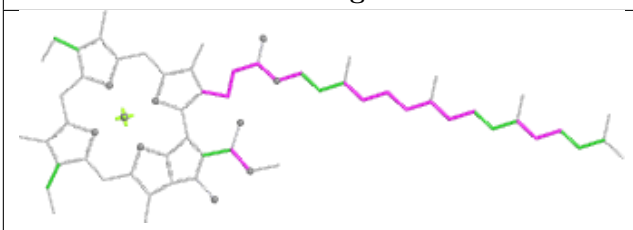
Ligand CLA A 1140



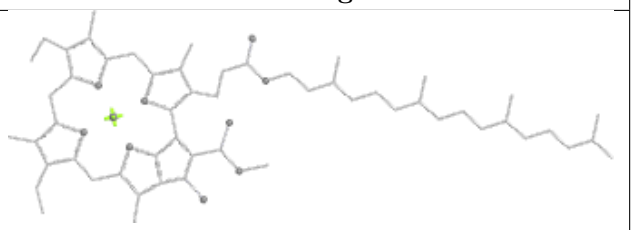
Bond lengths



Bond angles

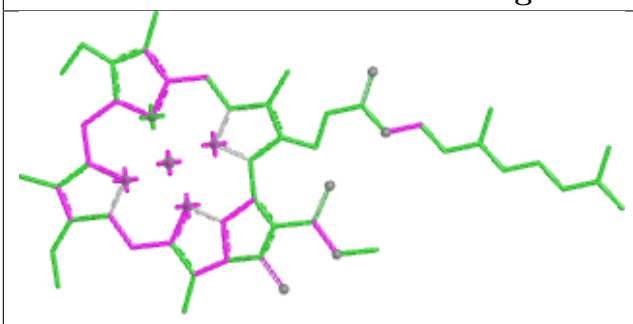


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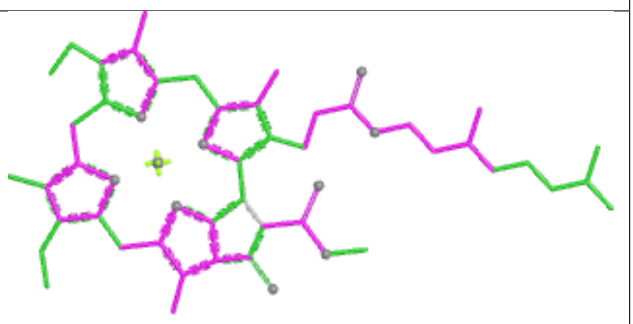


Rings

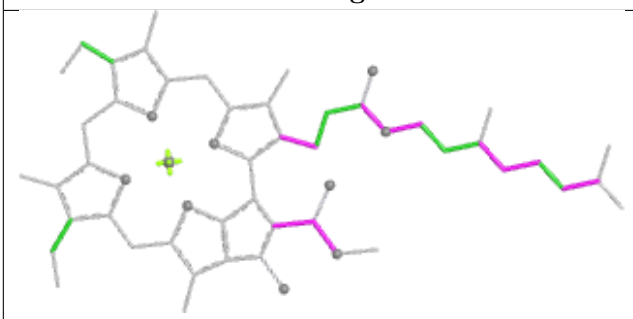
Ligand CLA A 1112



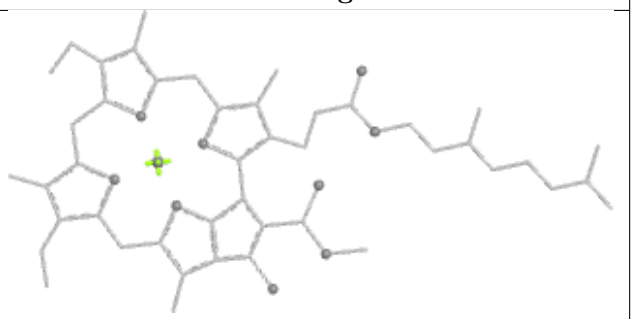
Bond lengths



Bond angles

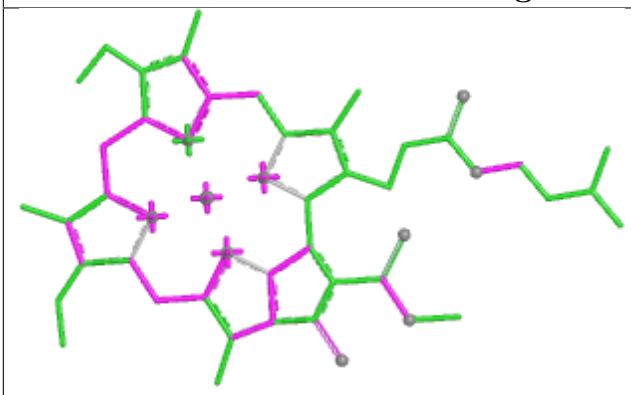


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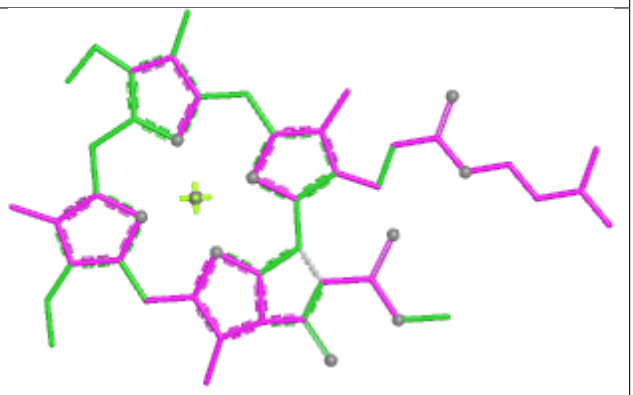


Rings

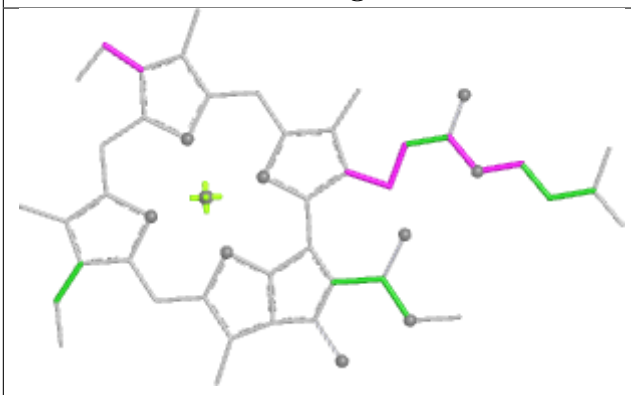
Ligand CLA A 1129



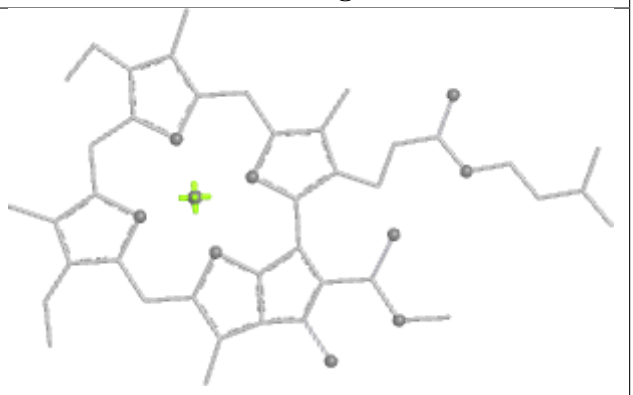
Bond lengths



Bond angles

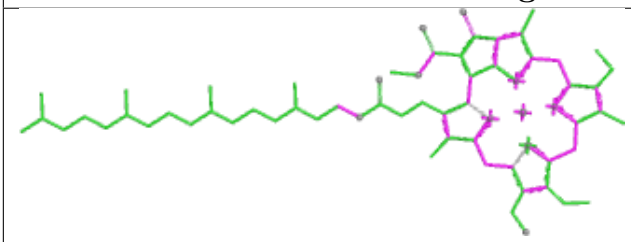


Torsions

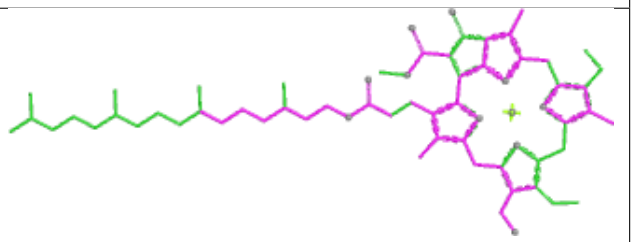


Rings

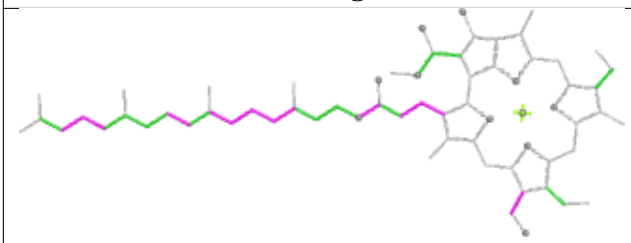
Ligand F6C H 1238



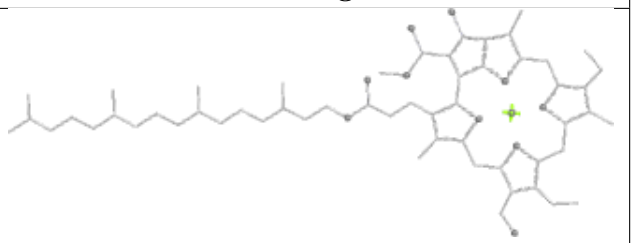
Bond lengths



Bond angles

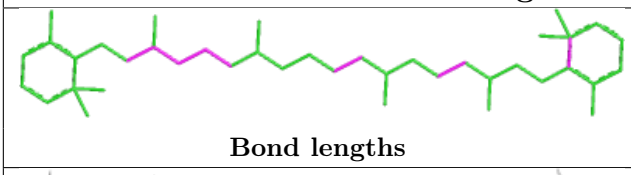


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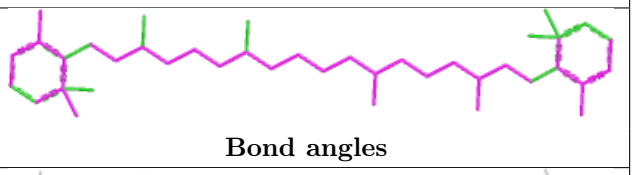


Rings

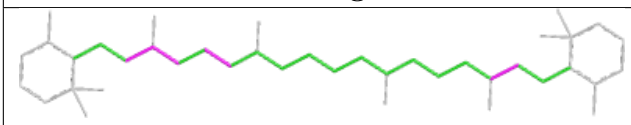
Ligand BCR b 4004



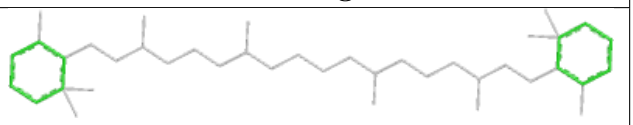
Bond lengths



Bond angles

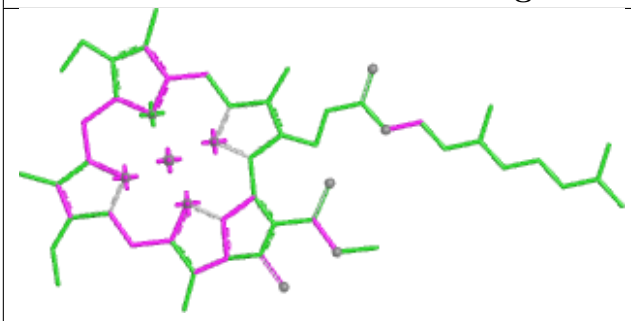


Torsions

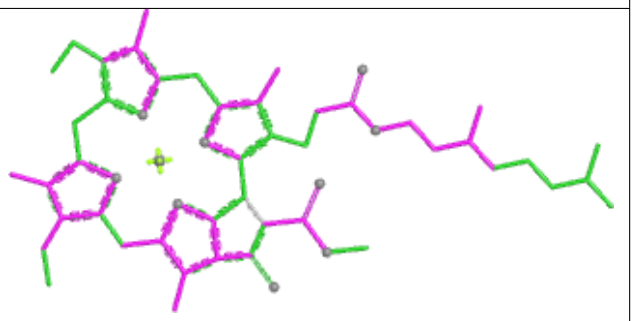


Rings

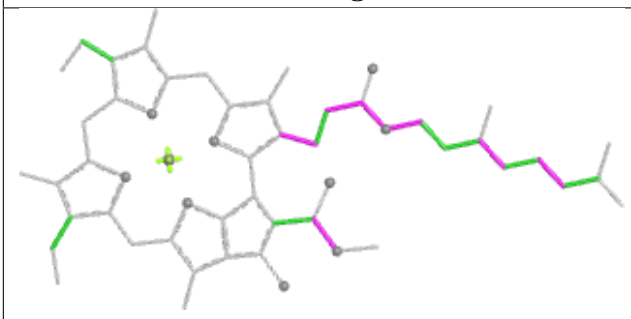
Ligand CLA X 1701



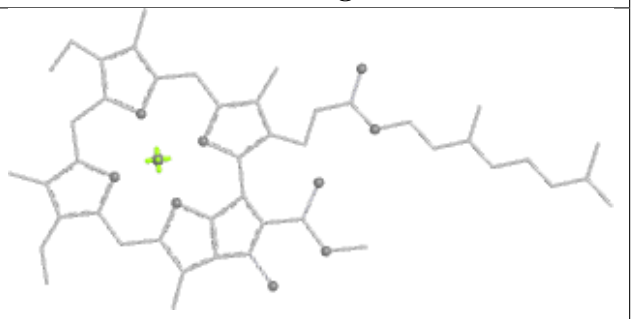
Bond lengths



Bond angles

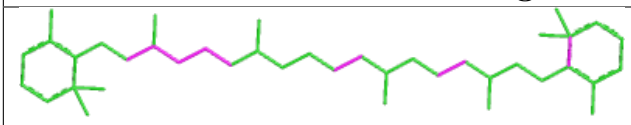


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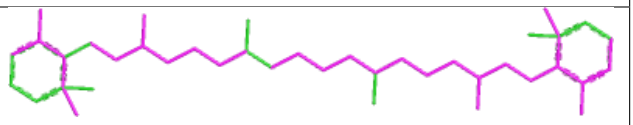


Rings

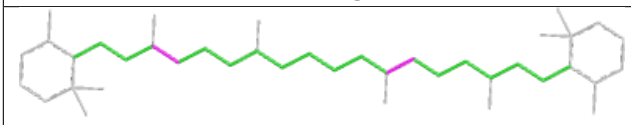
Ligand BCR b 4005



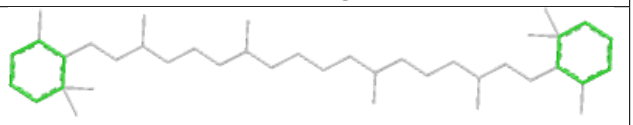
Bond lengths



Bond angles

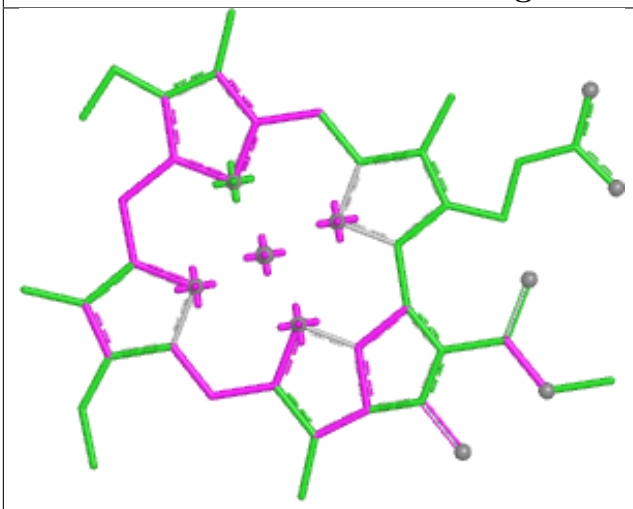


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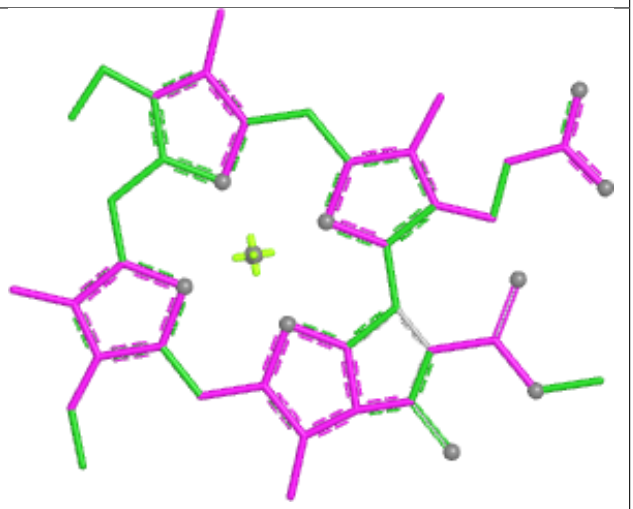


Rings

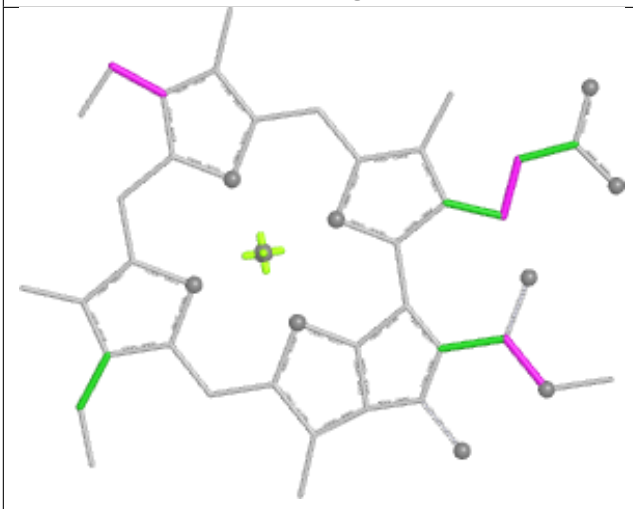
Ligand CLA A 1139



Bond lengths



Bond angles

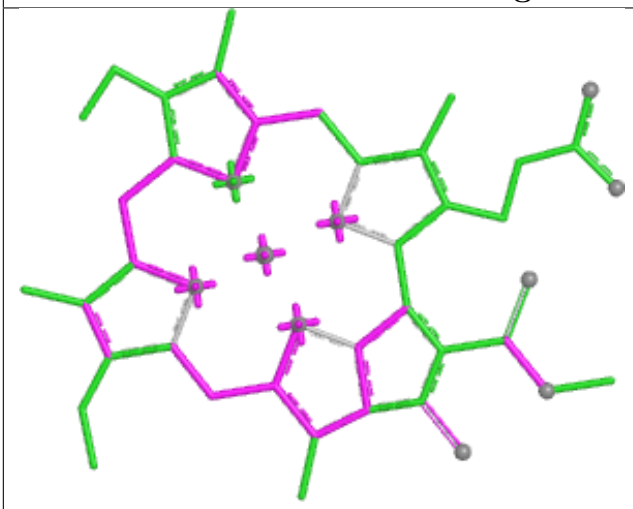


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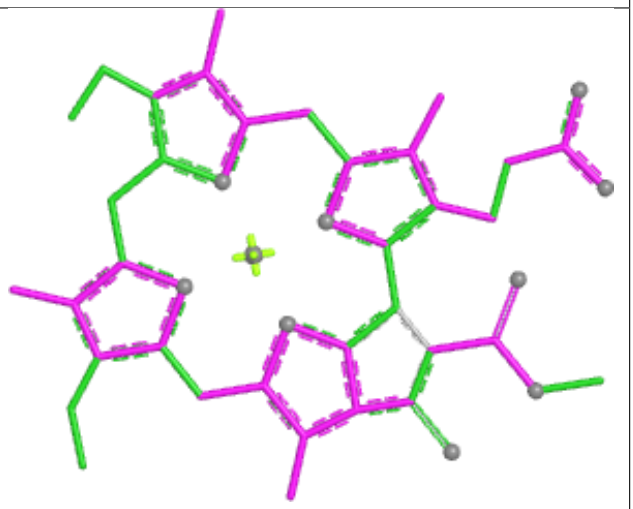


Rings

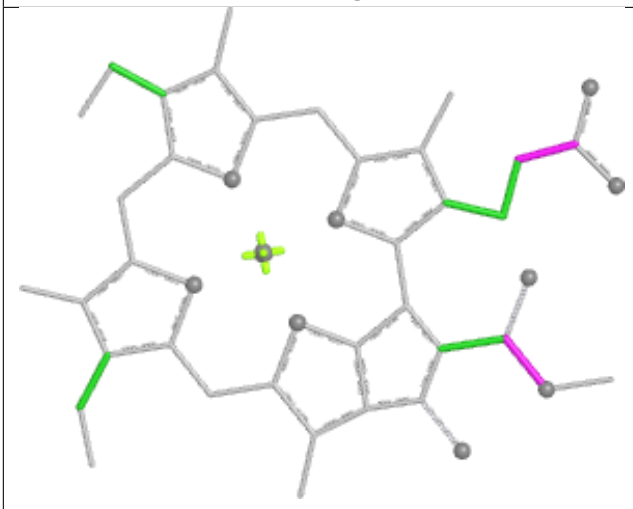
Ligand CLA G 1108



Bond lengths



Bond angles

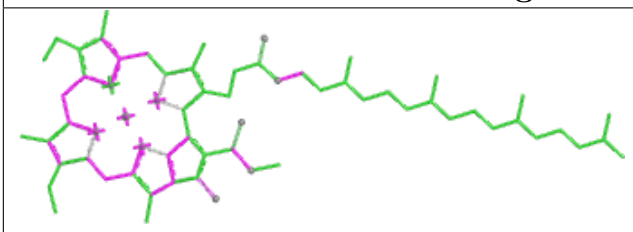


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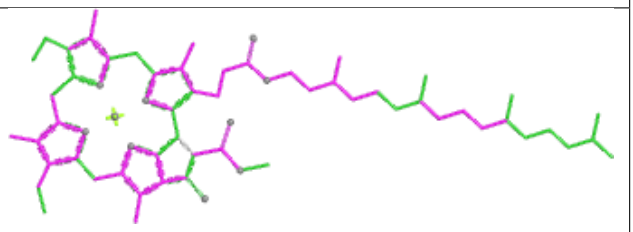


Rings

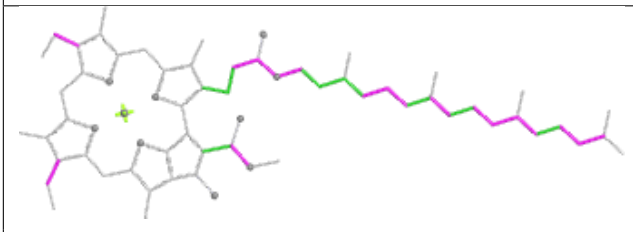
Ligand CLA B 1239



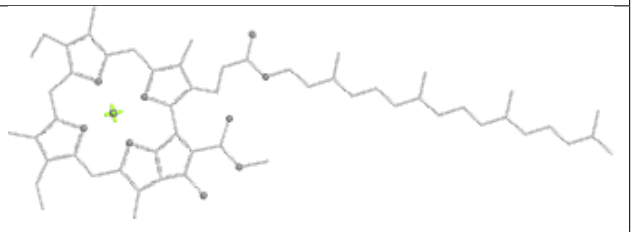
Bond lengths



Bond angles

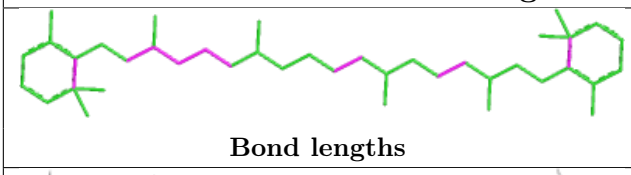


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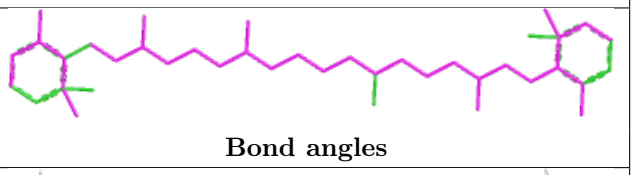


Rings

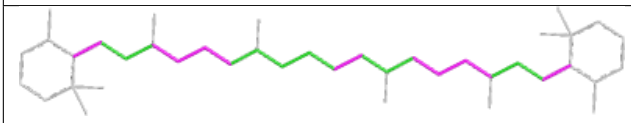
Ligand BCR I 4020



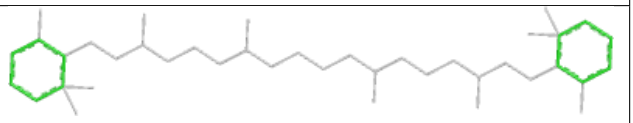
Bond lengths



Bond angles

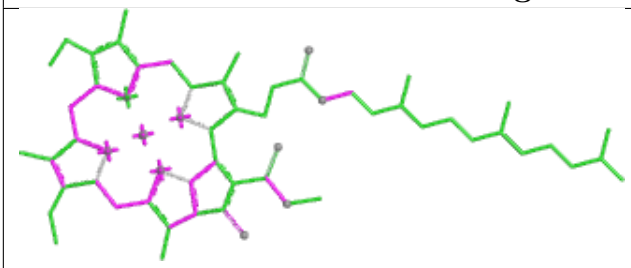


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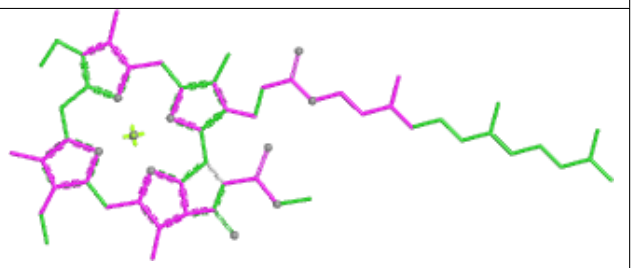


Rings

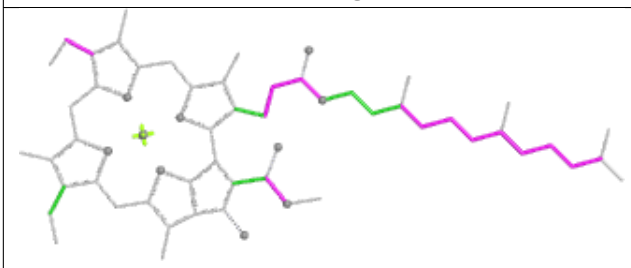
Ligand CLA G 1126



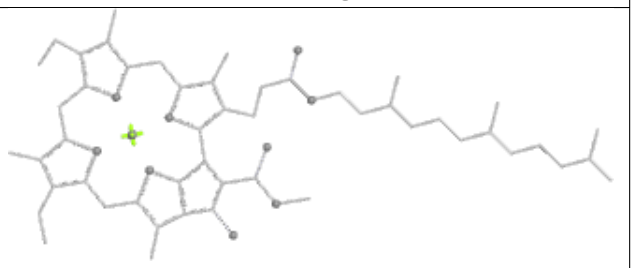
Bond lengths



Bond angles

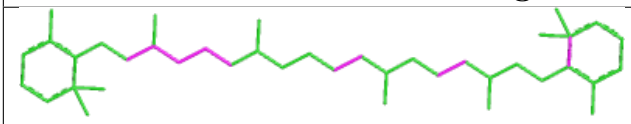


Torsions



Rings

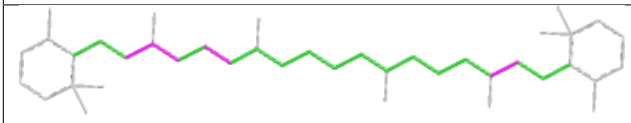
Ligand BCR B 4004



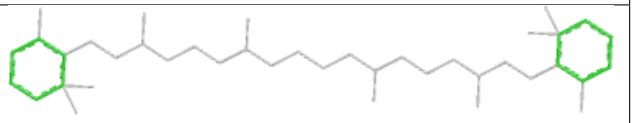
Bond lengths



Bond angles

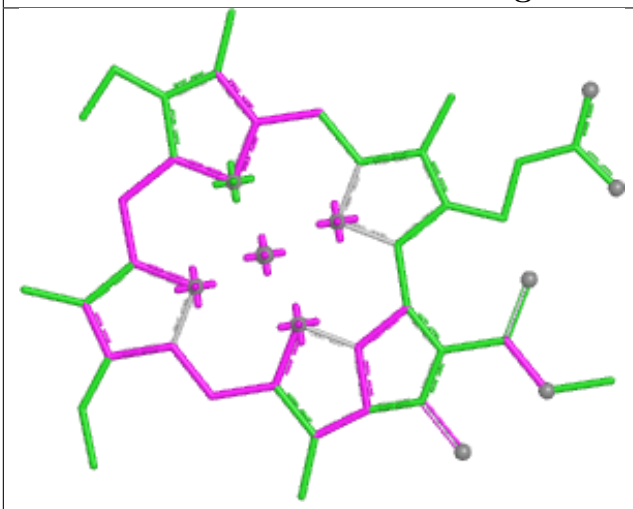


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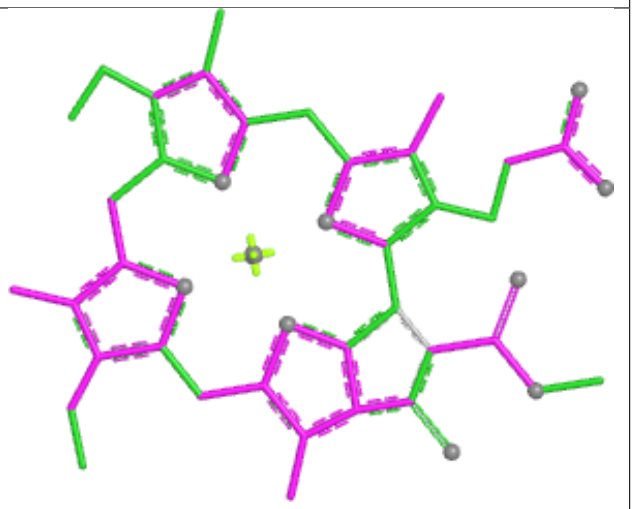


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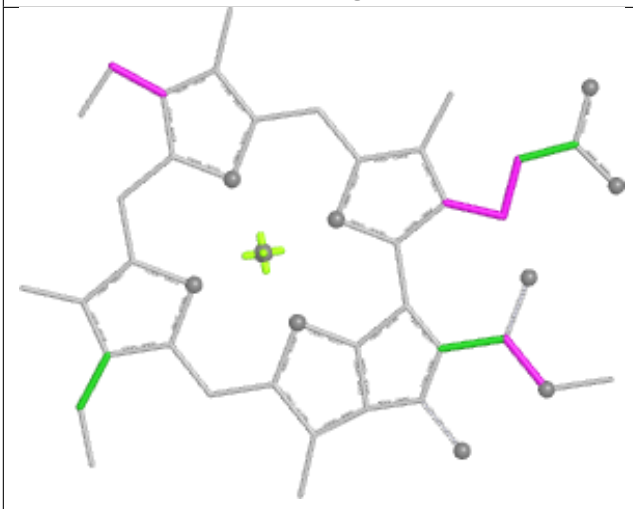
Ligand CLA H 1227



Bond lengths



Bond angles

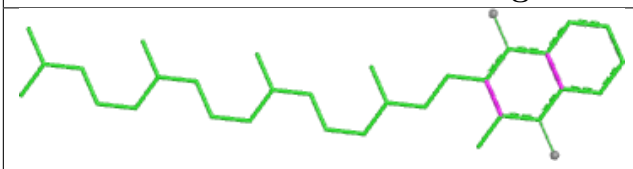


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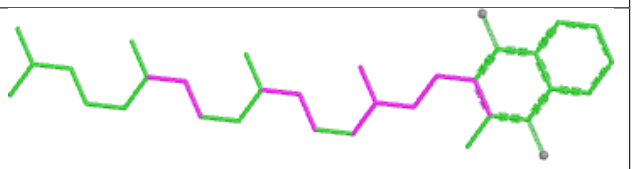


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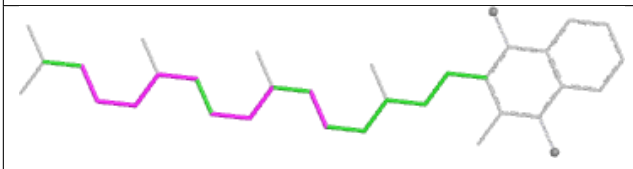
Ligand PQN G 2001



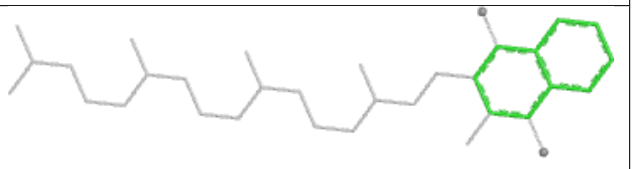
Bond lengths



Bond angles

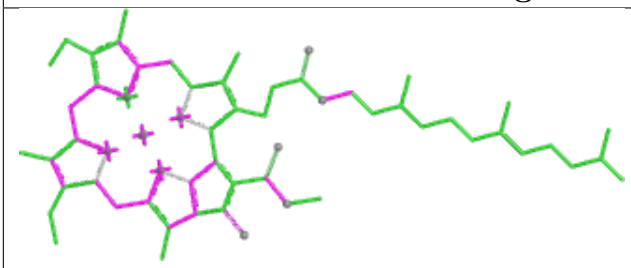


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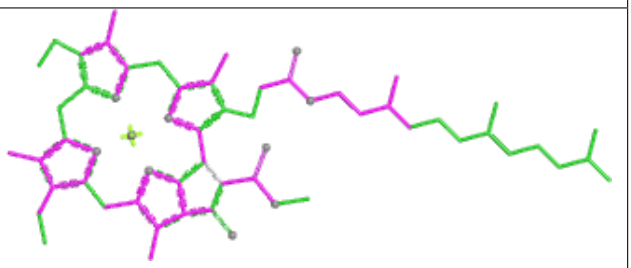


Rings

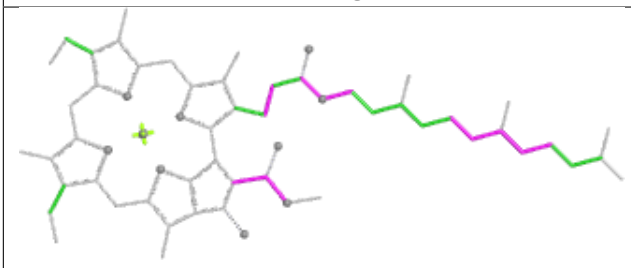
Ligand CLA A 1123



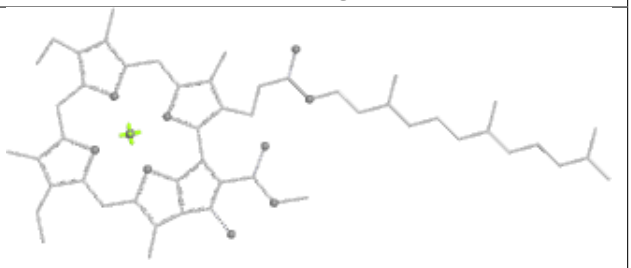
Bond lengths



Bond angles

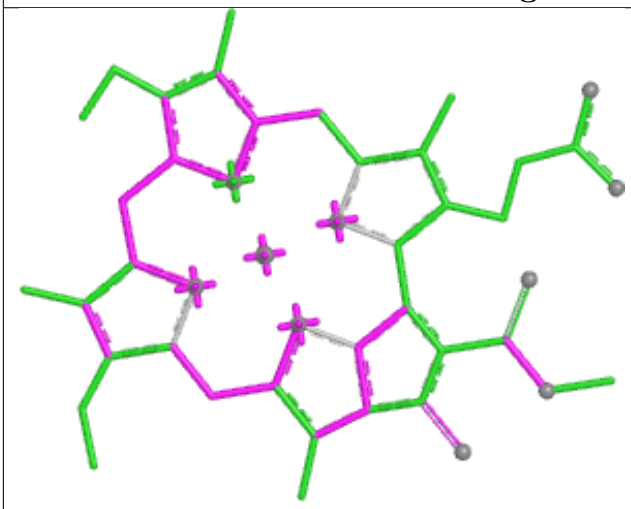


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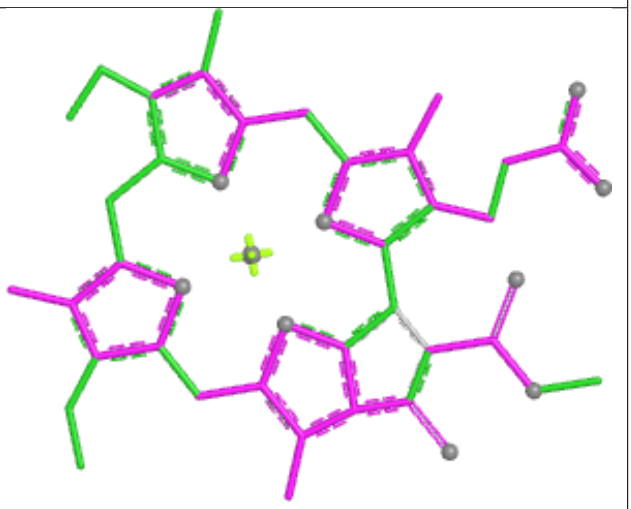


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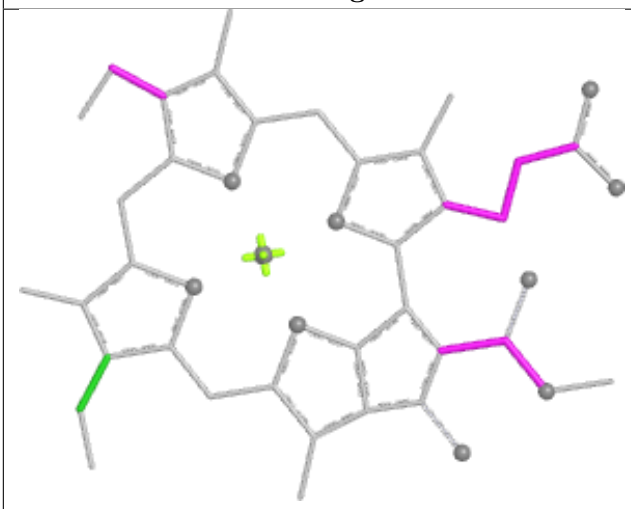
Ligand CLA a 1113



Bond lengths



Bond angles

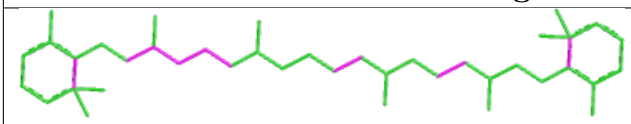


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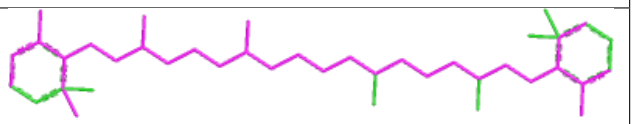


Rings

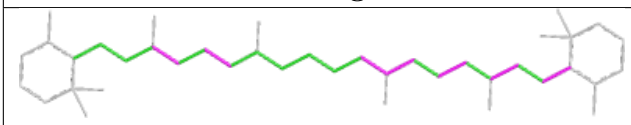
Ligand BCR A 4007



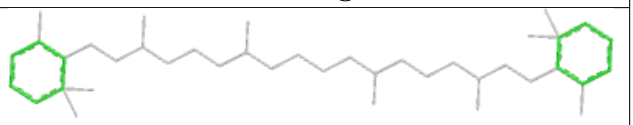
Bond lengths



Bond angles

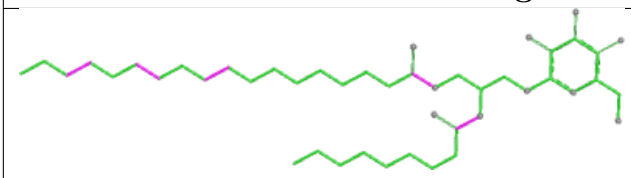


Torsions

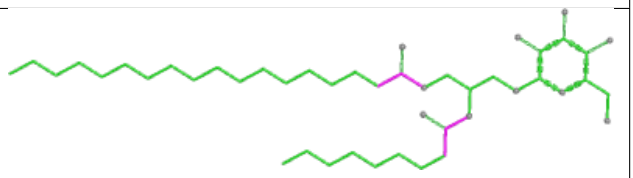


Rings

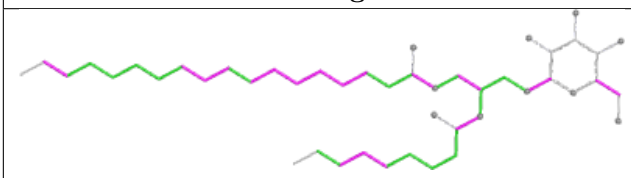
Ligand LMG a 5005



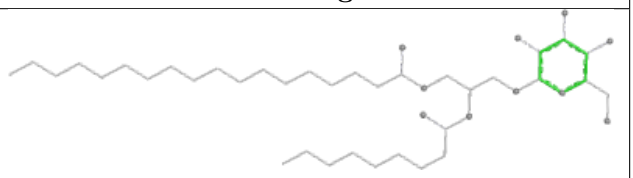
Bond lengths



Bond angles

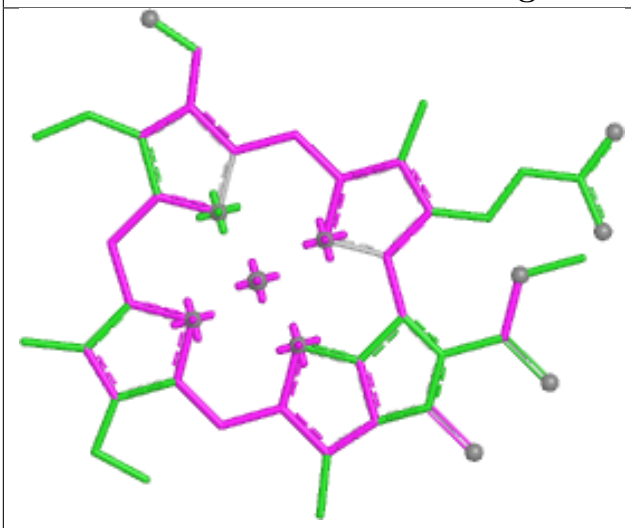


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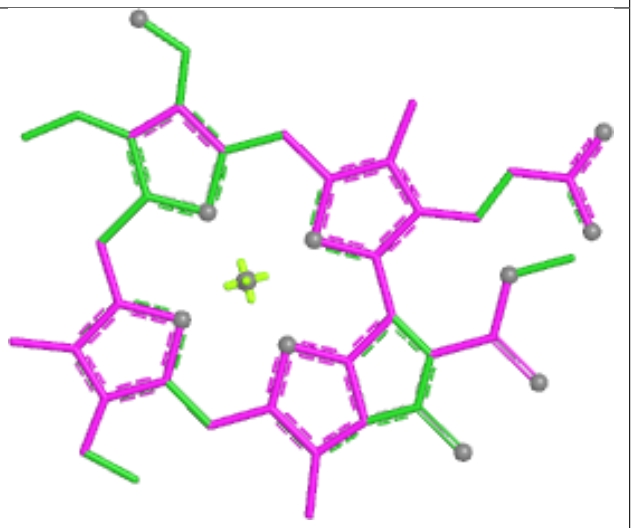


Rings

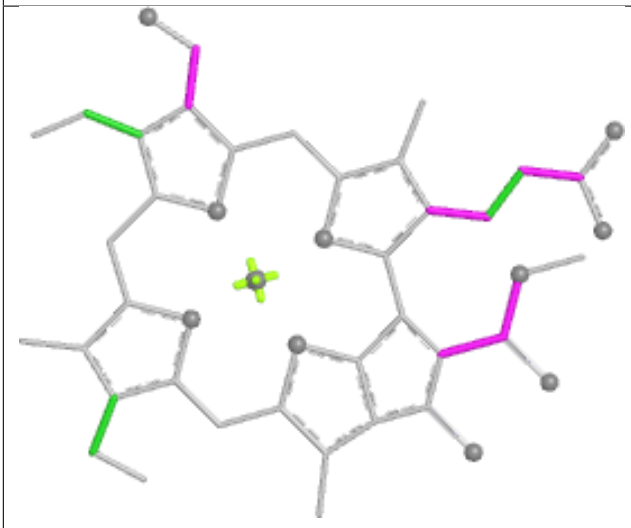
Ligand F6C H 1230



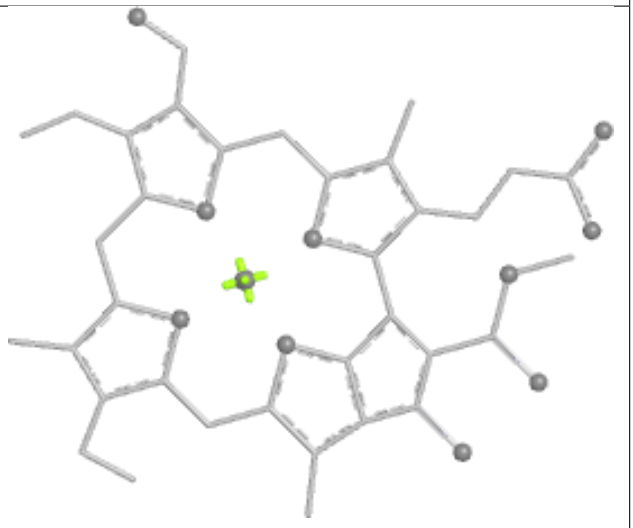
Bond lengths



Bond angles

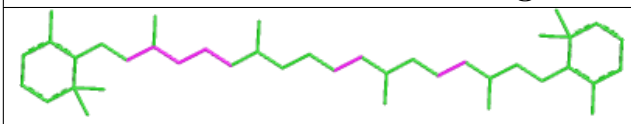


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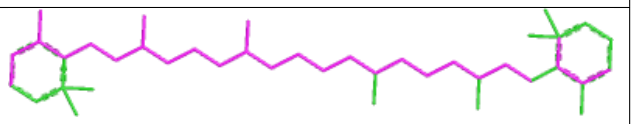


Rings

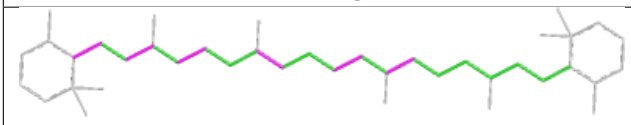
Ligand BCR b 4016



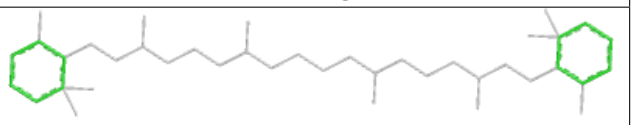
Bond lengths



Bond angles

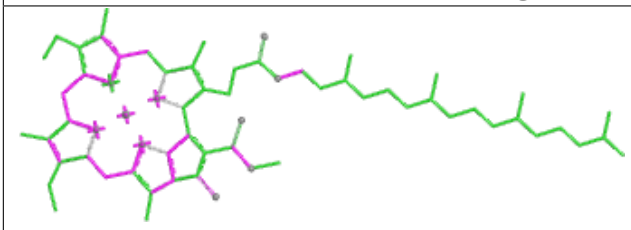


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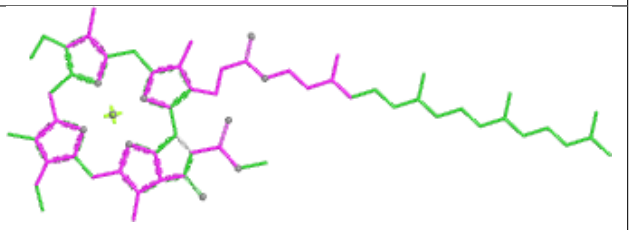


Rings

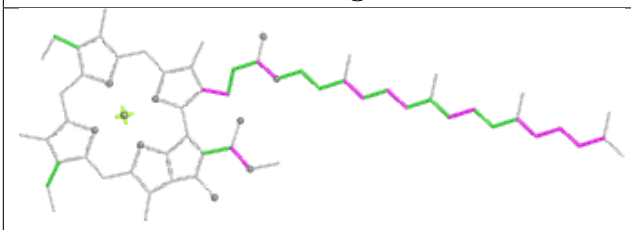
Ligand CLA U 1503



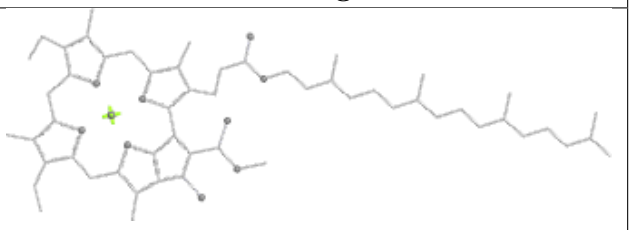
Bond lengths



Bond angles

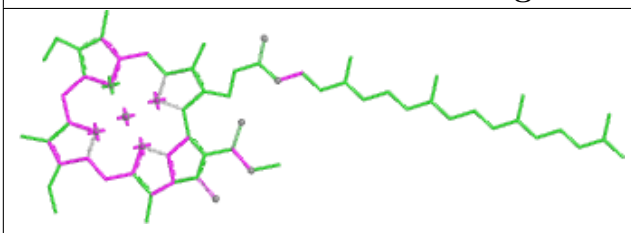


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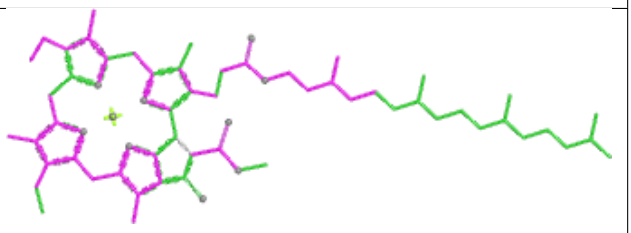


Rings

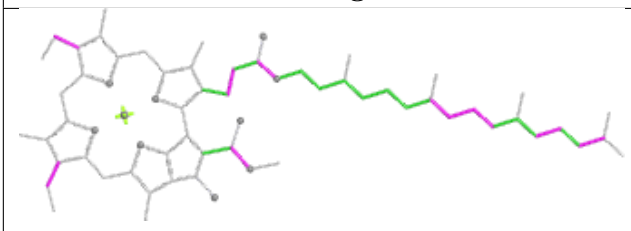
Ligand CLA H 1023



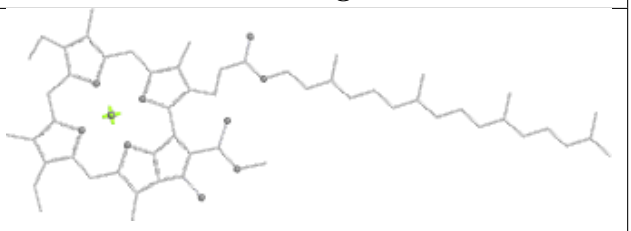
Bond lengths



Bond angles

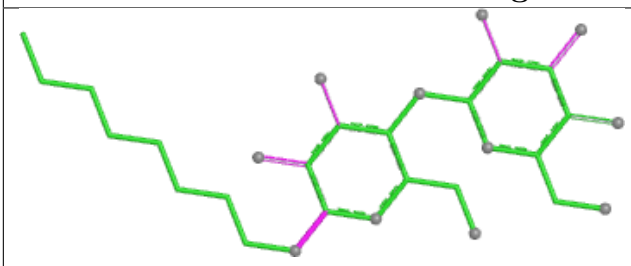


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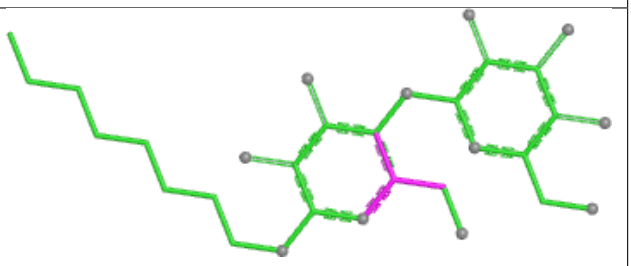


Rings

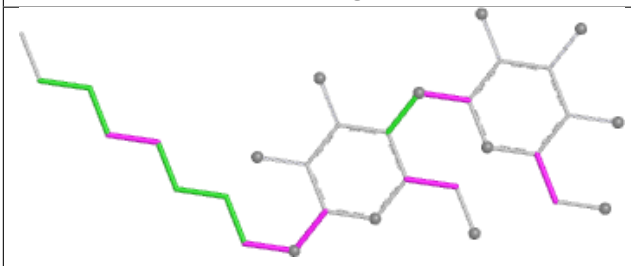
Ligand LMT G 6001



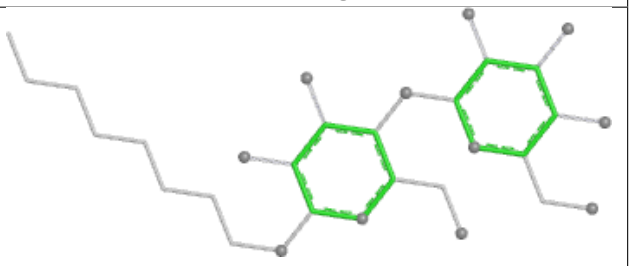
Bond lengths



Bond angles

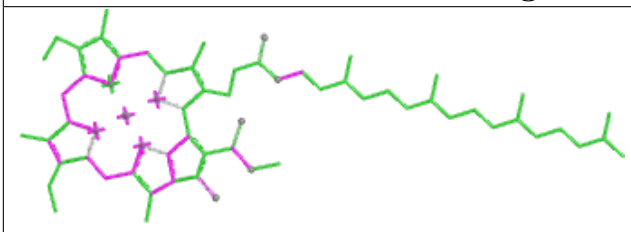


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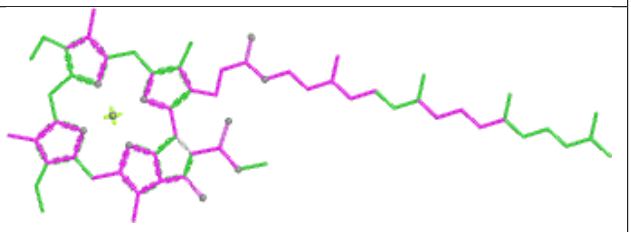


Rings

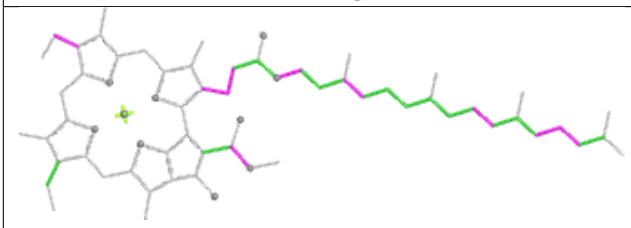
Ligand CLA a 1012



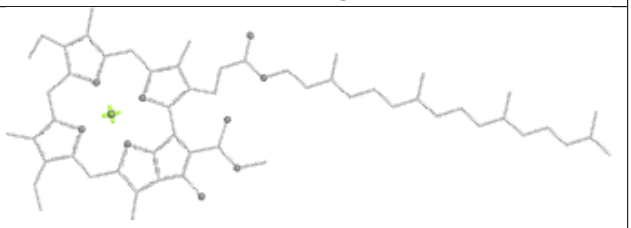
Bond lengths



Bond angles

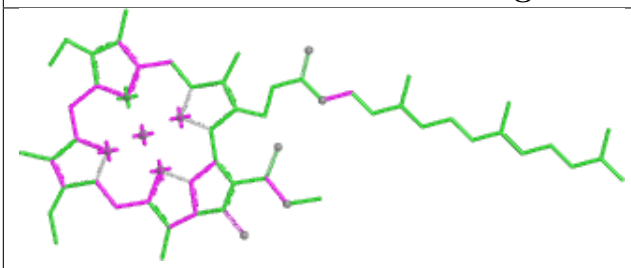


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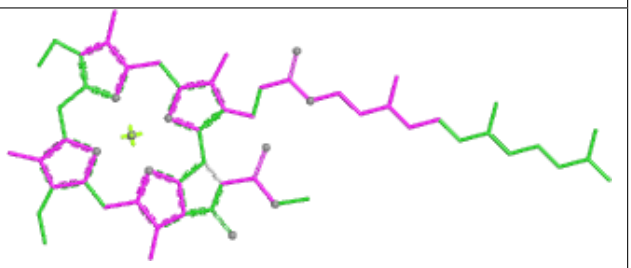


Rings

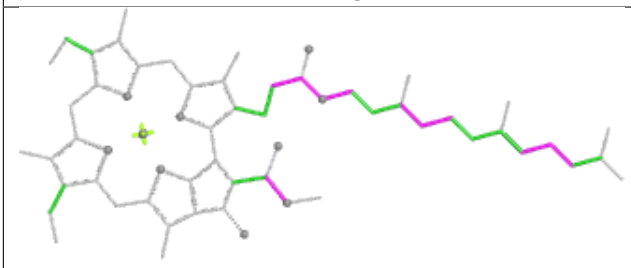
Ligand CLA H 1235



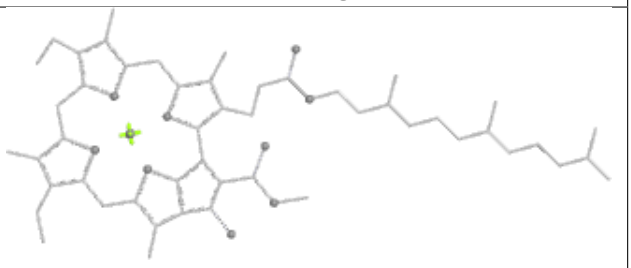
Bond lengths



Bond angles

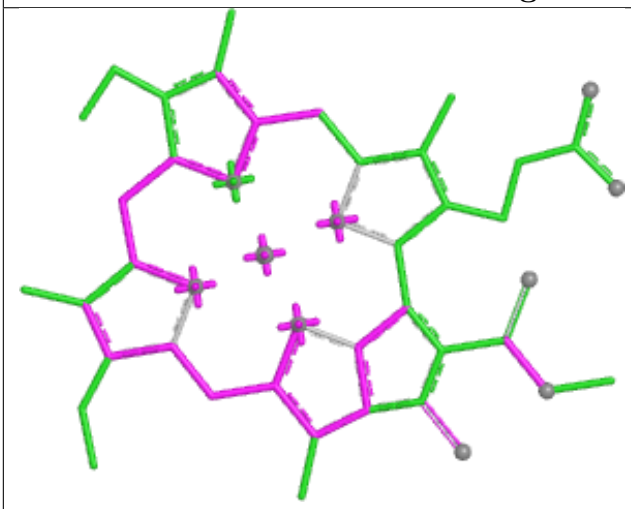


Torsions

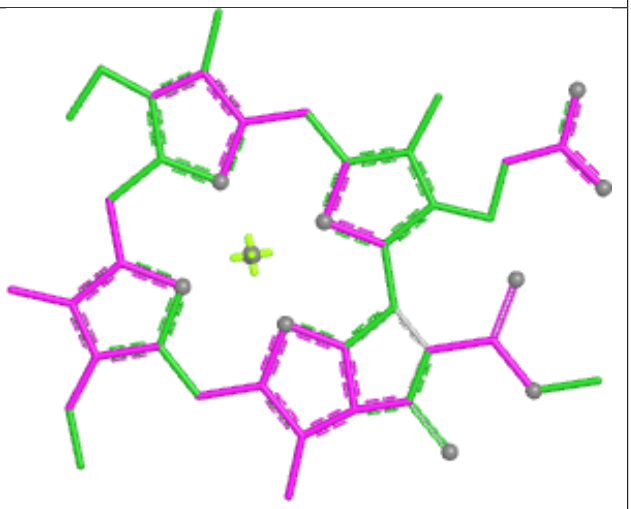


Rings

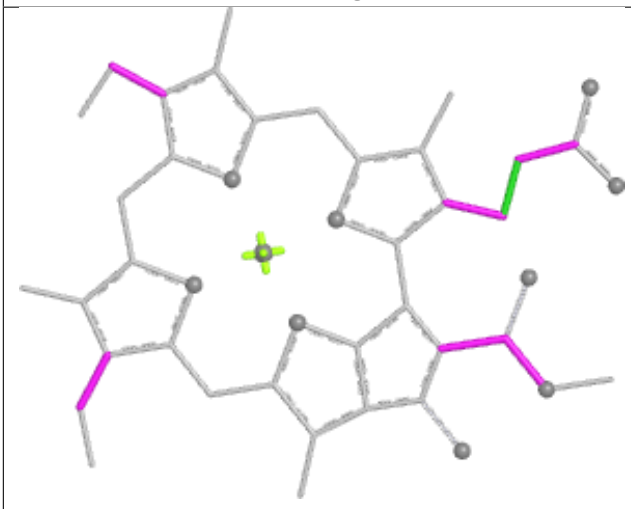
Ligand CLA a 1114



Bond lengths



Bond angles

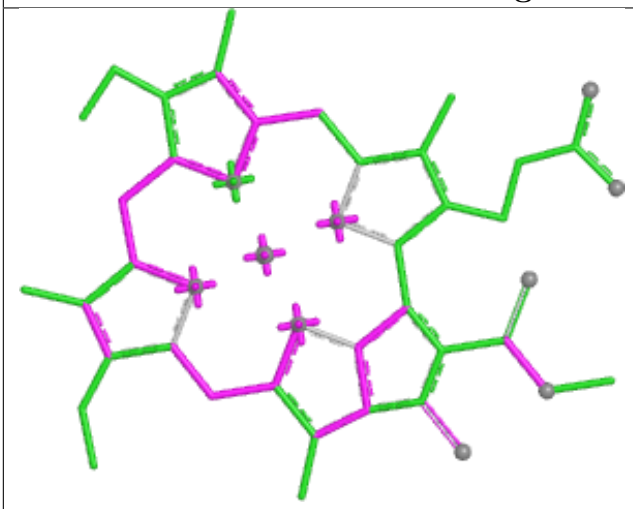


Torsions

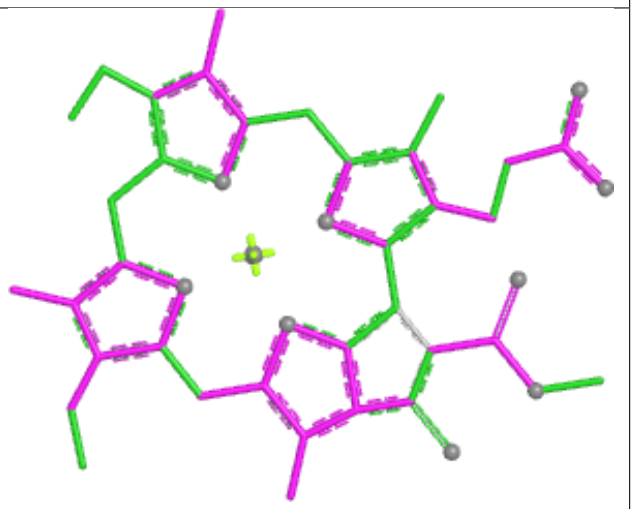


Rings

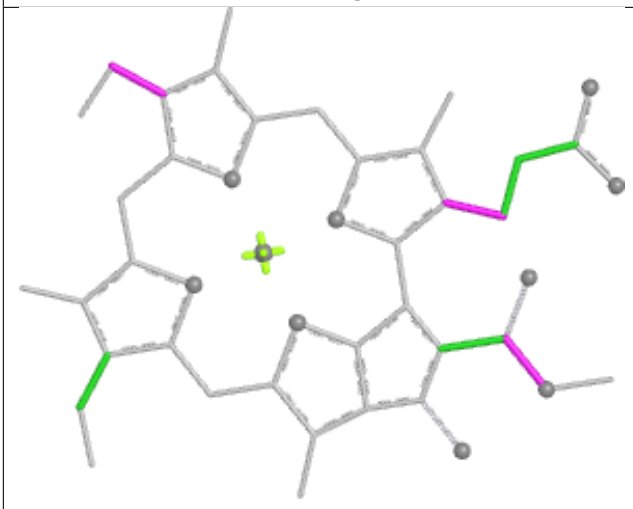
Ligand CLA A 1107



Bond lengths



Bond angles

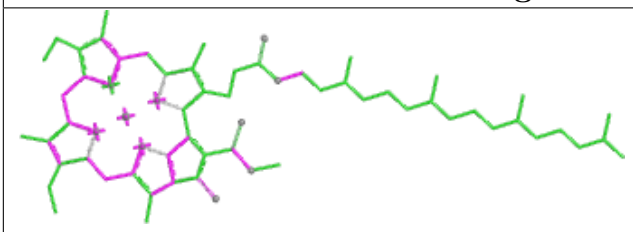


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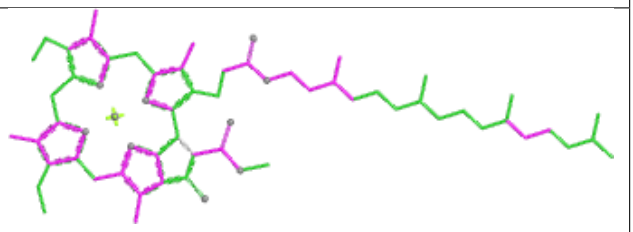


Rings

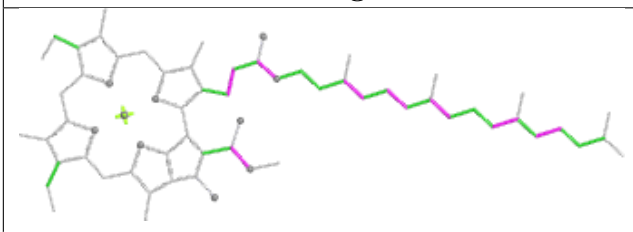
Ligand CLA U 1501



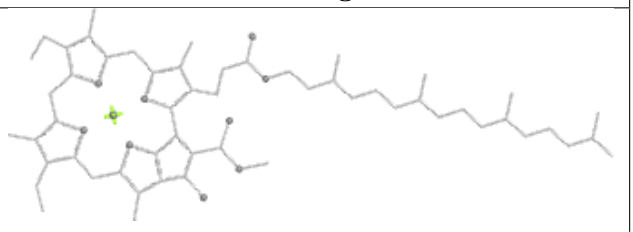
Bond lengths



Bond angles

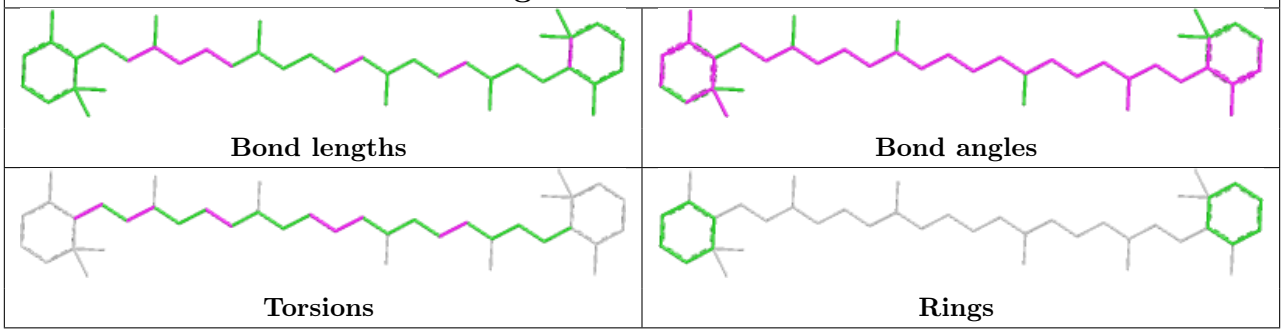


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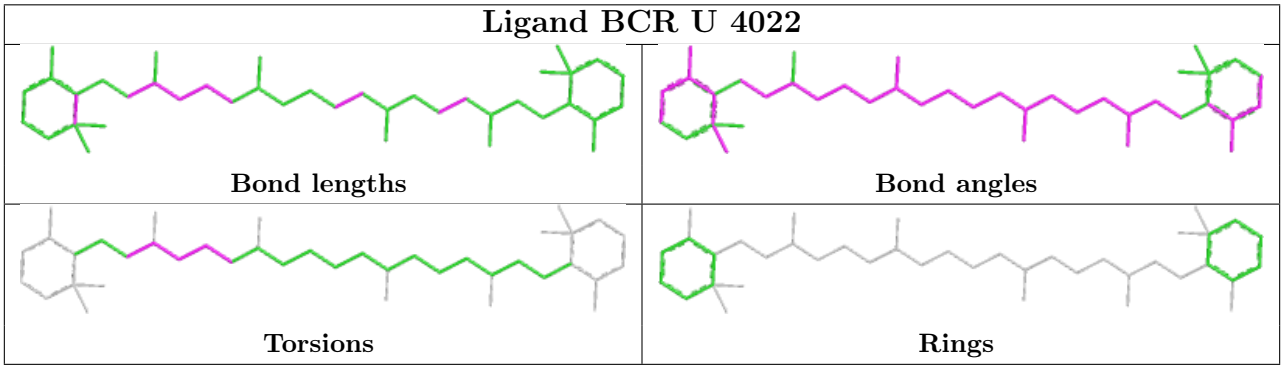


Rings

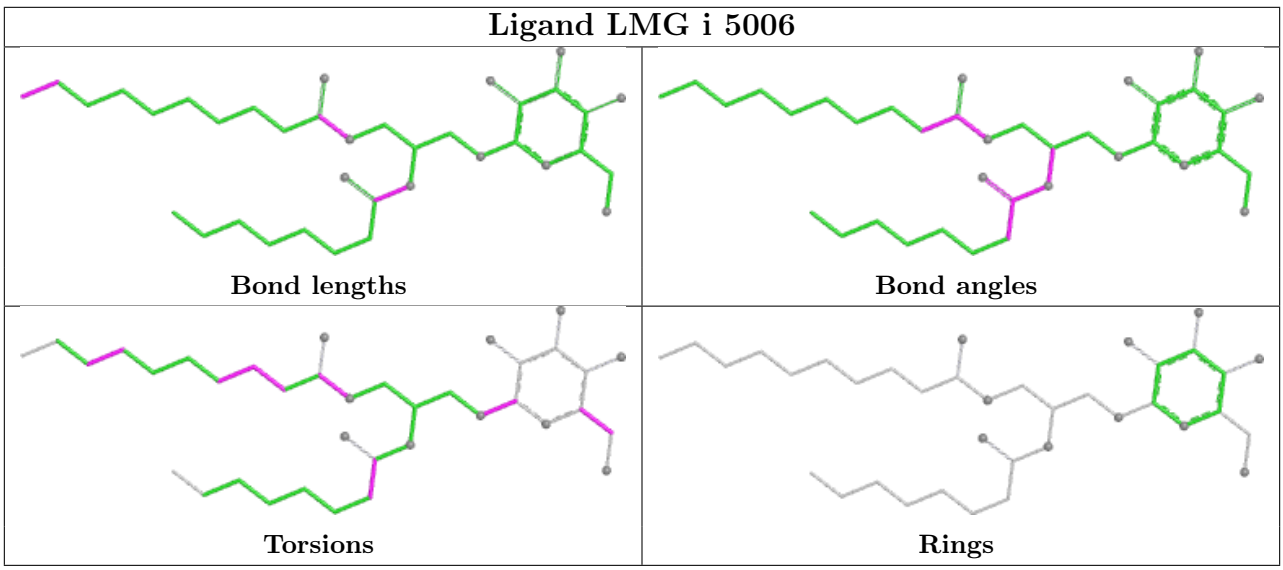
Ligand BCR R 4018



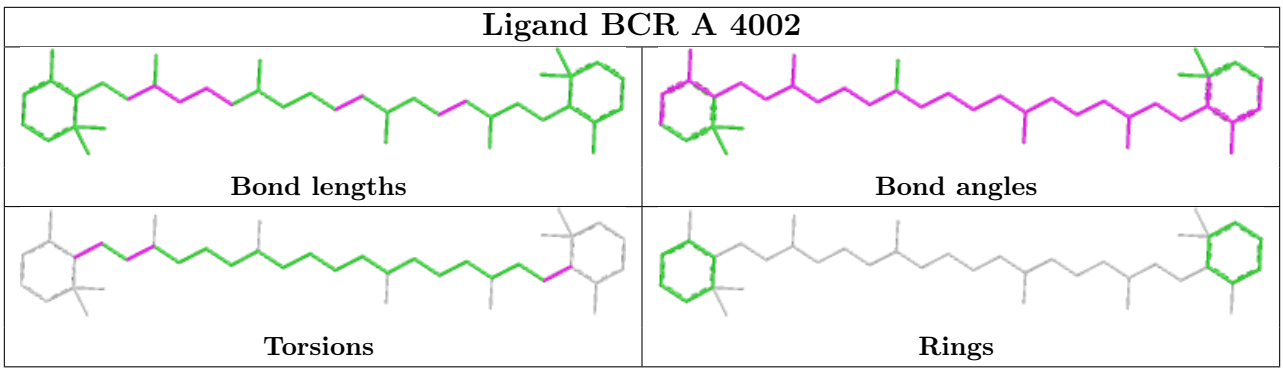
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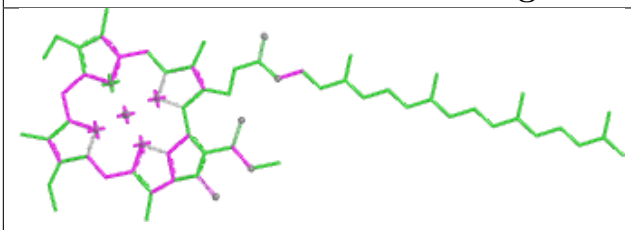
Ligand LMG i 5006



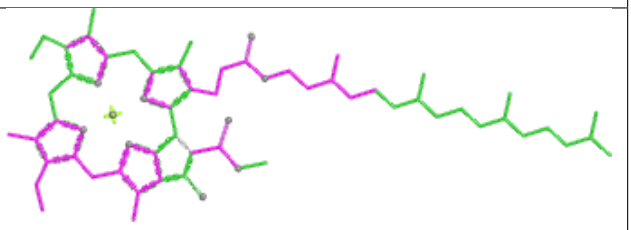
Ligand BCR A 4002



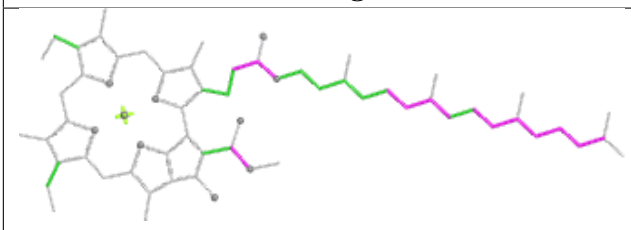
Ligand CLA b 1021



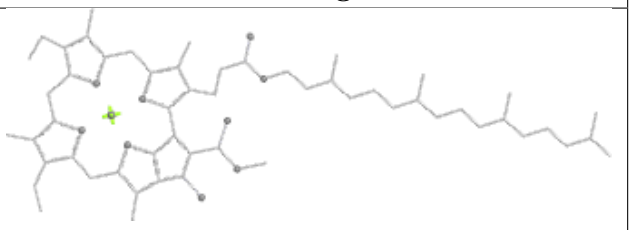
Bond lengths



Bond angles

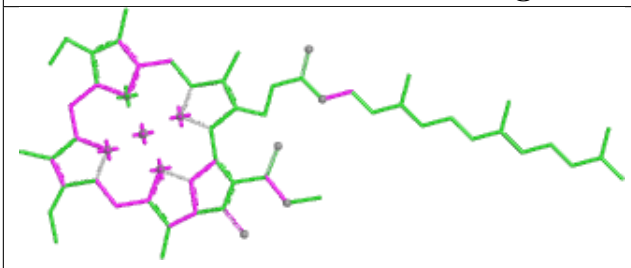


Torsions

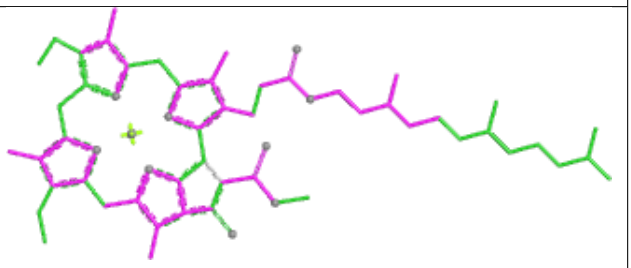


Rings

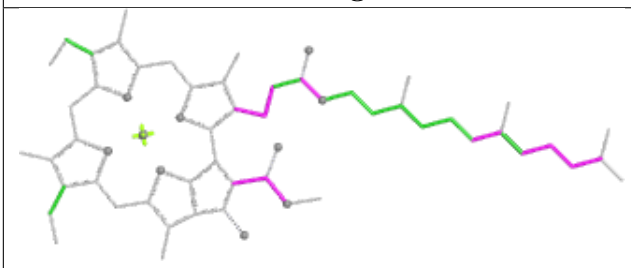
Ligand CLA A 1106



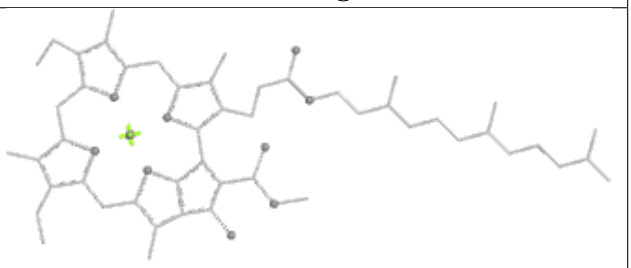
Bond lengths



Bond angles



Torsions

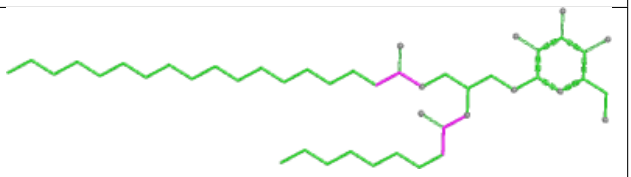


Rings

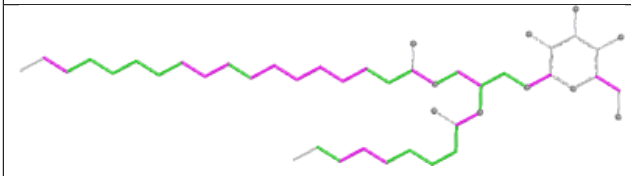
Ligand LMG G 5005



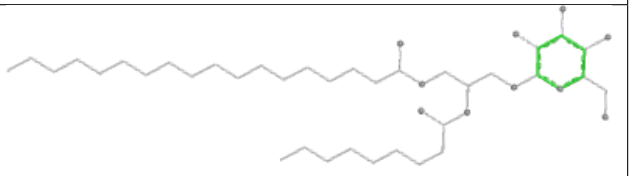
Bond lengths



Bond angles

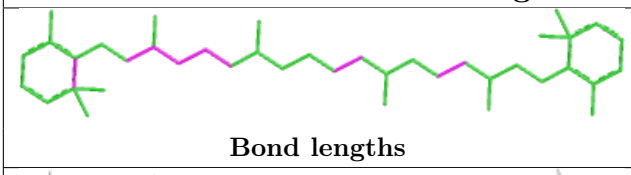


Torsions

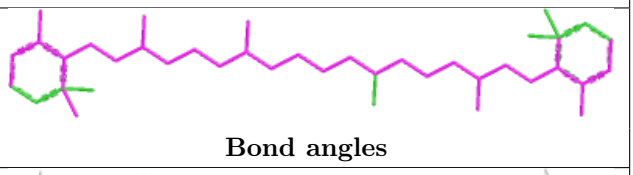


Rings

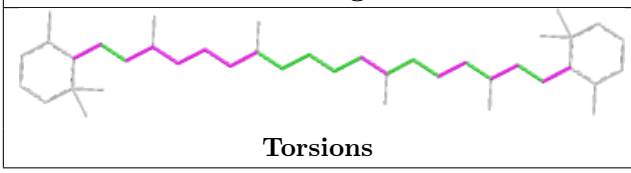
Ligand BCR A 4011



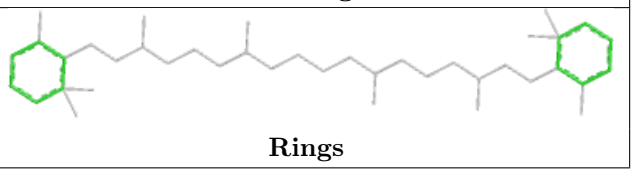
Bond lengths



Bond angles

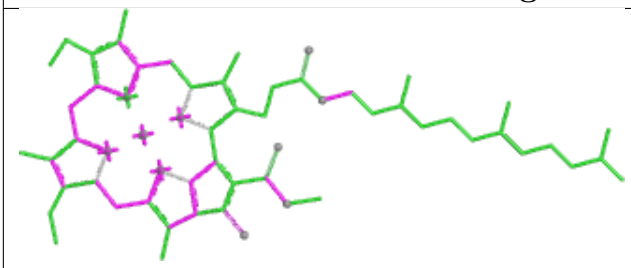


Torsions

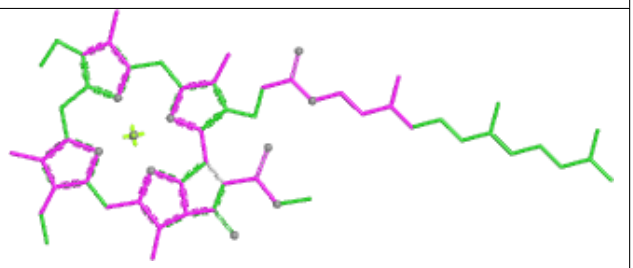


Rings

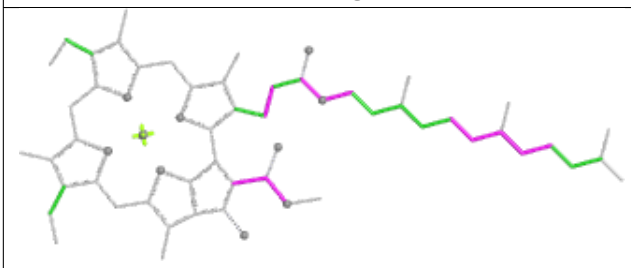
Ligand CLA a 1123



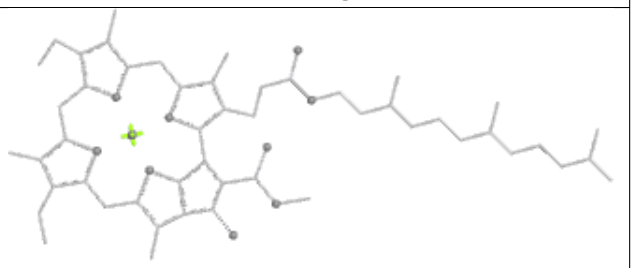
Bond lengths



Bond angles

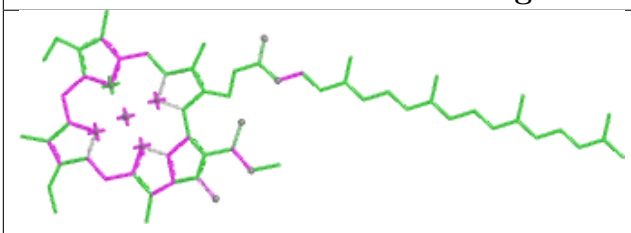


Torsions

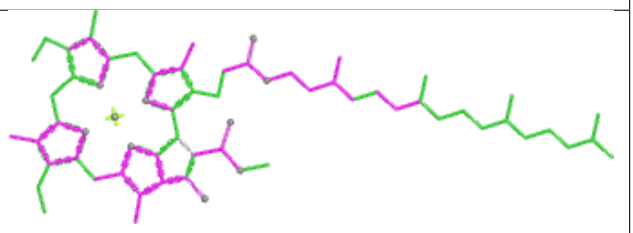


Rings

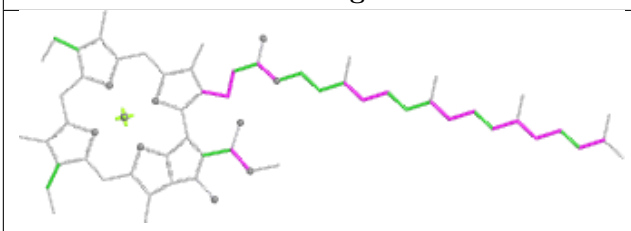
Ligand CLA A 1109



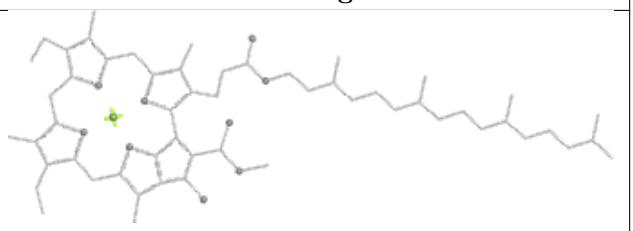
Bond lengths



Bond angles

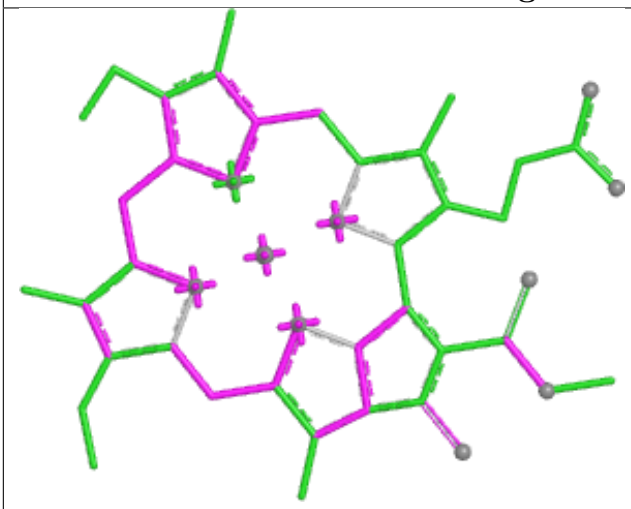


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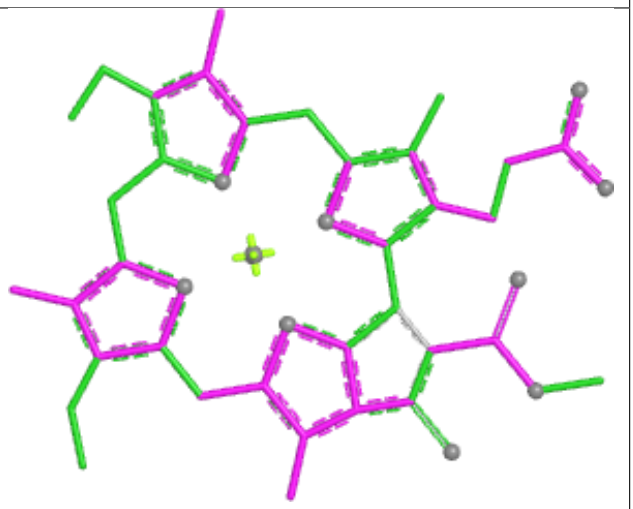


Rings

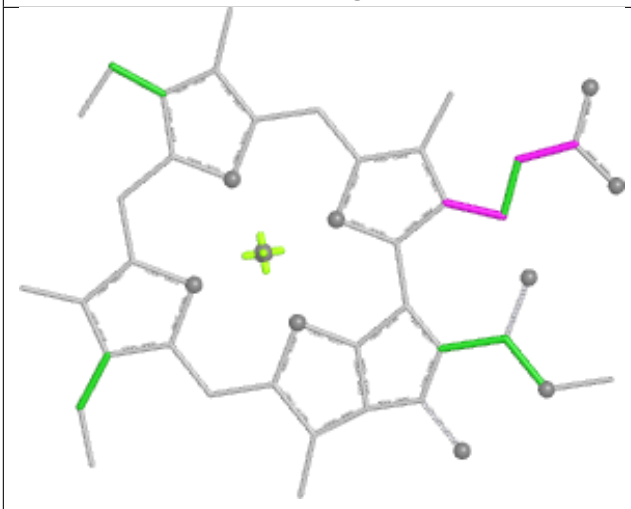
Ligand CLA b 1236



Bond lengths



Bond angles

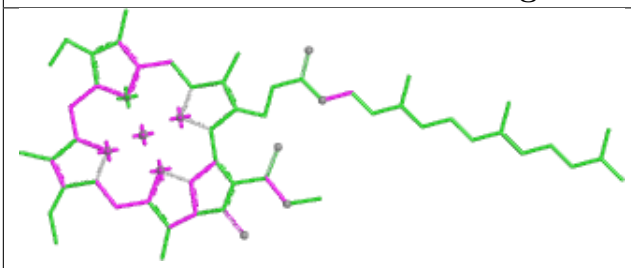


Torsions

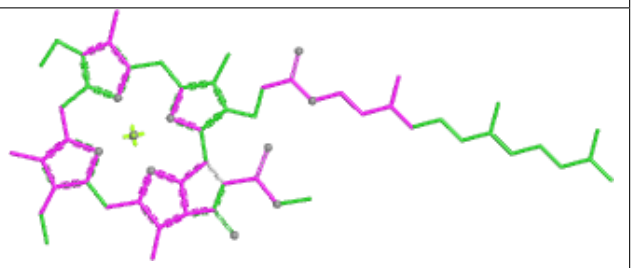


Rings

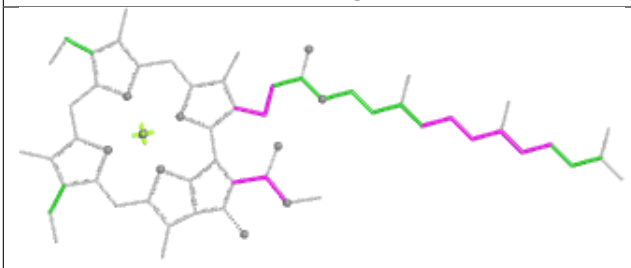
Ligand CLA a 1135



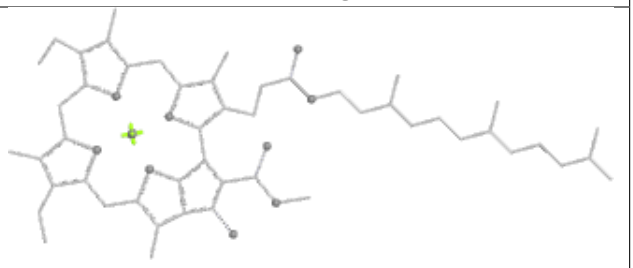
Bond lengths



Bond angles

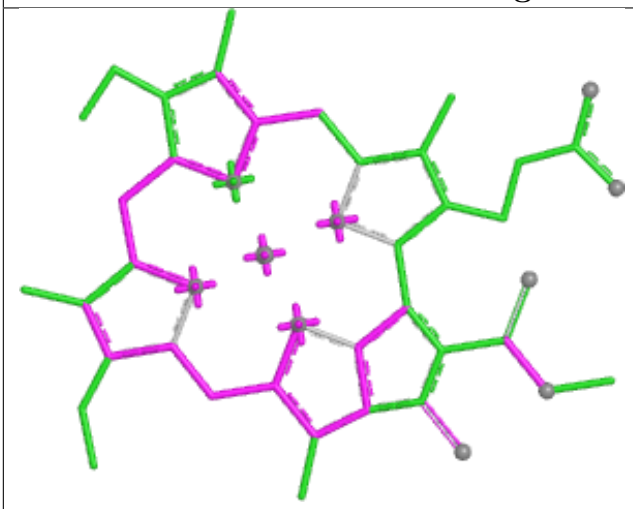


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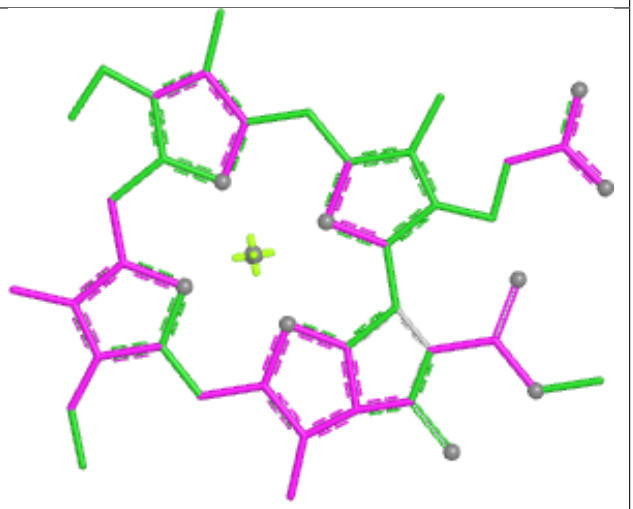


Rings

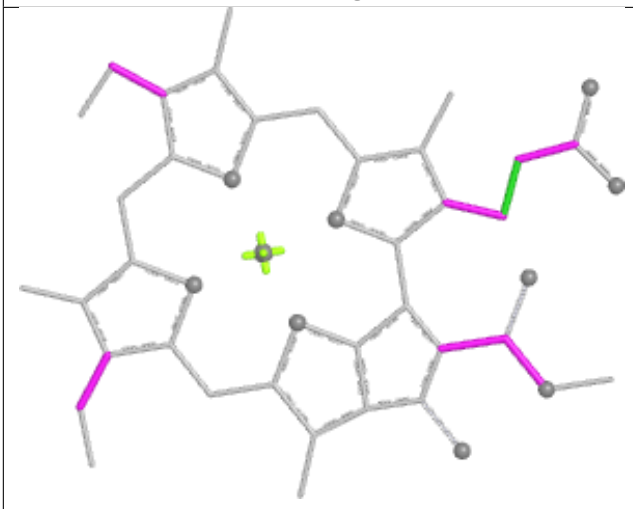
Ligand CLA G 1114



Bond lengths



Bond angles

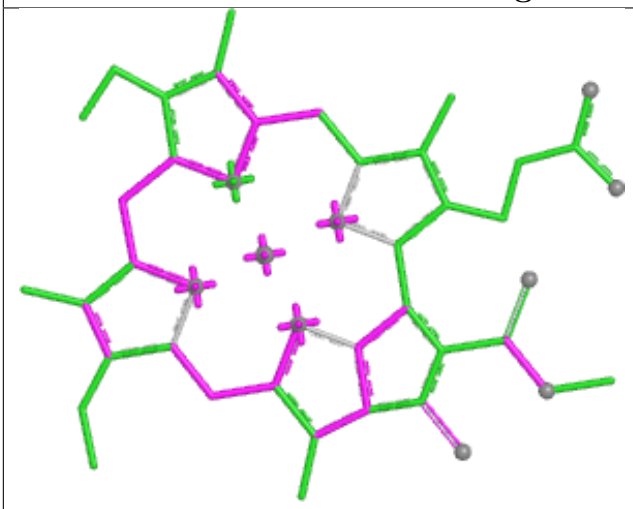


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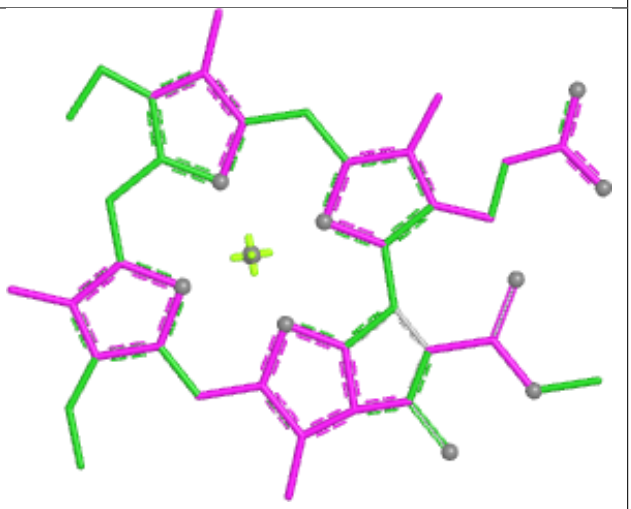


Rings

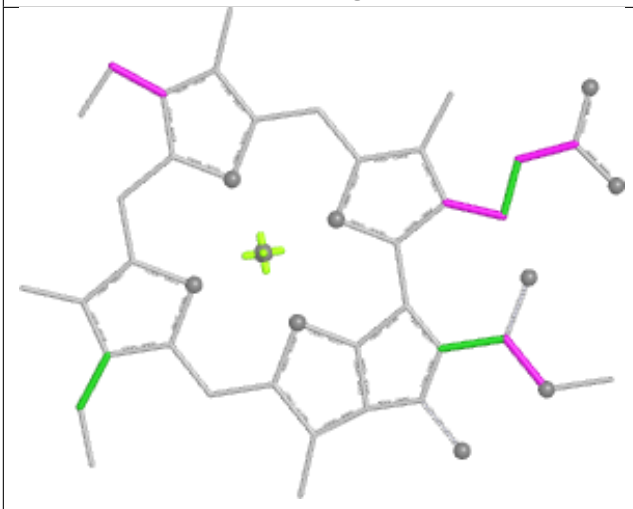
Ligand CLA A 1110



Bond lengths



Bond angles

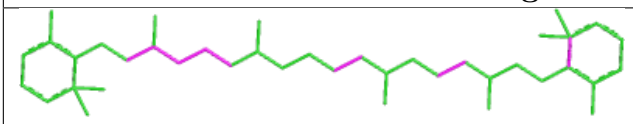


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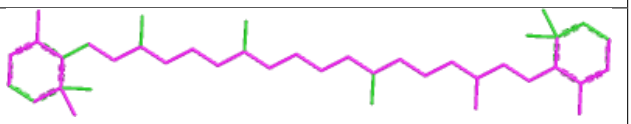


Rings

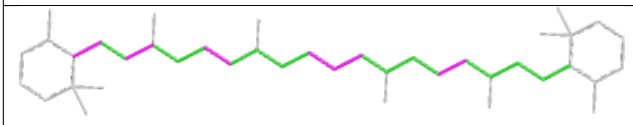
Ligand BCR i 4018



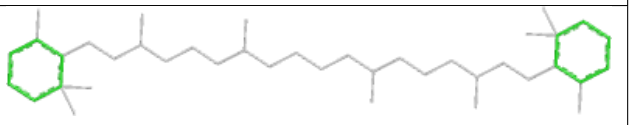
Bond lengths



Bond angles

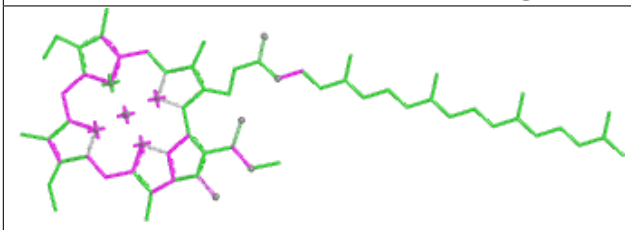


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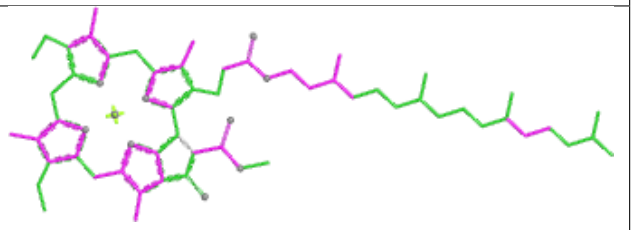


Rings

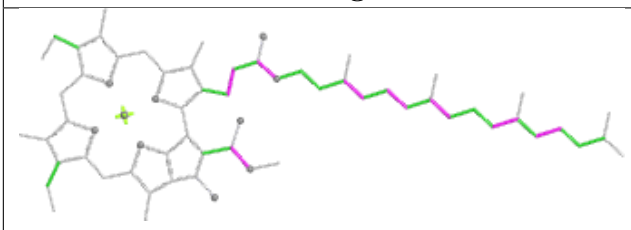
Ligand CLA L 1501



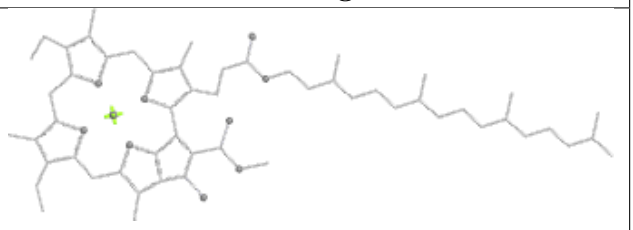
Bond lengths



Bond angles

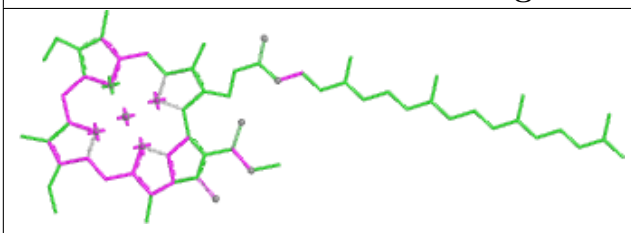


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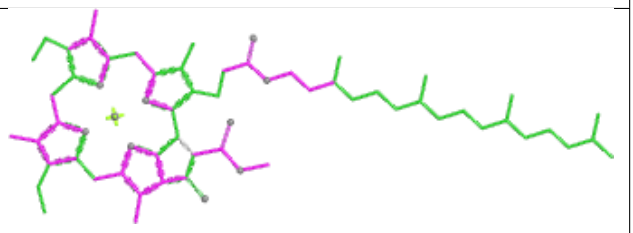


Rings

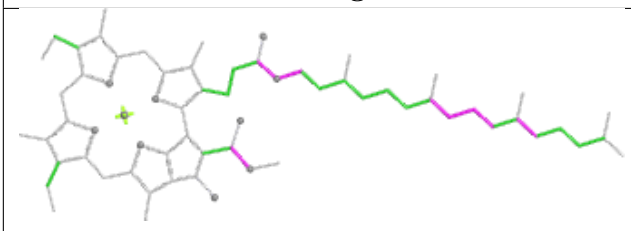
Ligand CLA A 1119



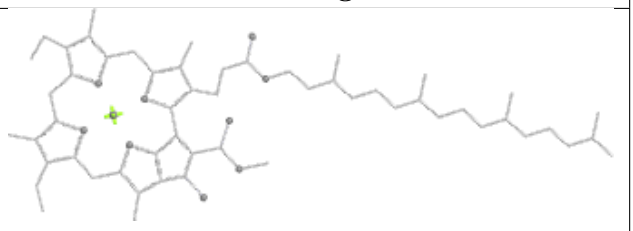
Bond lengths



Bond angles

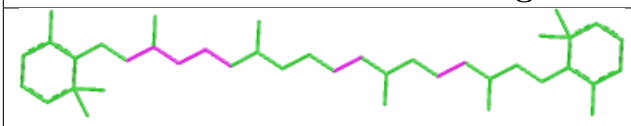


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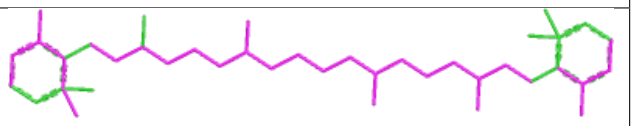


Rings

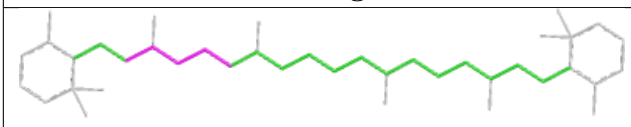
Ligand BCR L 4022



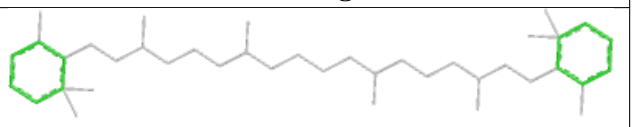
Bond lengths



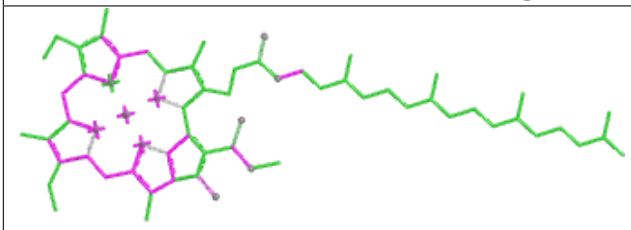
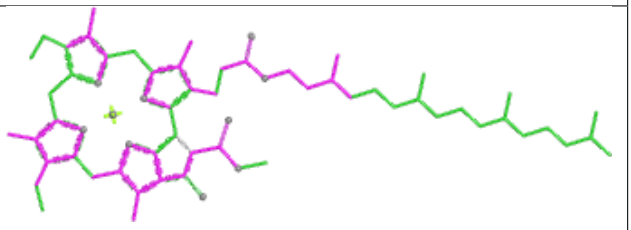
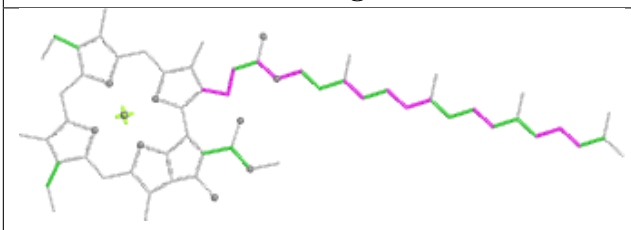
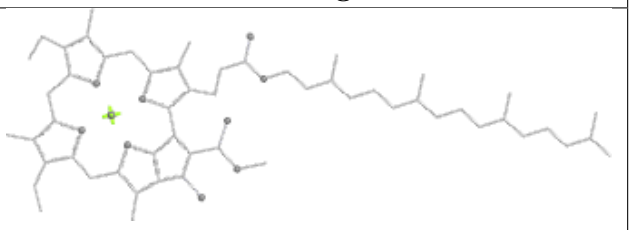
Bond angles

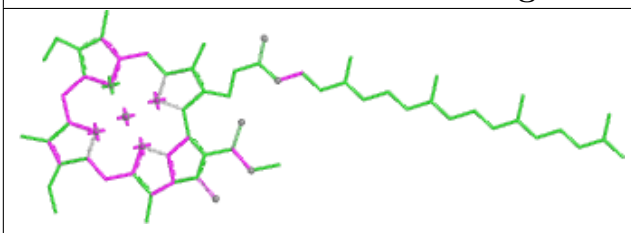
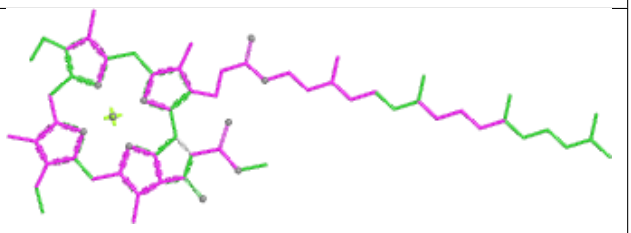
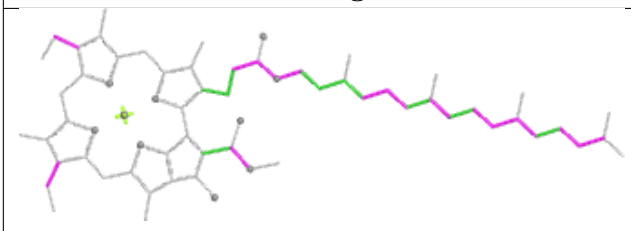
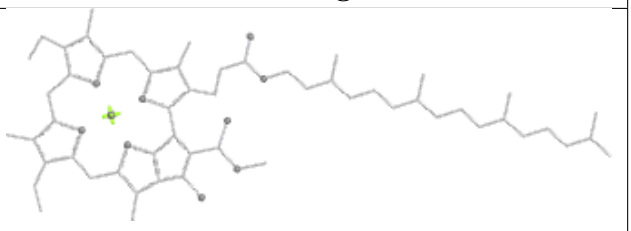


Torsions

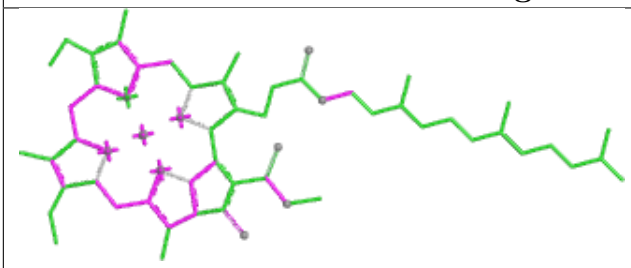


Rings

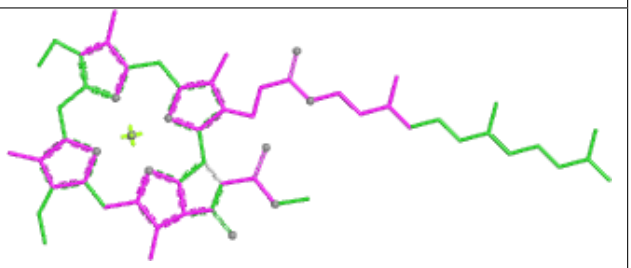
Ligand CLA b 1210	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1239	
	
Bond lengths	Bond angles
	
Torsions	Rings

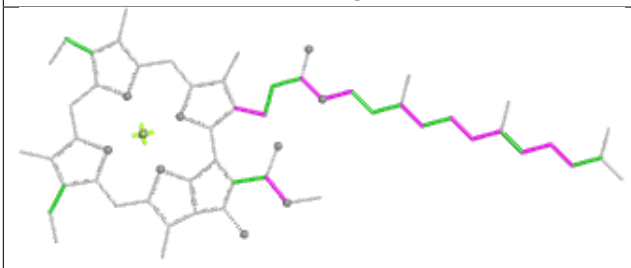
Ligand CLA H 1229



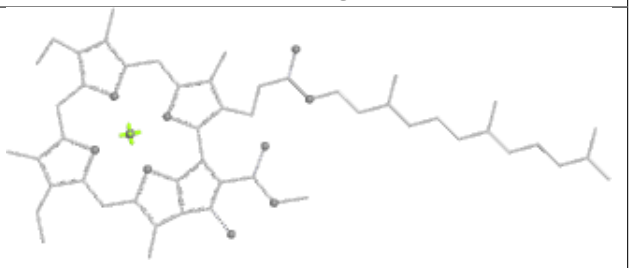
Bond lengths



Bond angles

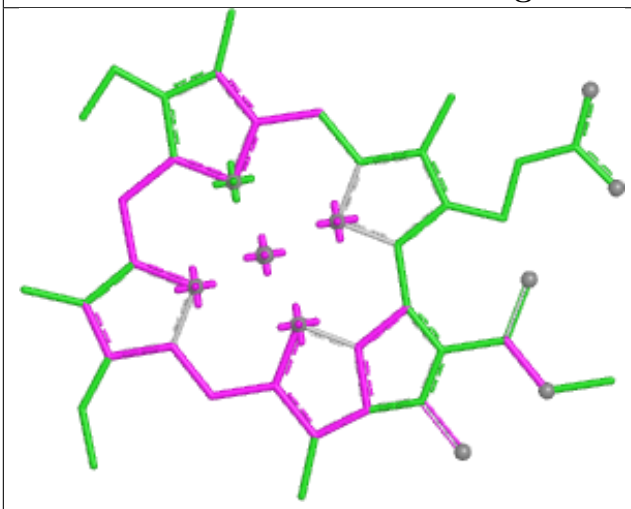


Torsions

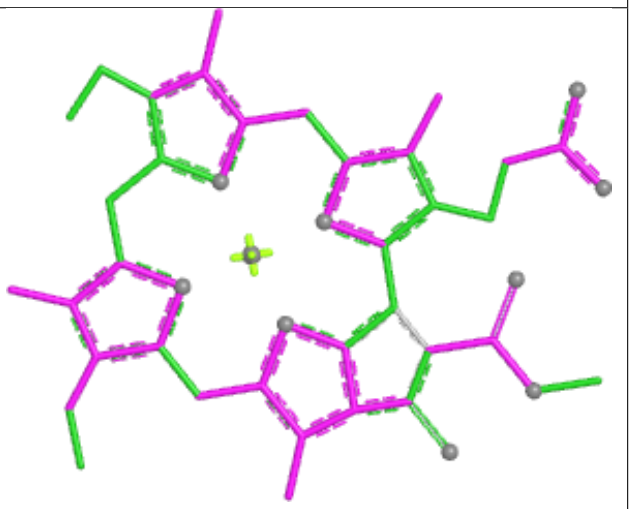


Rings

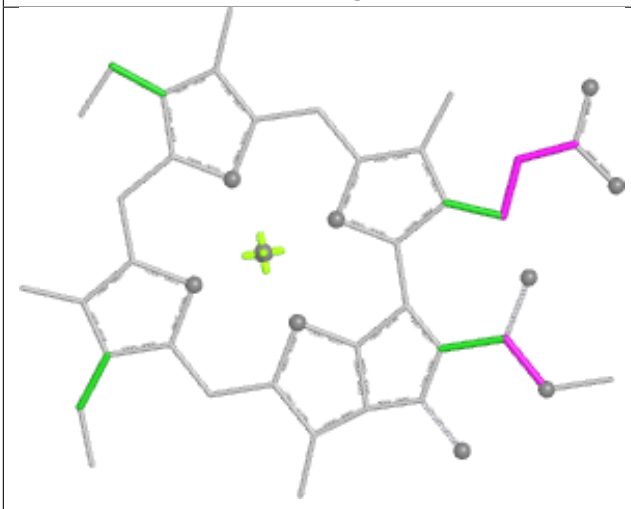
Ligand CLA A 1134



Bond lengths



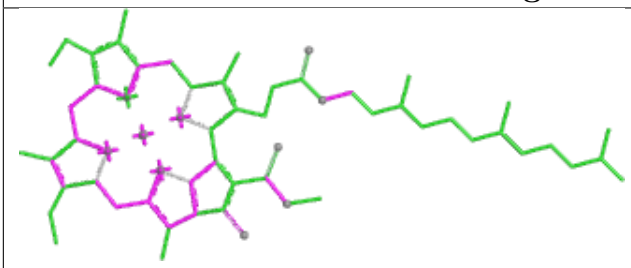
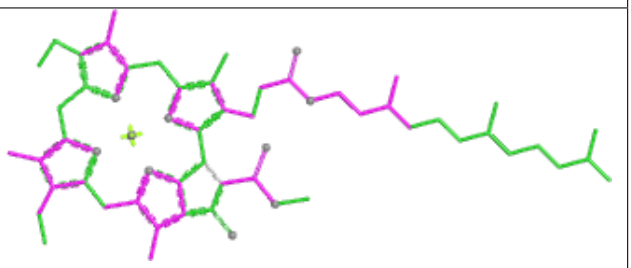
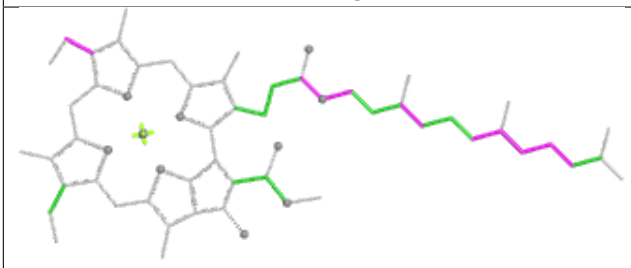
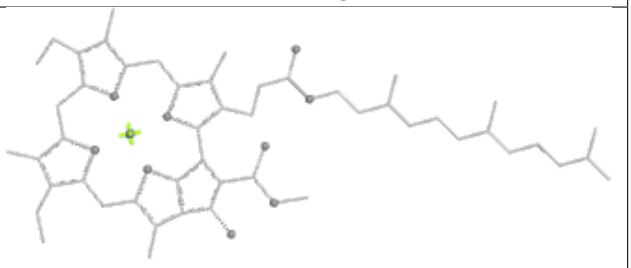
Bond angles

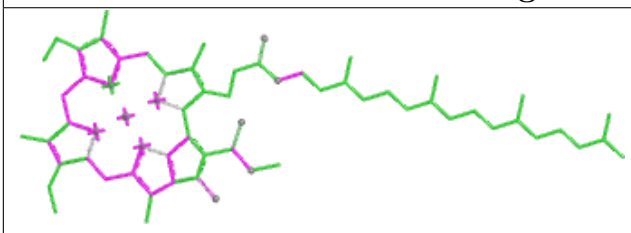
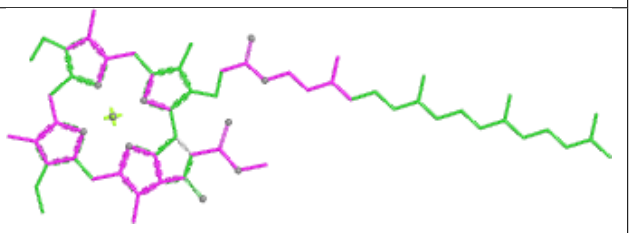
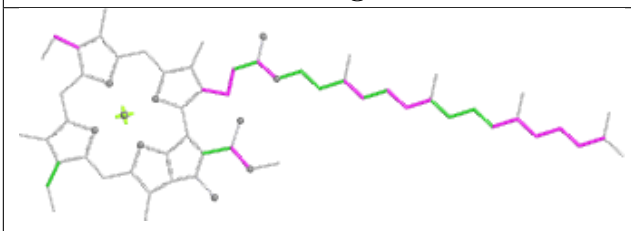
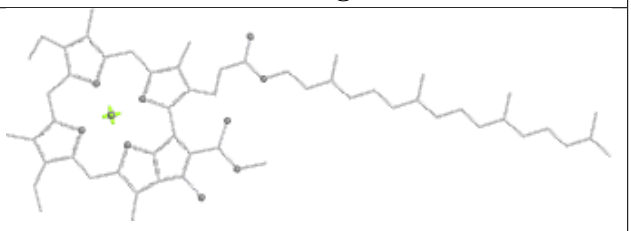


Torsions

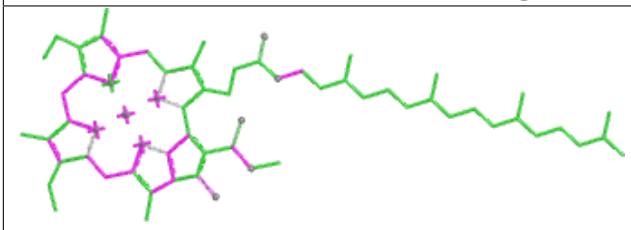


Rings

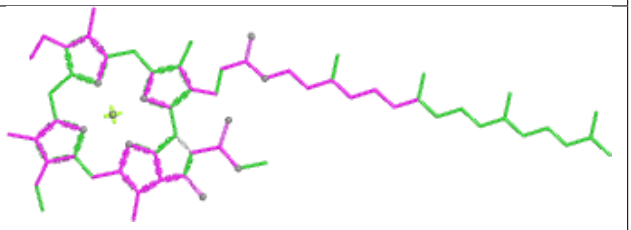
Ligand CLA l 1502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1216	
	
Bond lengths	Bond angles
	
Torsions	Rings

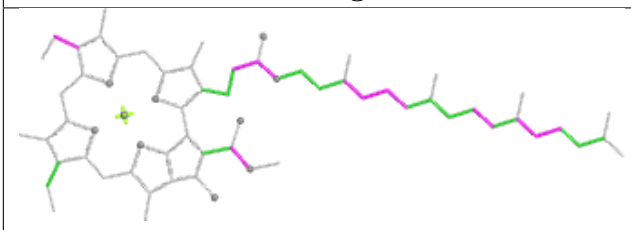
Ligand CLA B 1204



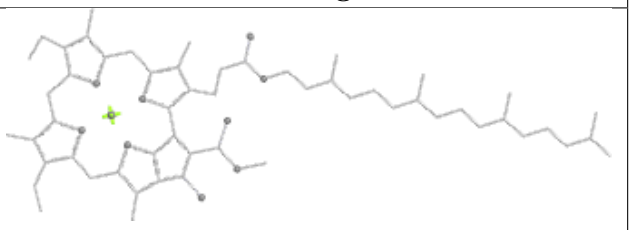
Bond lengths



Bond angles

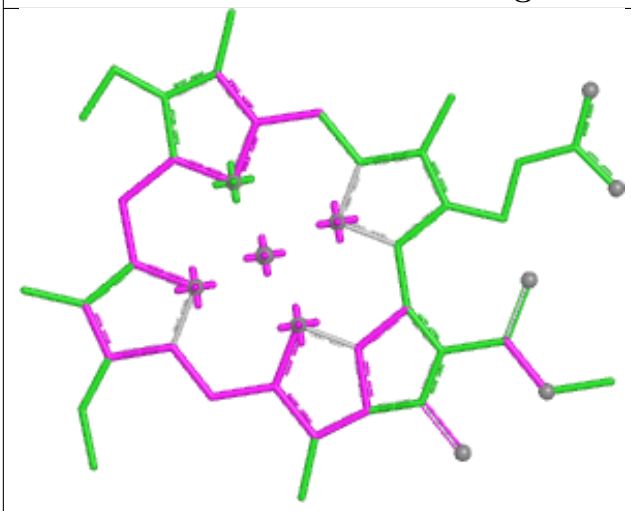


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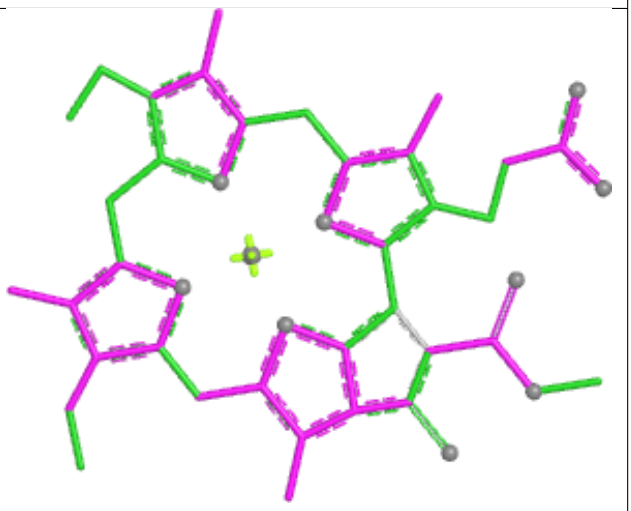


Rings

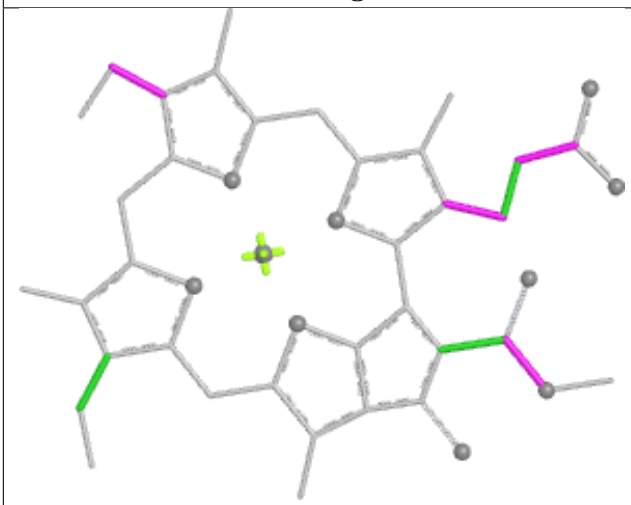
Ligand CLA H 1233



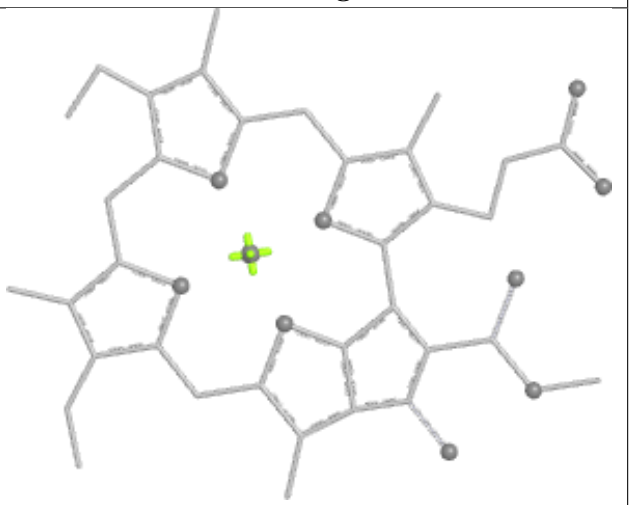
Bond lengths



Bond angles

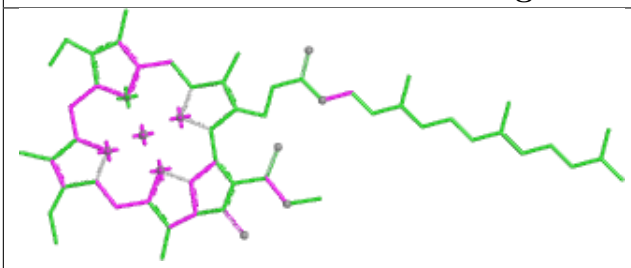


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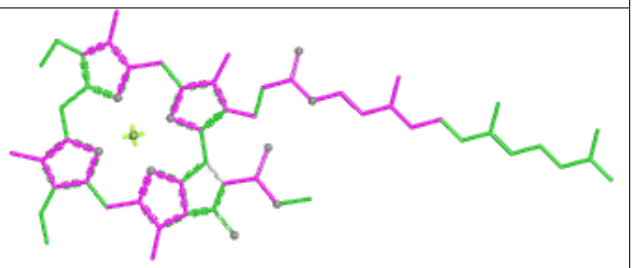


Rings

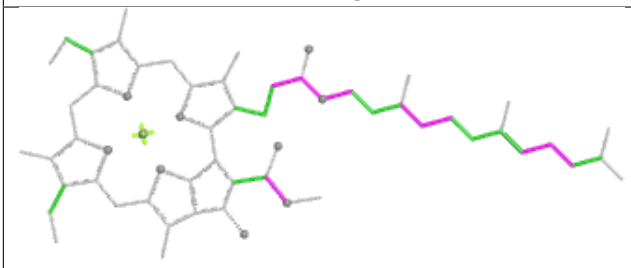
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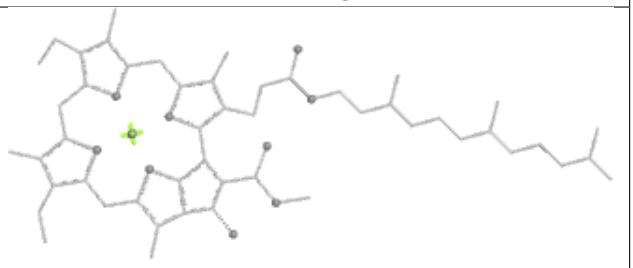
Bond lengths



Bond angles

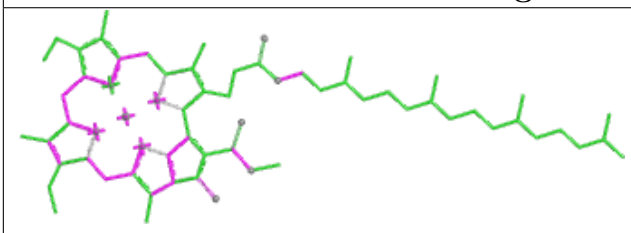


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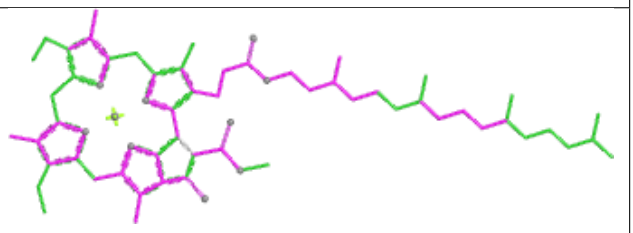


Rings

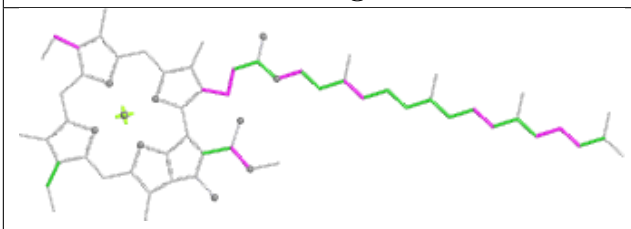
Ligand CLA A 1012



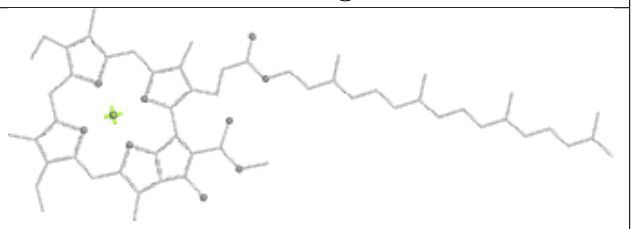
Bond lengths



Bond angles

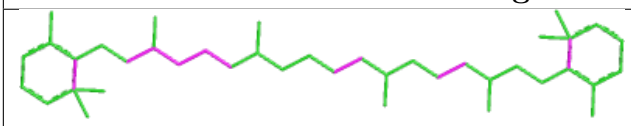


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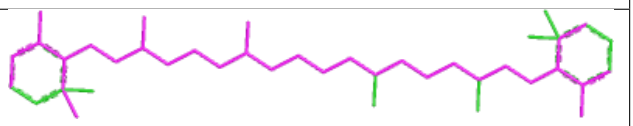


Rings

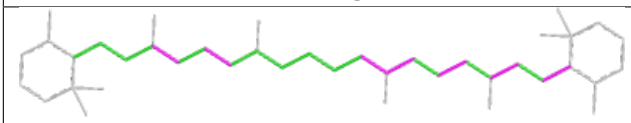
Ligand BCR G 4007



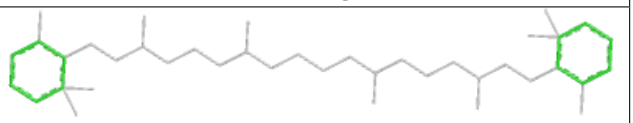
Bond lengths



Bond angles

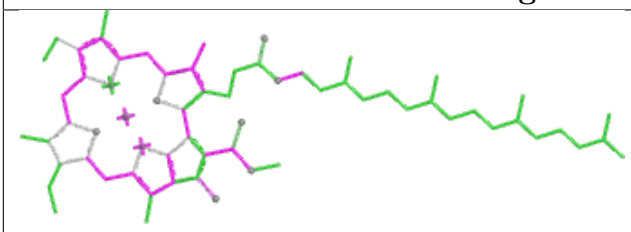


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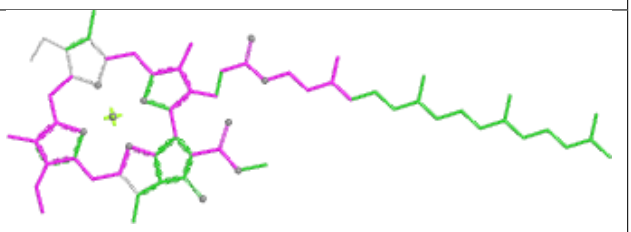


Rings

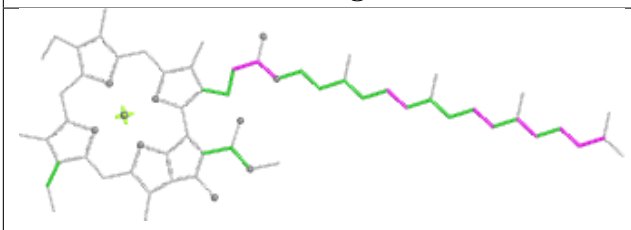
Ligand CL0 G 1011



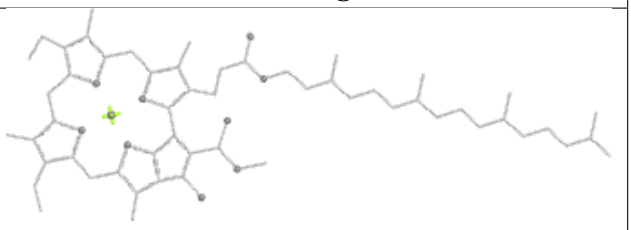
Bond lengths



Bond angles

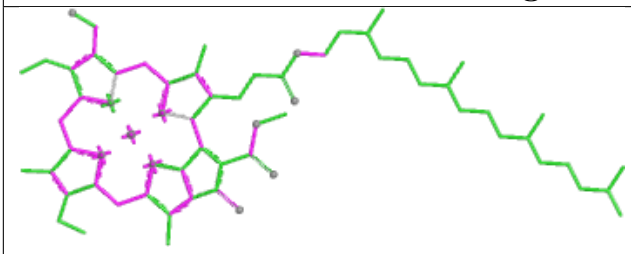


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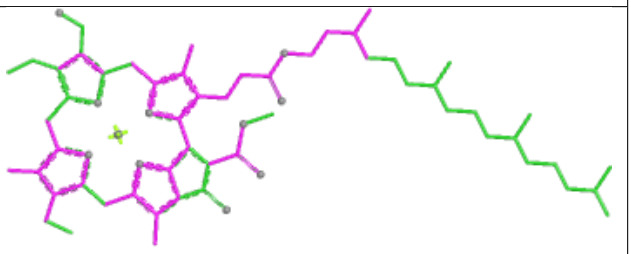


Rings

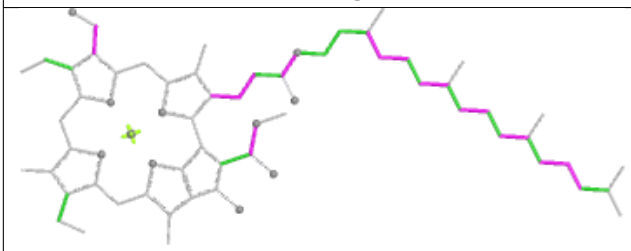
Ligand F6C b 1237



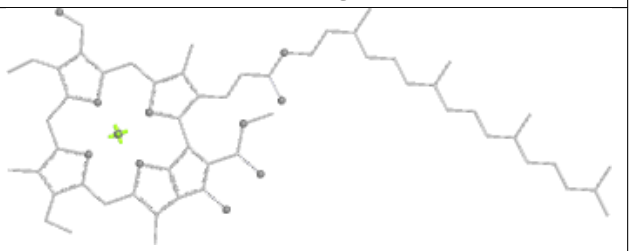
Bond lengths



Bond angles

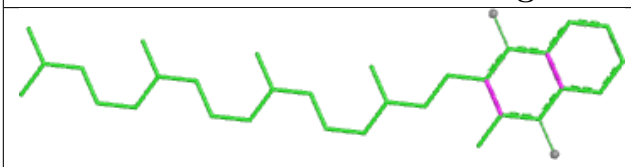


Torsions

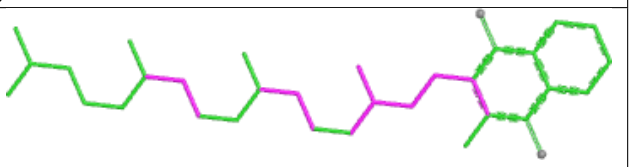


Rings

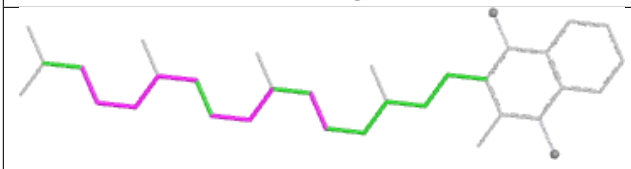
Ligand PQN a 2001



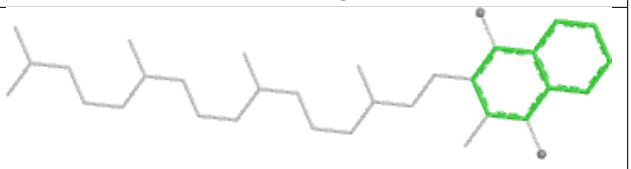
Bond lengths



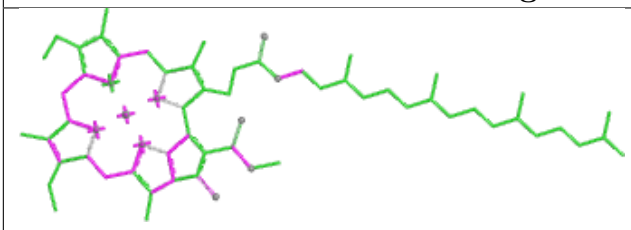
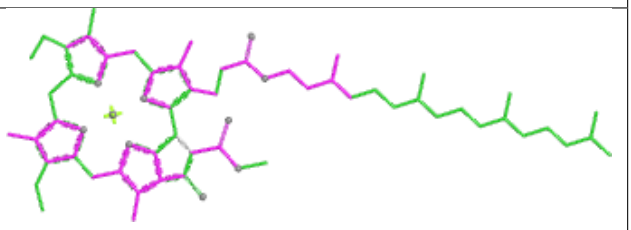
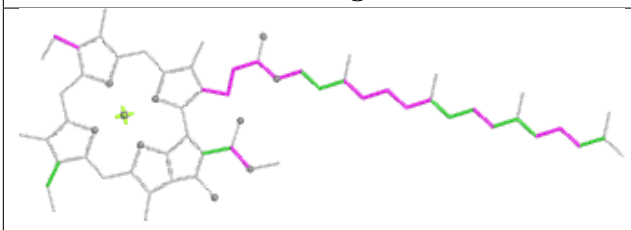
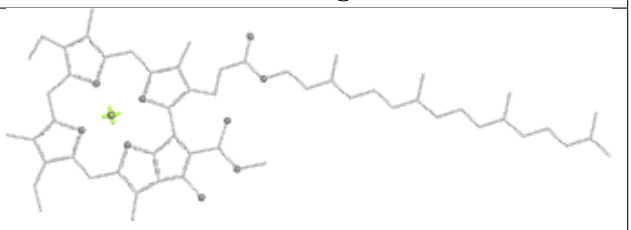
Bond angles

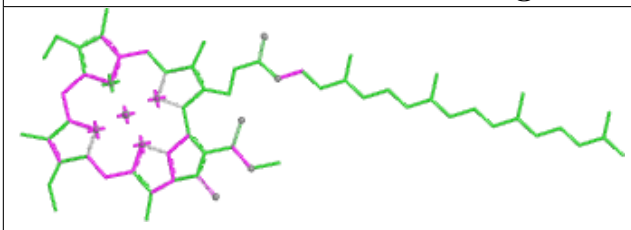
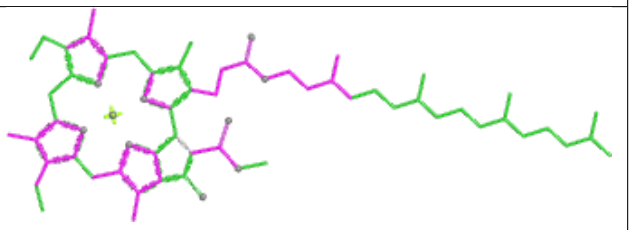
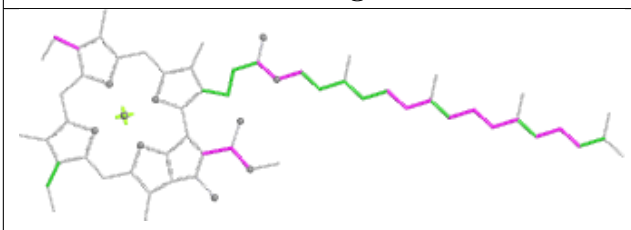
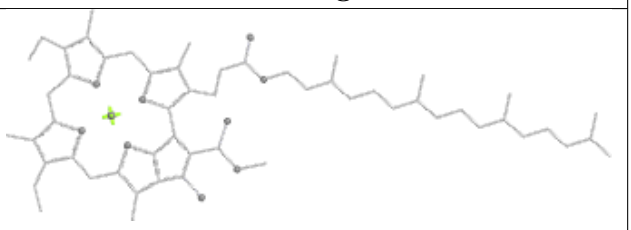


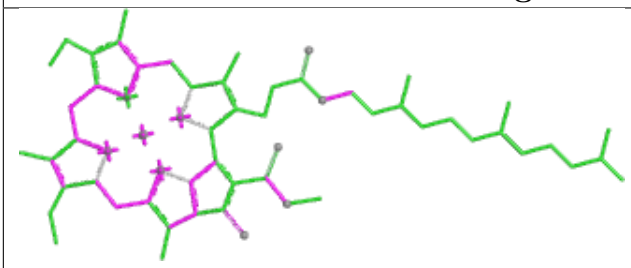
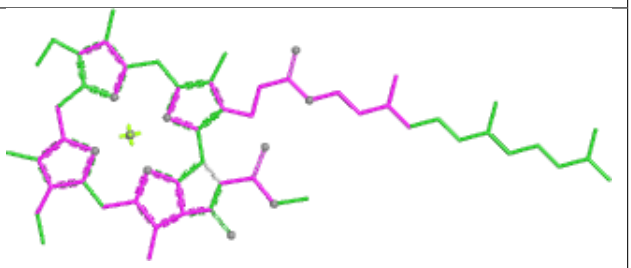
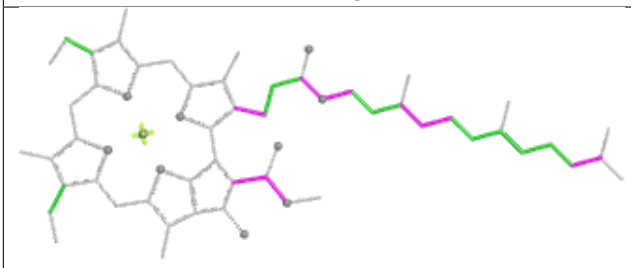
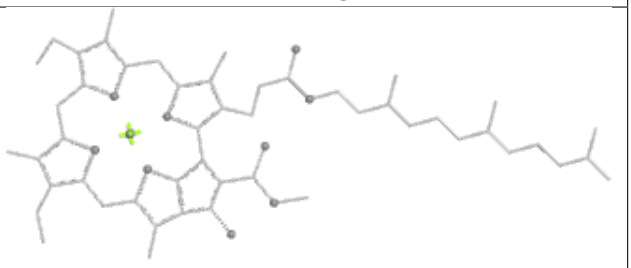
Torsions

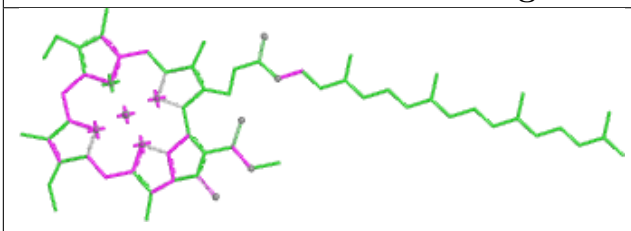
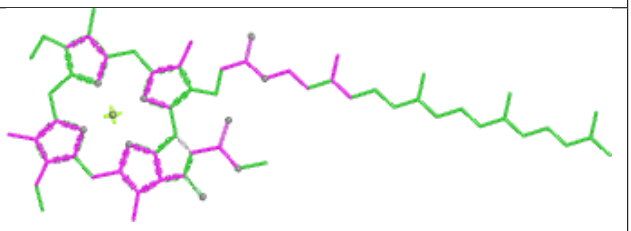
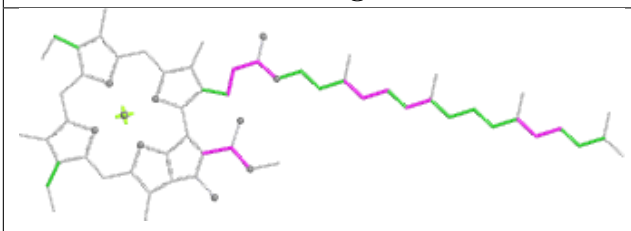
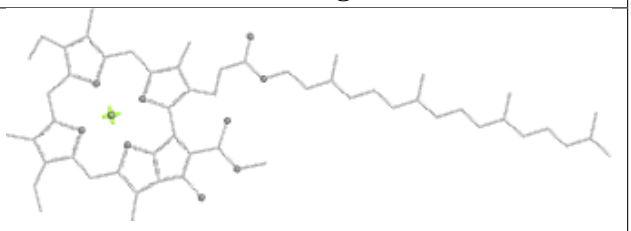


Rings

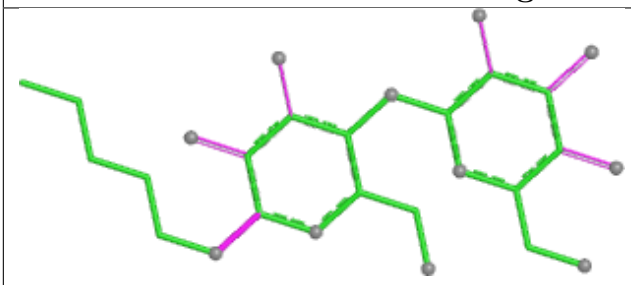
Ligand CLA a 1136	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 1234	
	
Bond lengths	Bond angles
	
Torsions	Rings

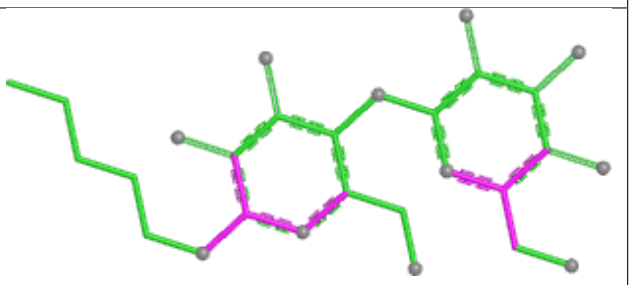
Ligand CLA A 1103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 1213	
	
Bond lengths	Bond angles
	
Torsions	Rings

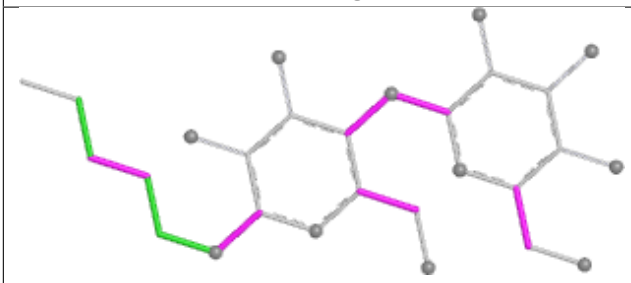
Ligand LMT a 6002



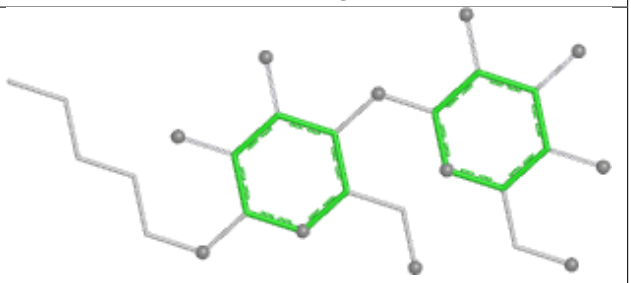
Bond lengths



Bond angles

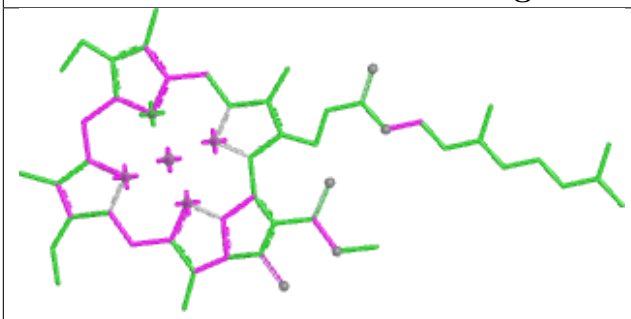


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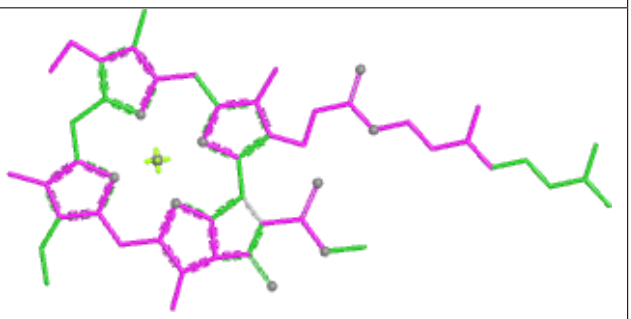


Rings

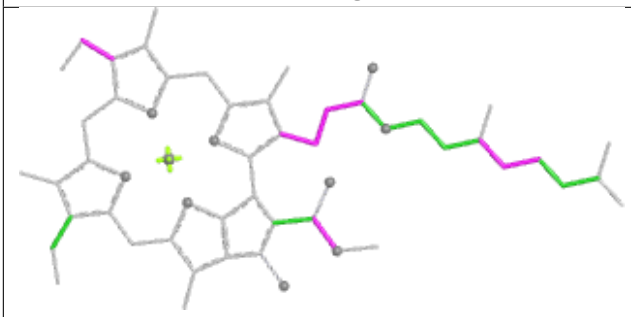
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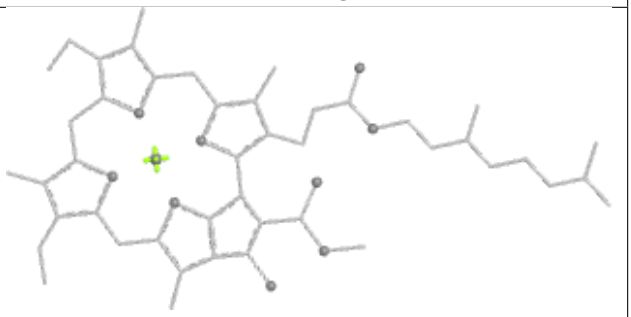
Bond lengths



Bond angles

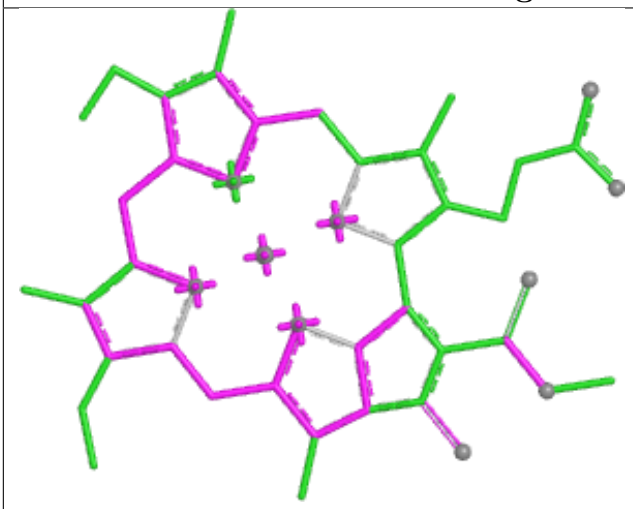


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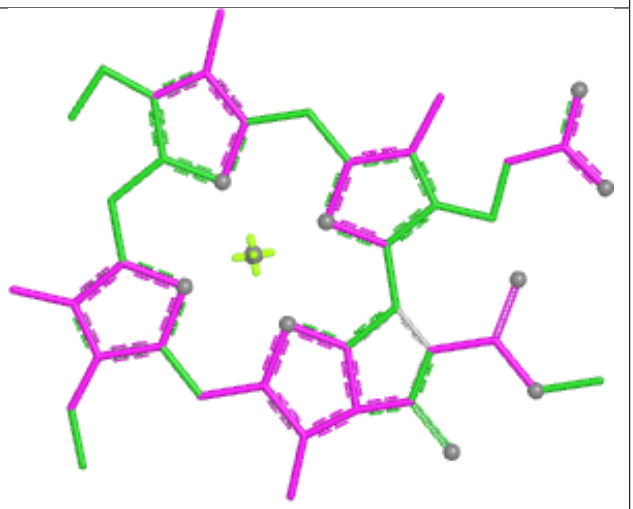


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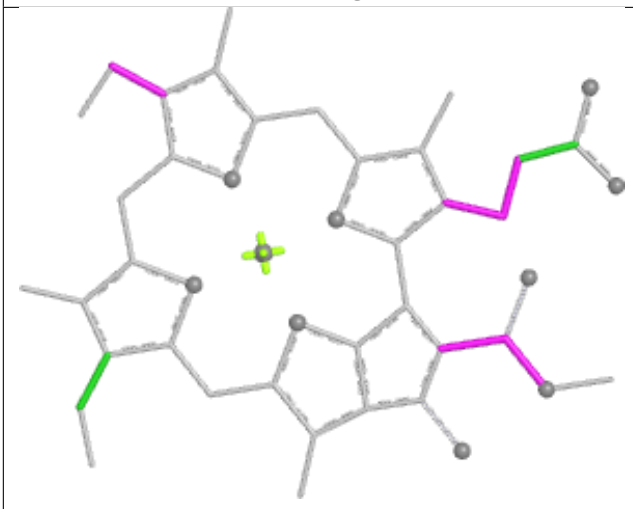
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Bond lengths



Bond angles

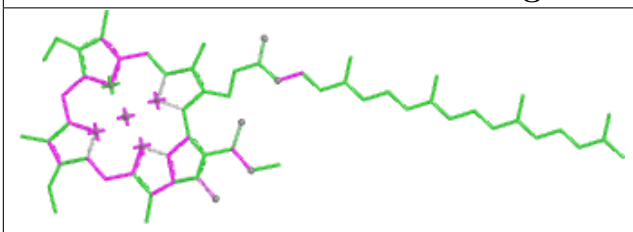


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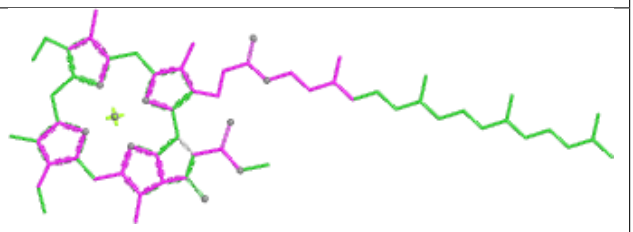


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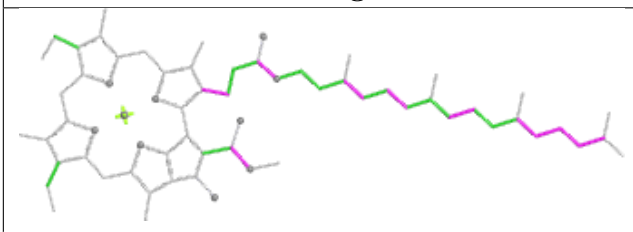
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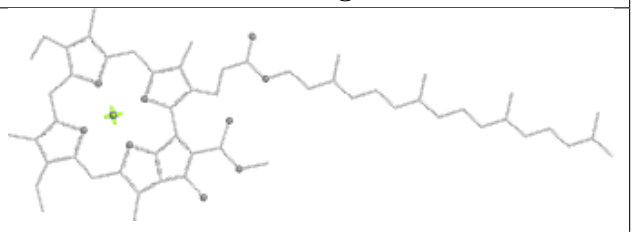
Bond lengths



Bond angles

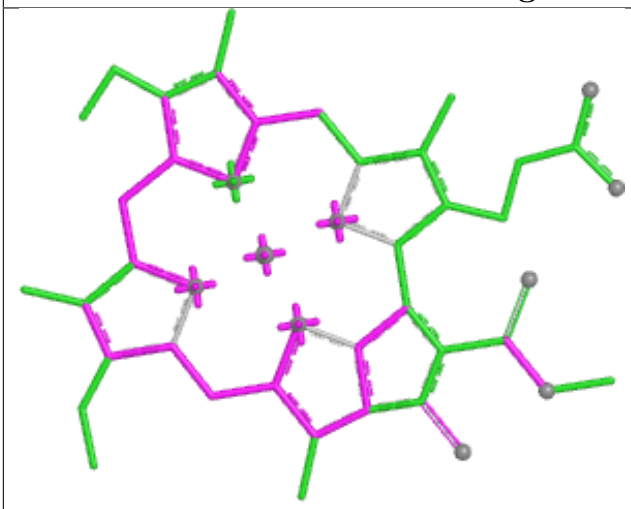


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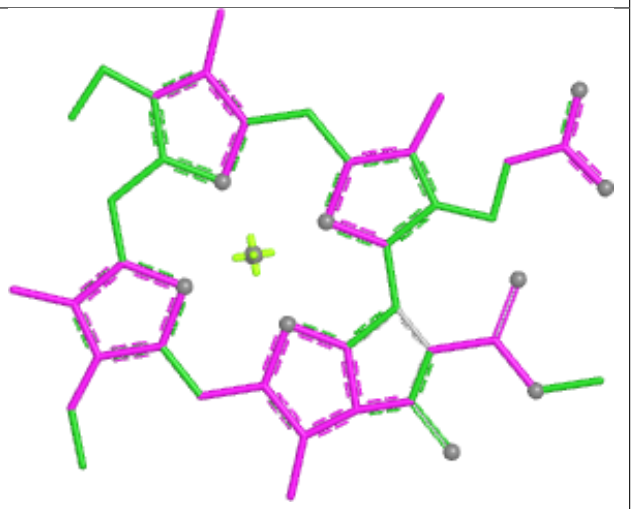


Rings

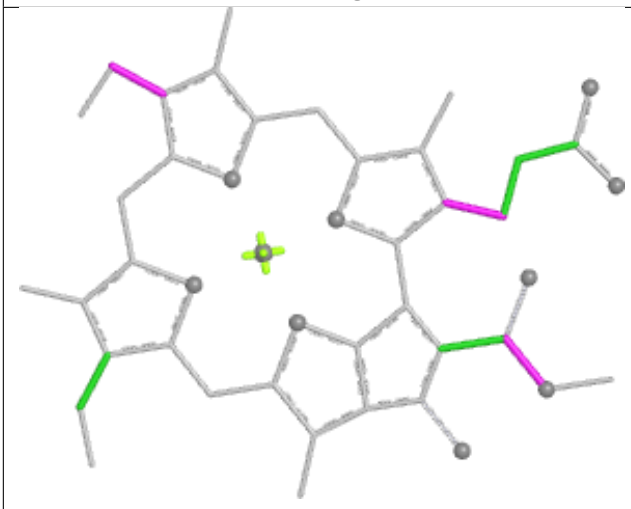
Ligand CLA b 1219



Bond lengths



Bond angles

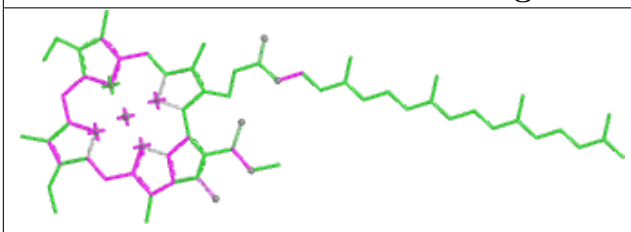


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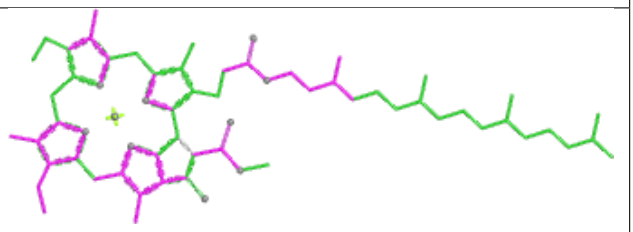


Rings

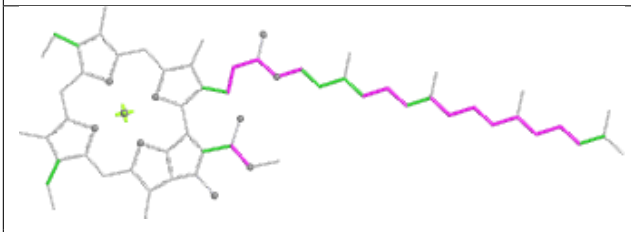
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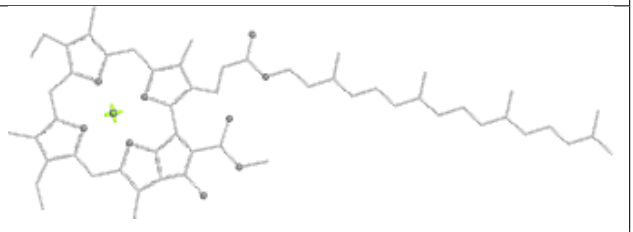
Bond lengths



Bond angles

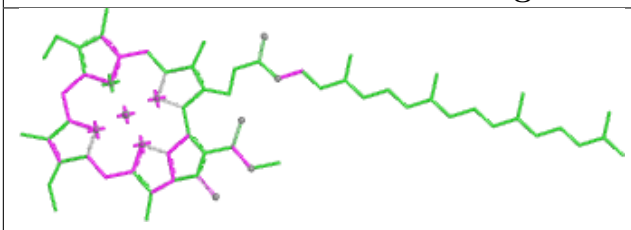


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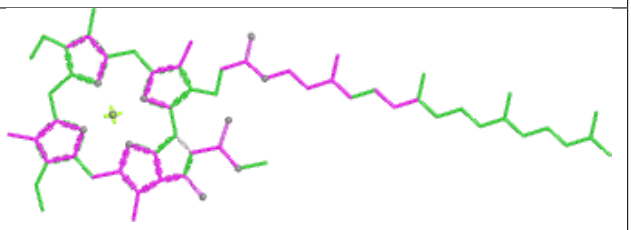


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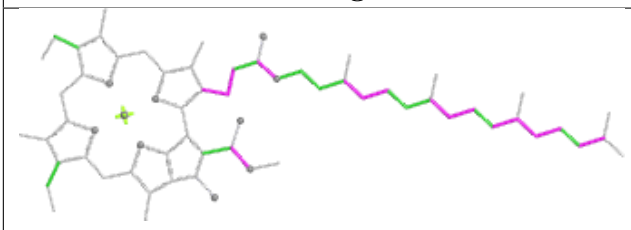
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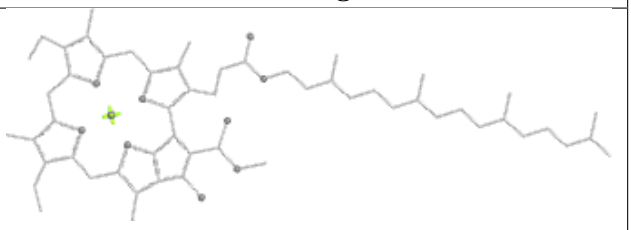
Bond lengths



Bond angles

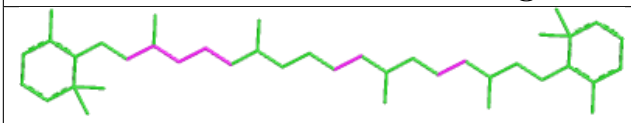


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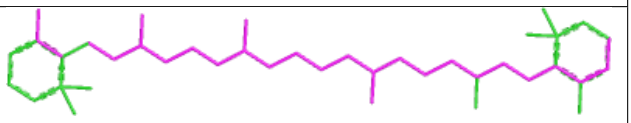


Rings

Ligand BCR a 4008



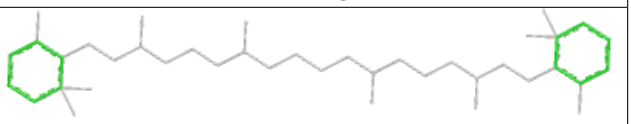
Bond lengths



Bond angles

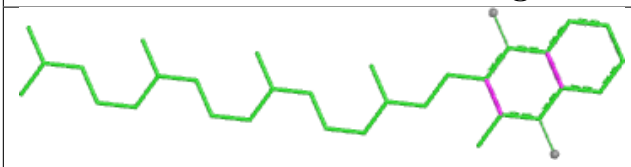


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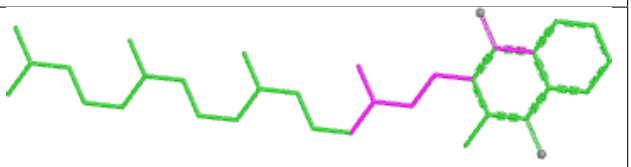


Rings

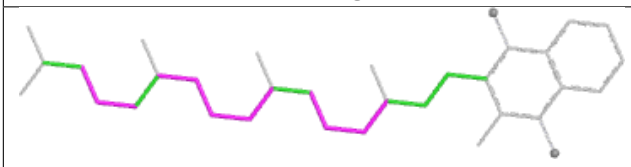
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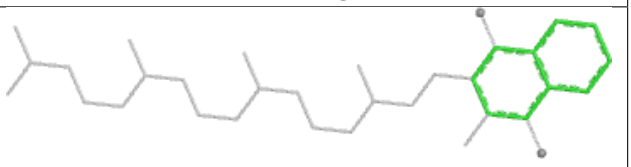
Bond lengths



Bond angles

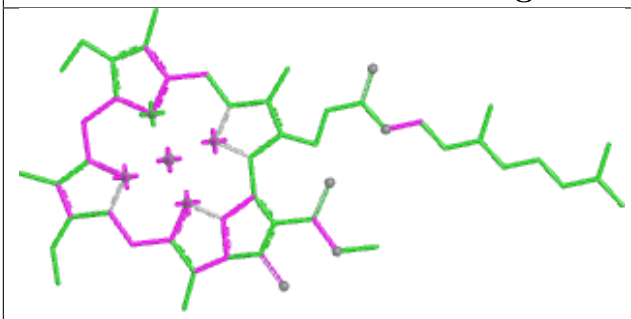


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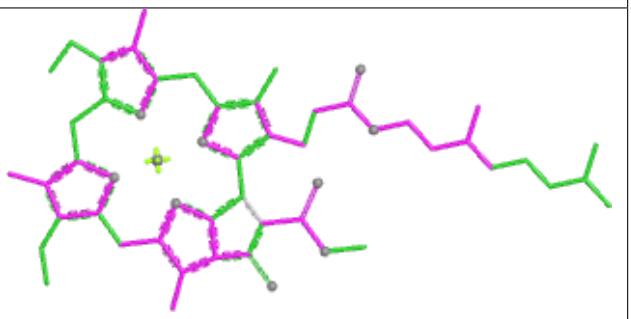


Rings

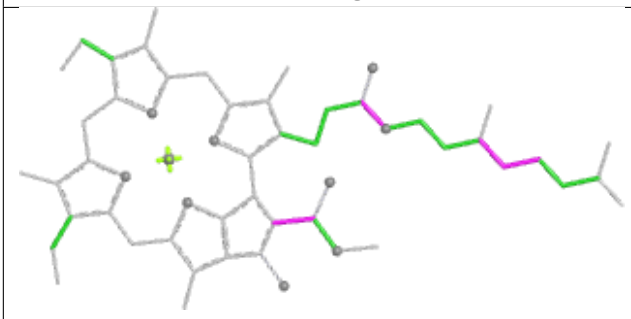
Ligand CLA B 1201



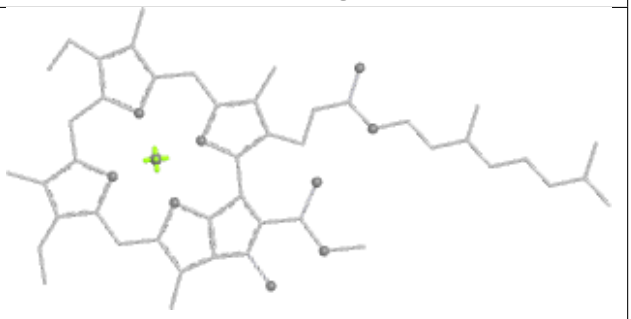
Bond lengths



Bond angles

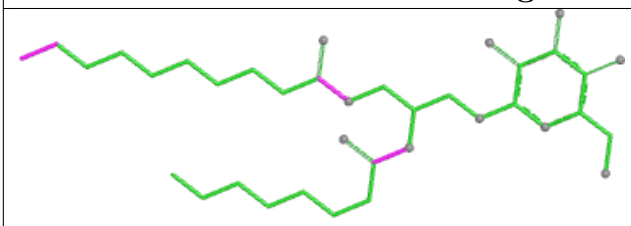


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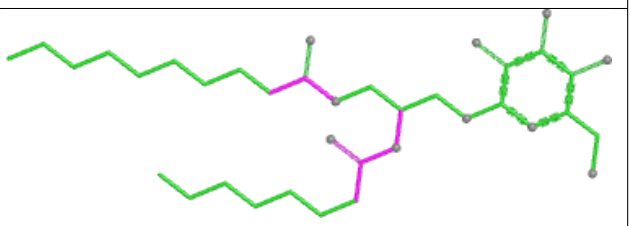


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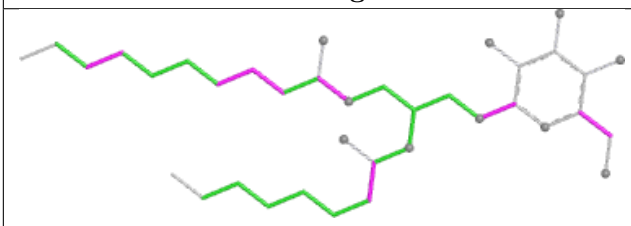
Ligand LMG I 5006



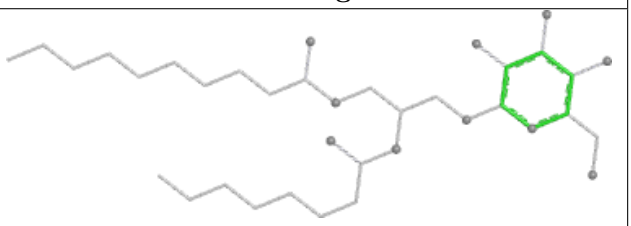
Bond lengths



Bond angles

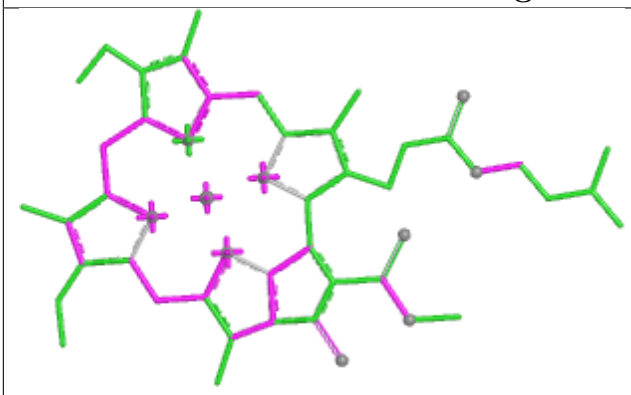


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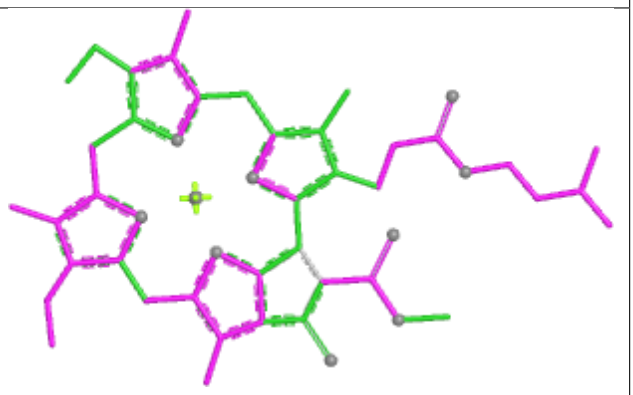


Rings

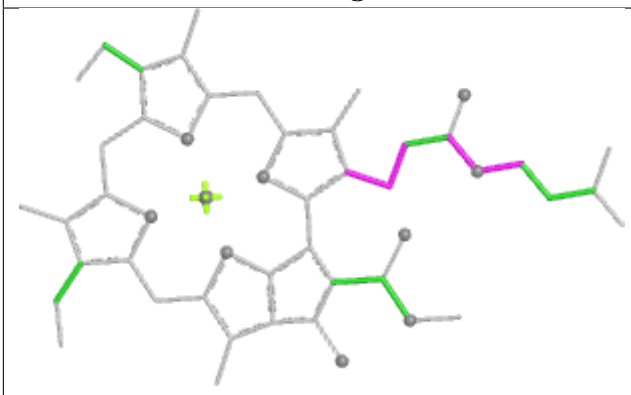
Ligand CLA A 1137



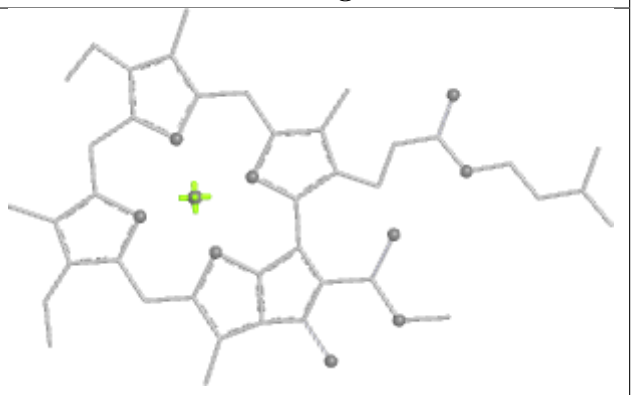
Bond lengths



Bond angles

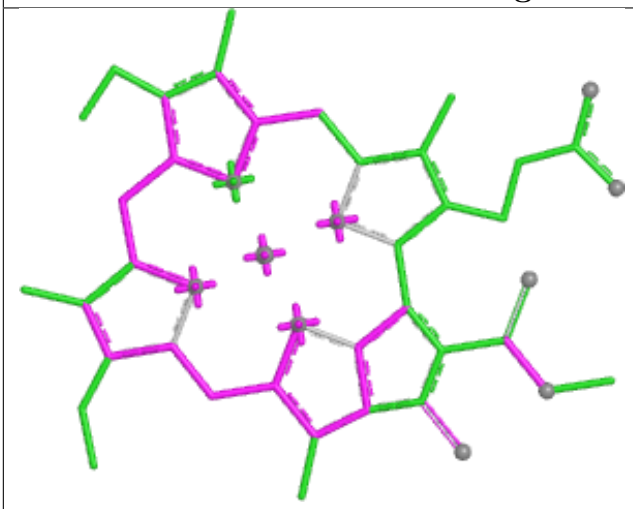


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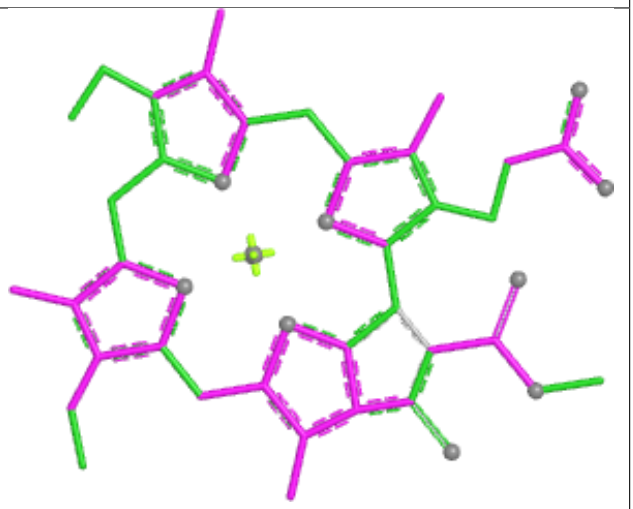


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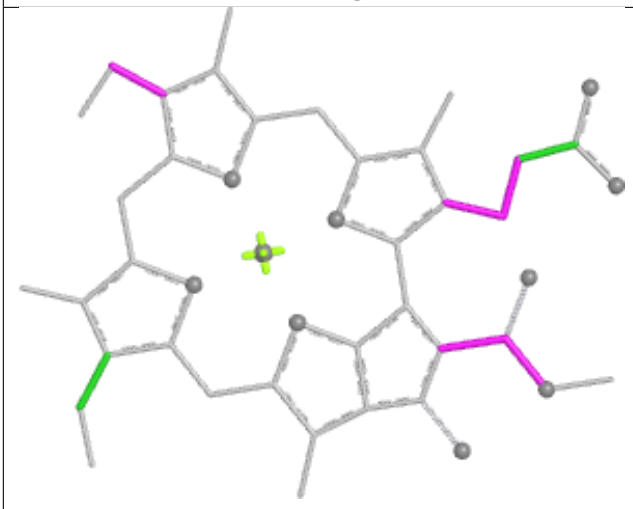
Ligand CLA K 1401



Bond lengths



Bond angles

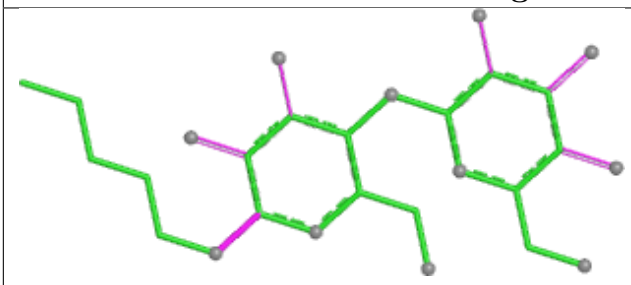


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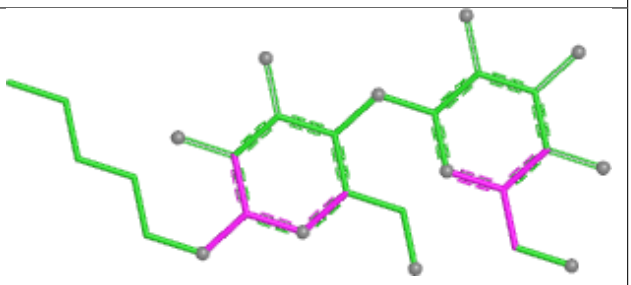


Rings

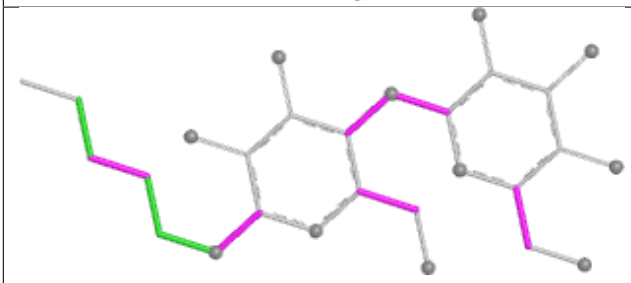
Ligand LMT G 6002



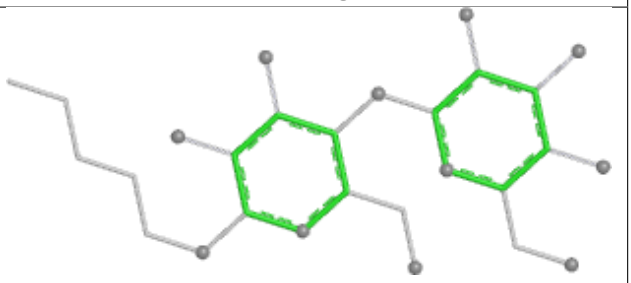
Bond lengths



Bond angles

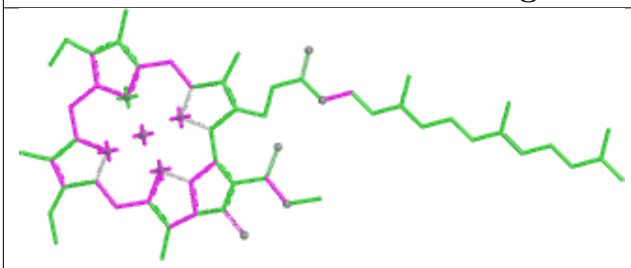


Torsions

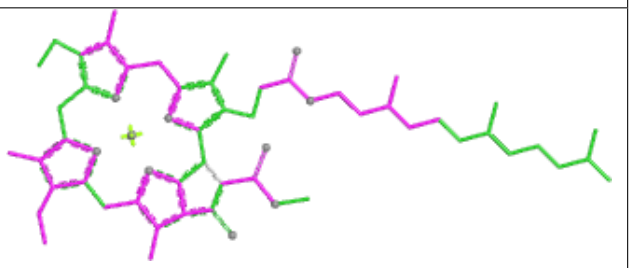


Rings

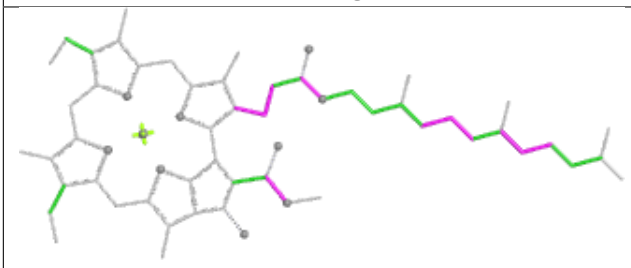
Ligand CLA a 1013



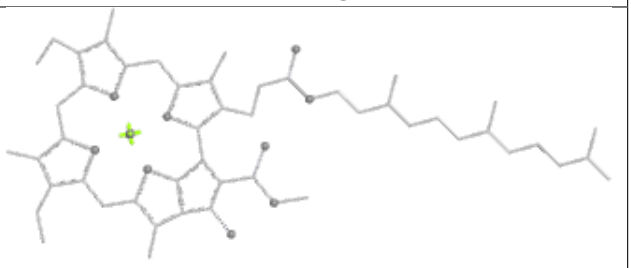
Bond lengths



Bond angles

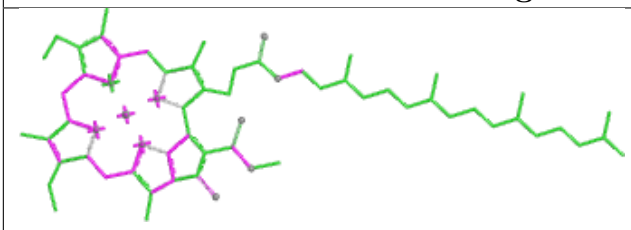


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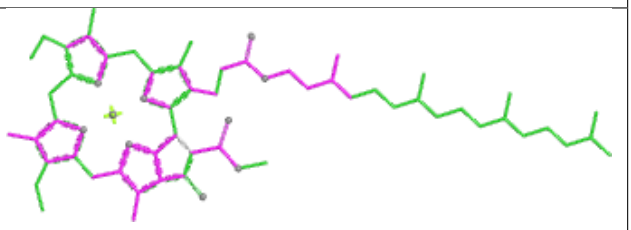


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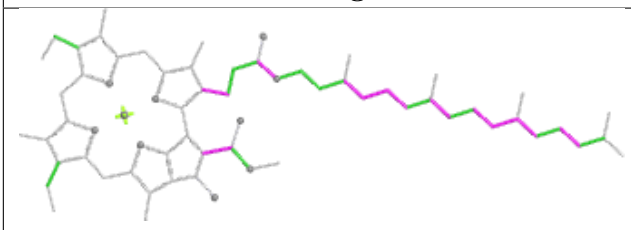
Ligand CLA B 1203



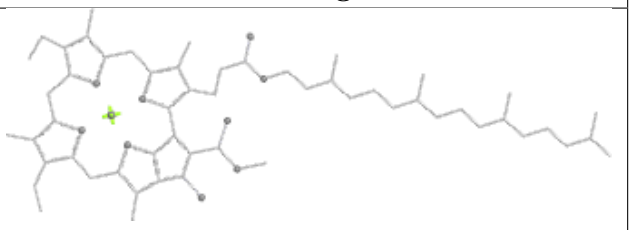
Bond lengths



Bond angles

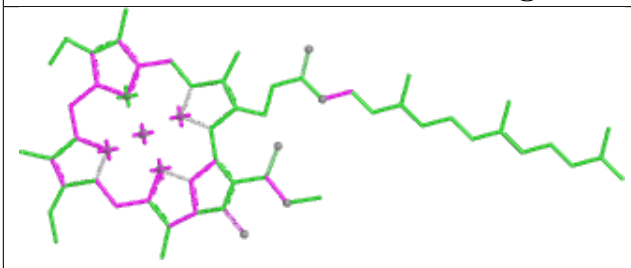


Torsions

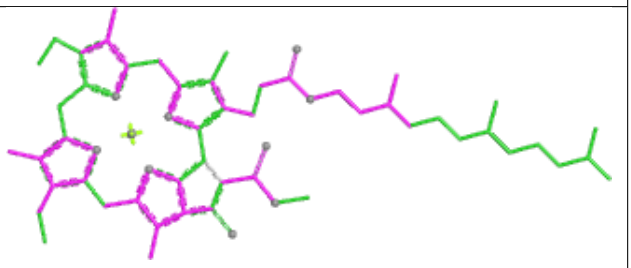


Rings

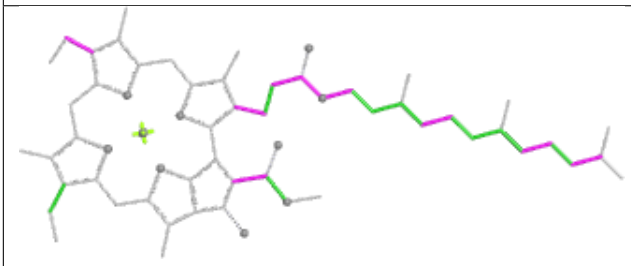
Ligand CLA b 1202



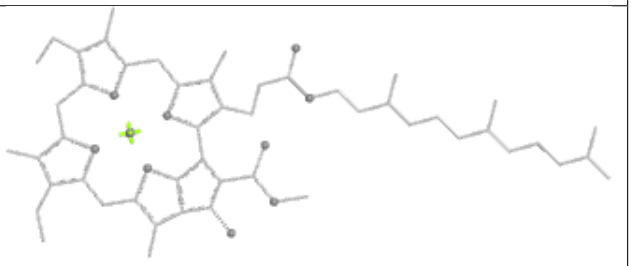
Bond lengths



Bond angles

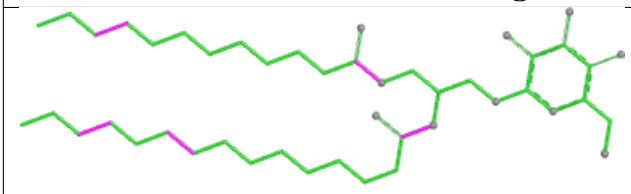


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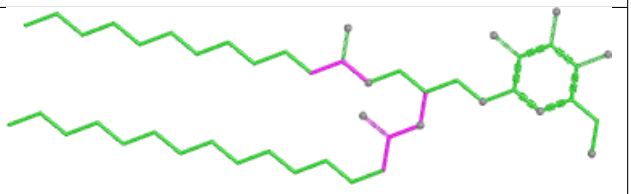


Rings

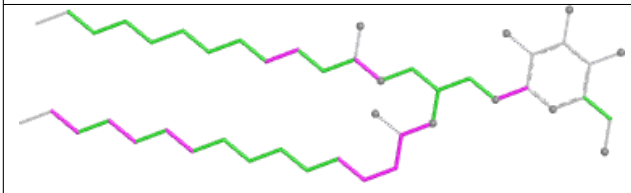
Ligand LMG B 5002



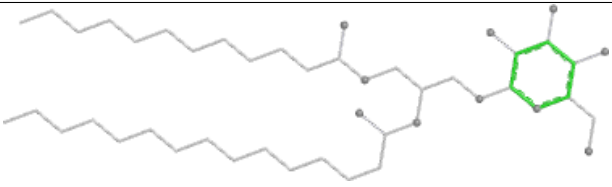
Bond lengths



Bond angles

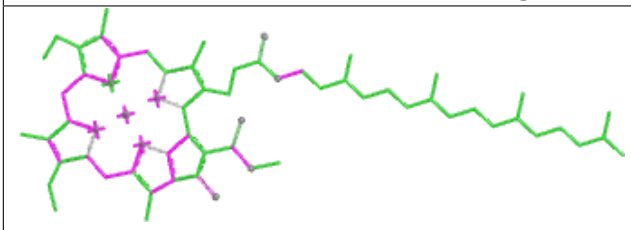


Torsions

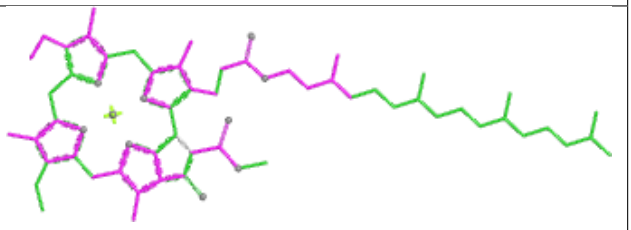


Rings

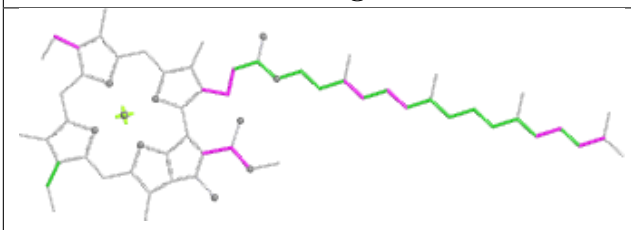
Ligand CLA A 1132



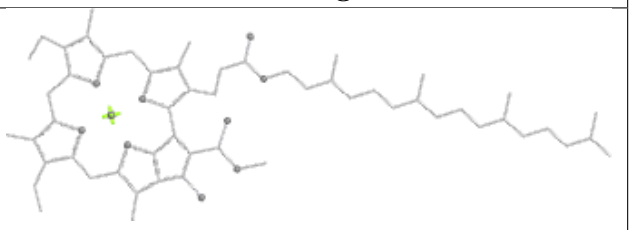
Bond lengths



Bond angles

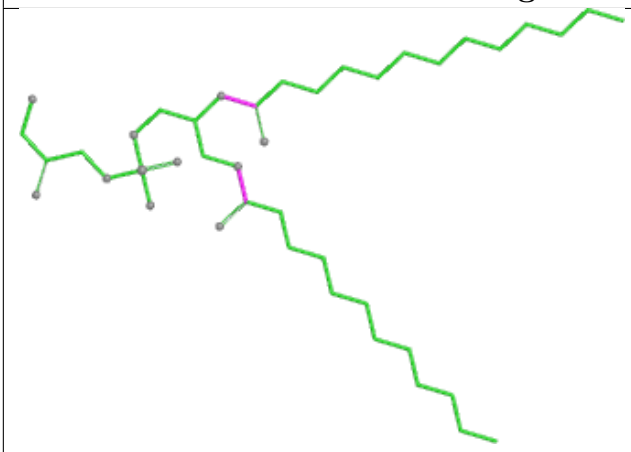


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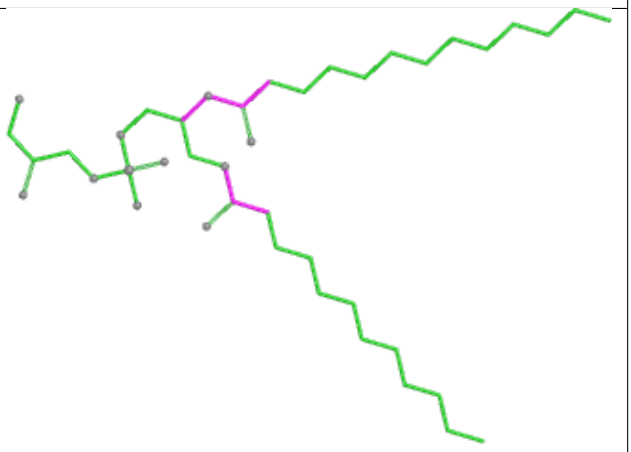


Rings

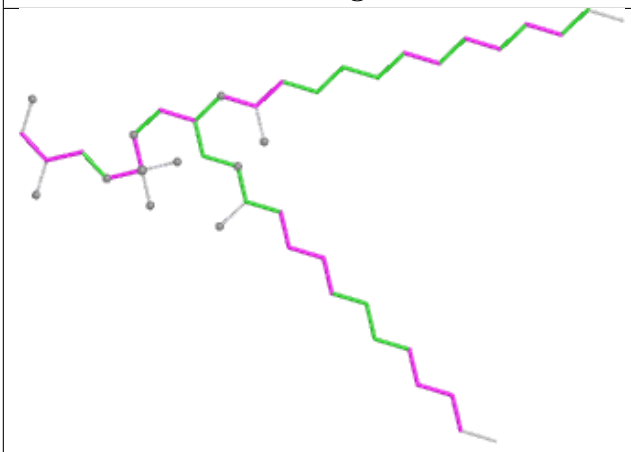
Ligand LHG a 5001



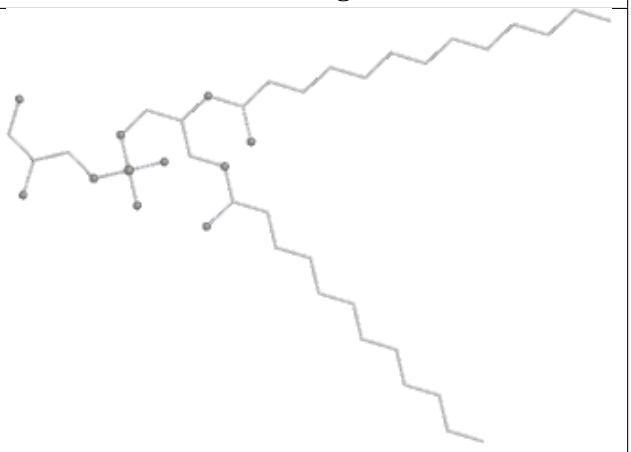
Bond lengths



Bond angles

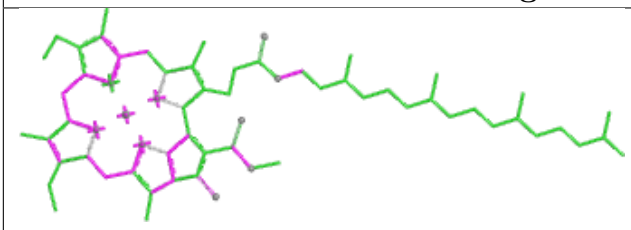


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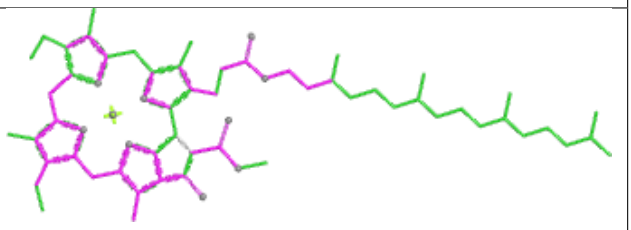


Rings

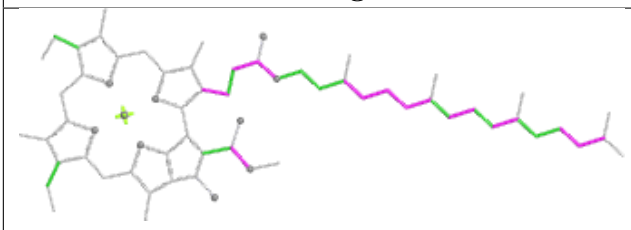
Ligand CLA a 1125



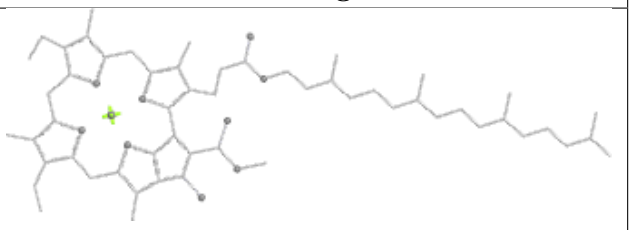
Bond lengths



Bond angles

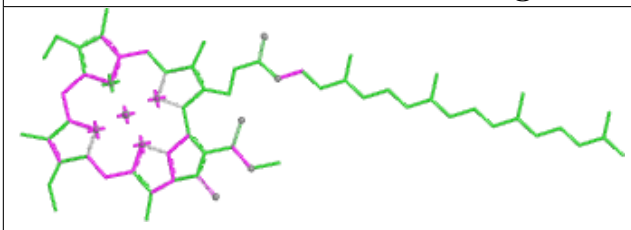


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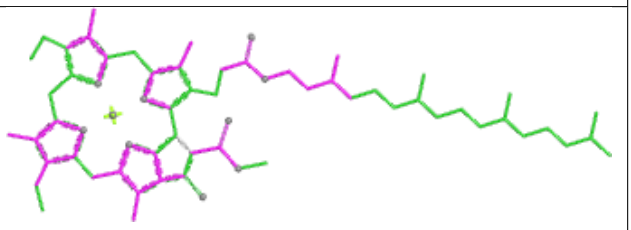


Rings

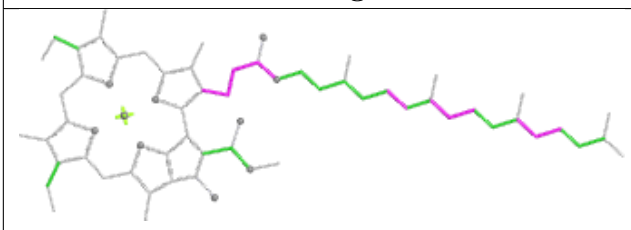
Ligand CLA G 1127



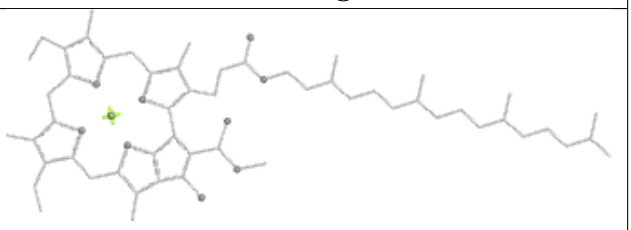
Bond lengths



Bond angles

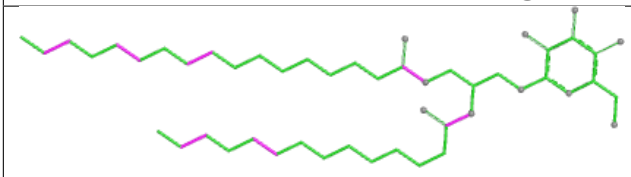


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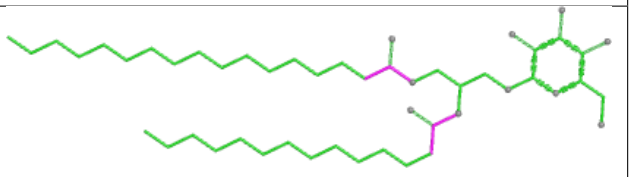


Rings

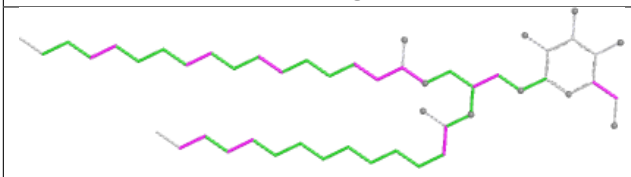
Ligand LMG l 5007



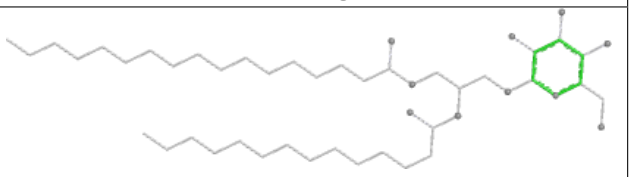
Bond lengths



Bond angles

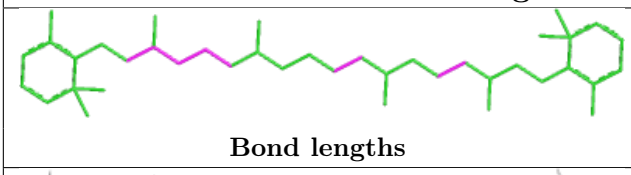


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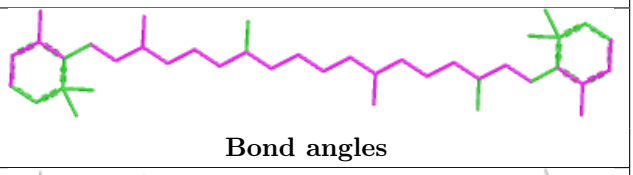


Rings

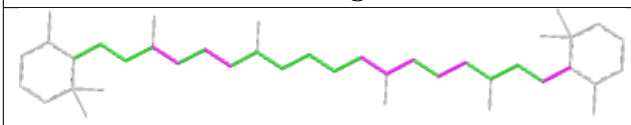
Ligand BCR H 4010



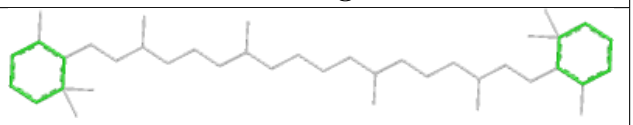
Bond lengths



Bond angles

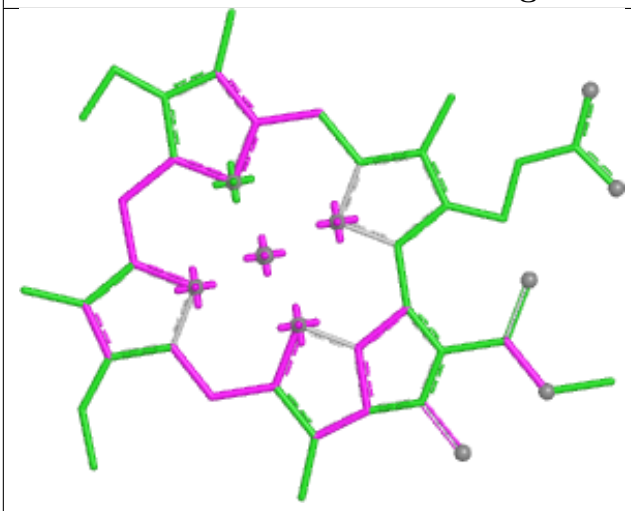


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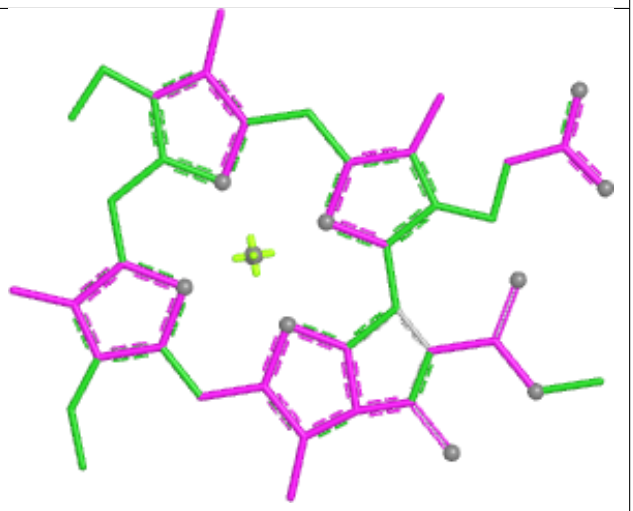


Rings

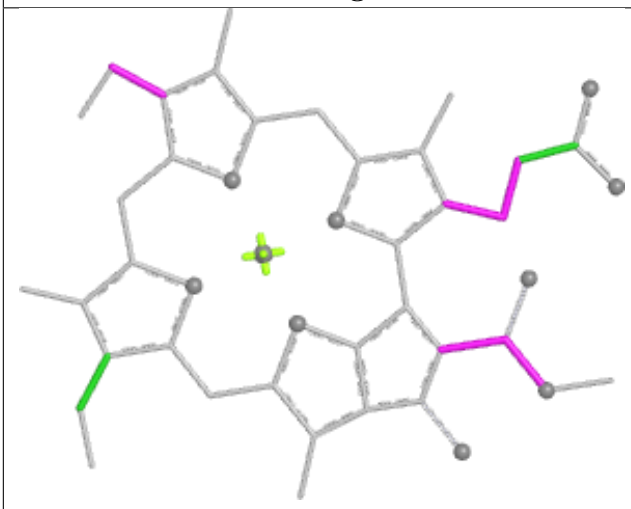
Ligand CLA a 1120



Bond lengths



Bond angles

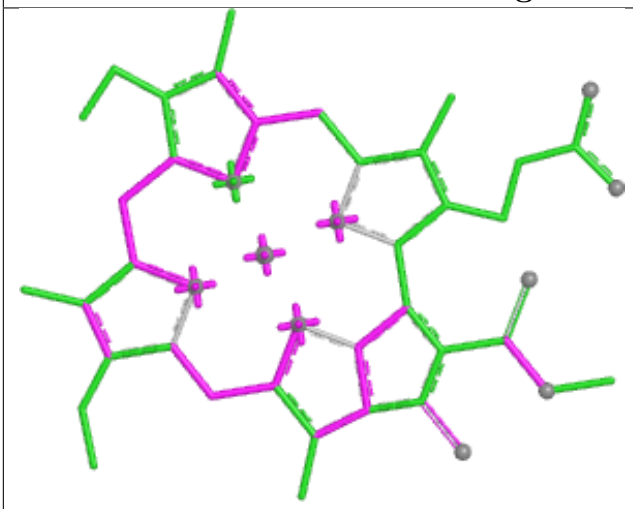


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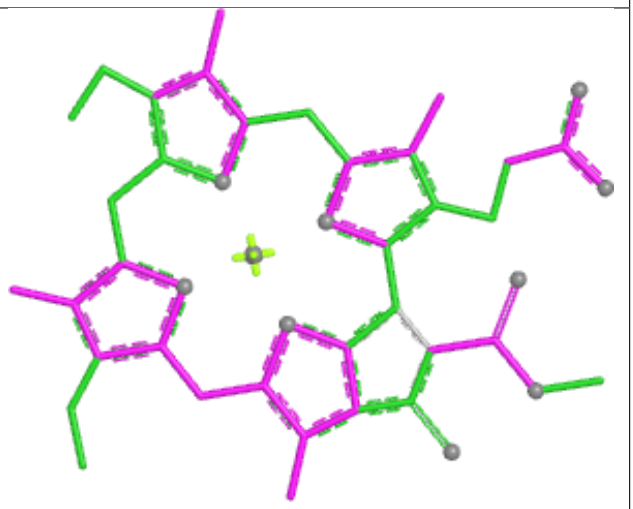


Rings

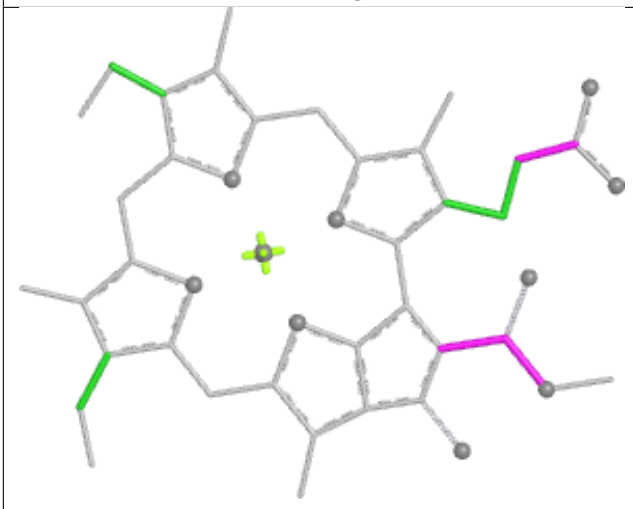
Ligand CLA B 1218



Bond lengths



Bond angles

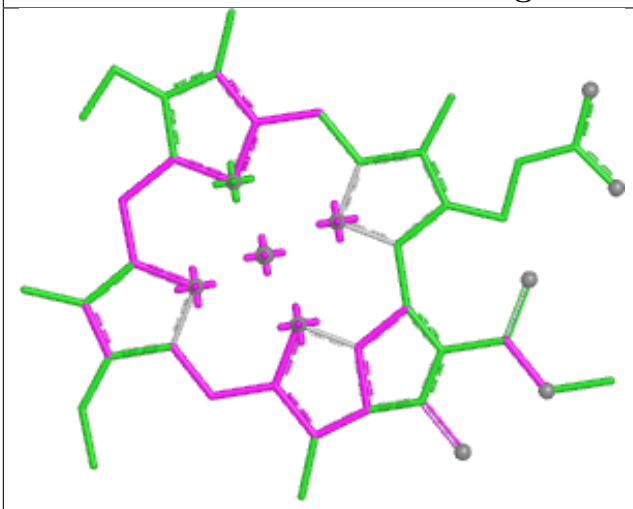


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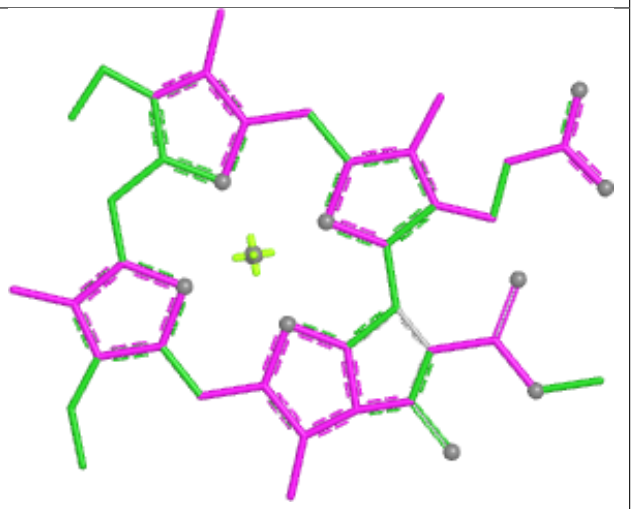


Rings

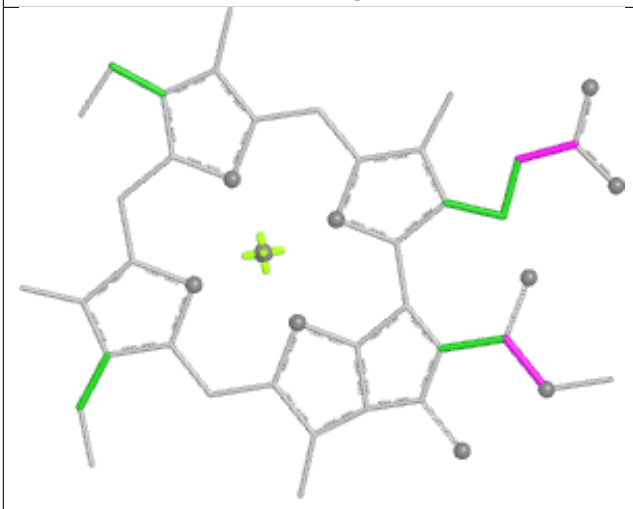
Ligand CLA A 1108



Bond lengths



Bond angles

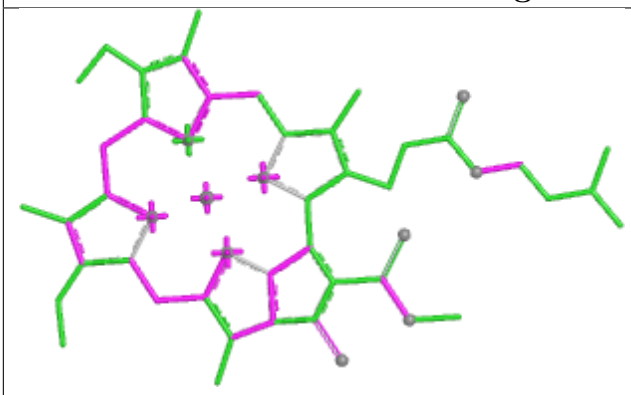


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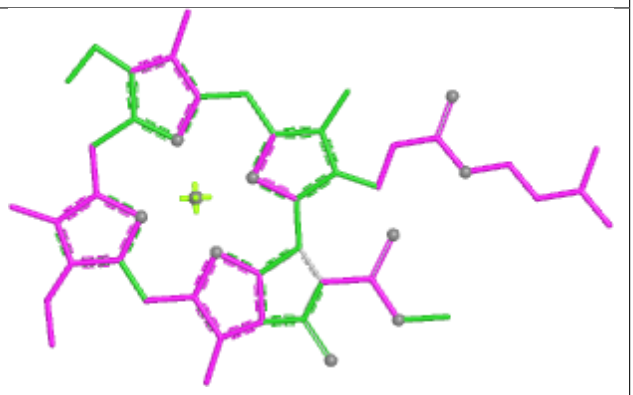


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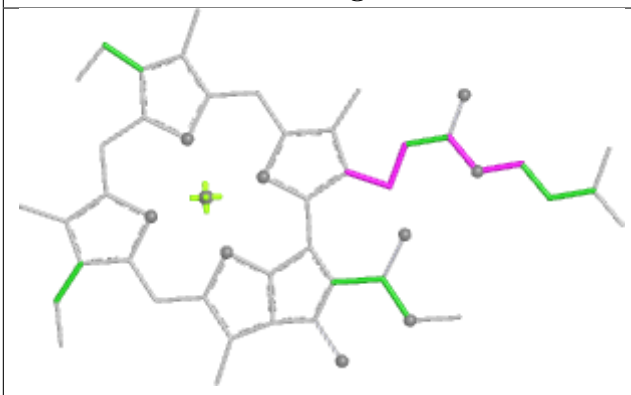
Ligand CLA G 1137



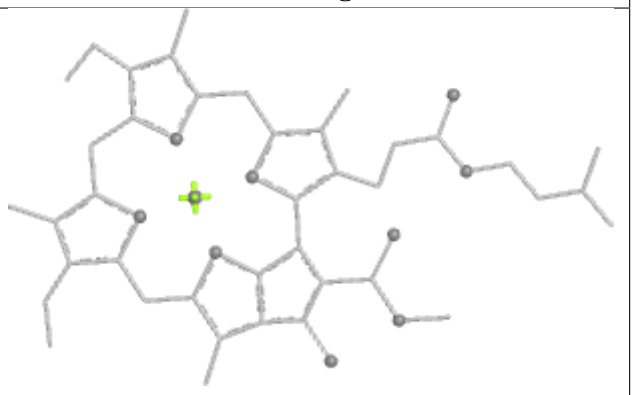
Bond lengths



Bond angles

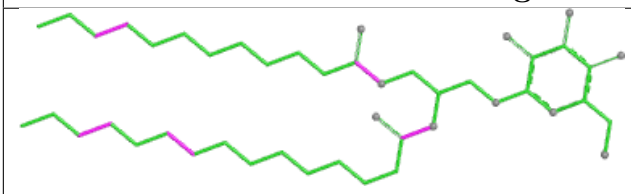


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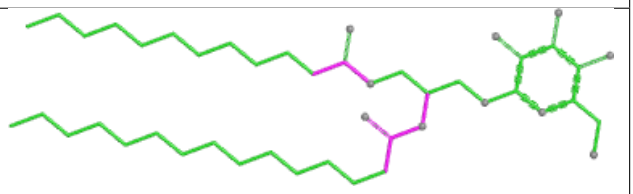


Rings

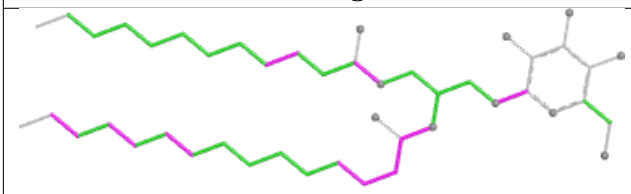
Ligand LMG b 5002



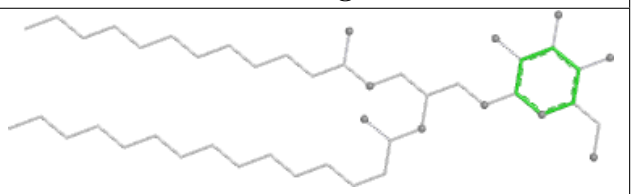
Bond lengths



Bond angles

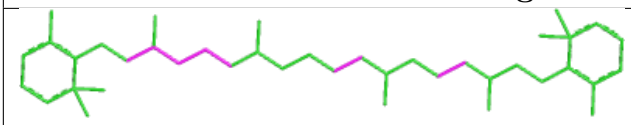


Torsions



Rings

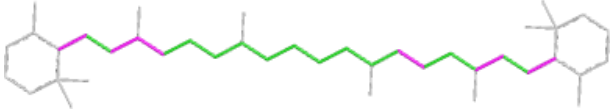
Ligand BCR b 4006



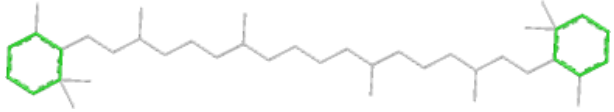
Bond lengths



Bond angles

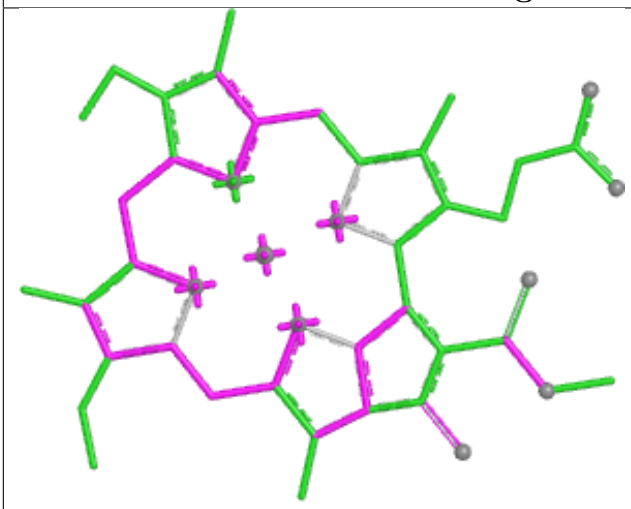


Torsions

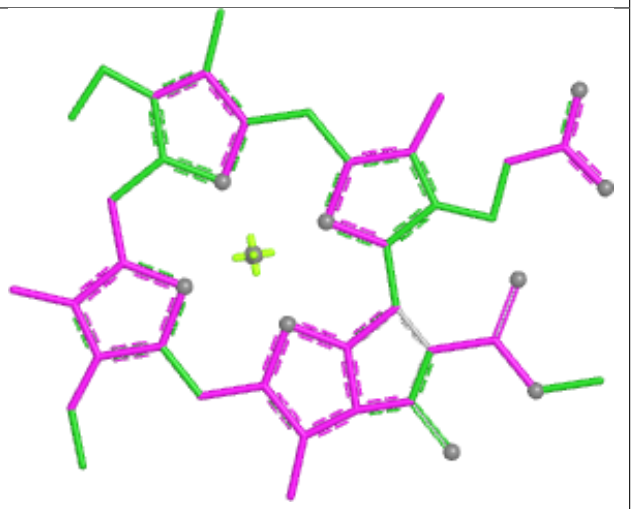


Rings

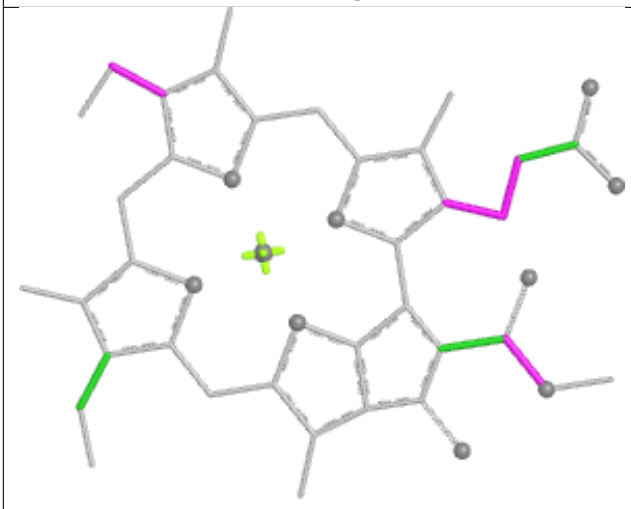
Ligand CLA B 1227



Bond lengths



Bond angles

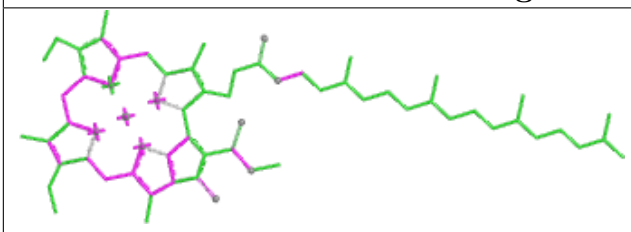


Torsions

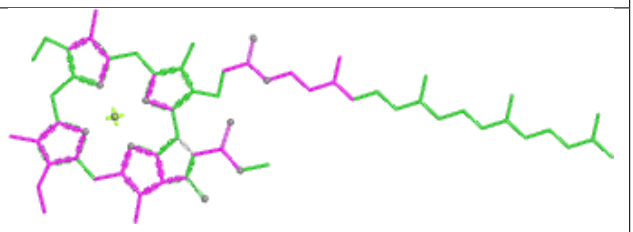


Rings

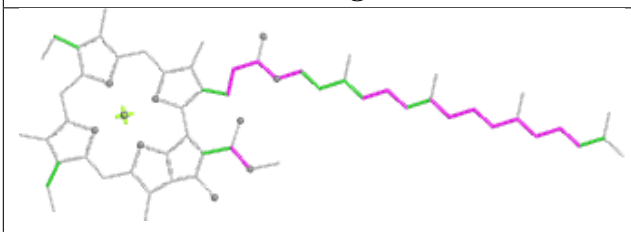
Ligand CLA B 1211



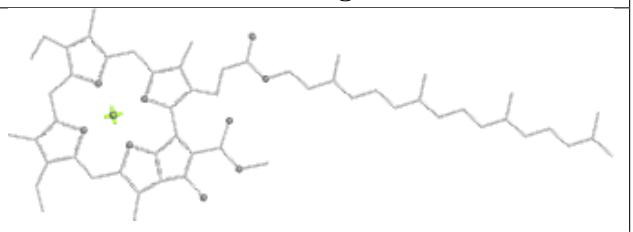
Bond lengths



Bond angles

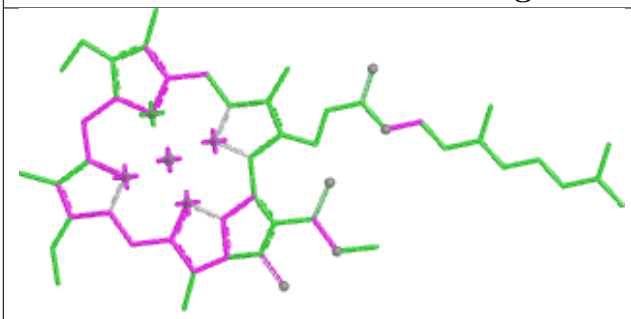


Torsions

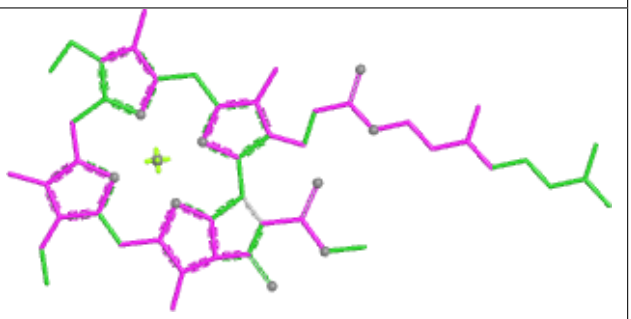


Rings

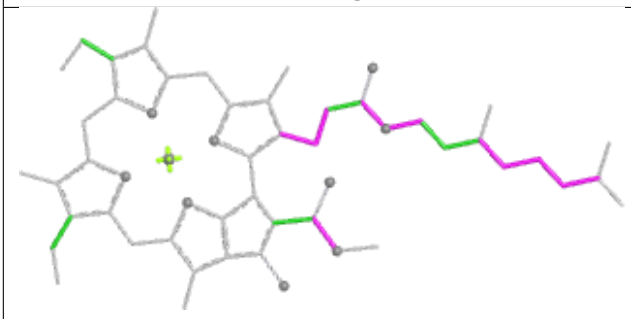
Ligand CLA H 1228



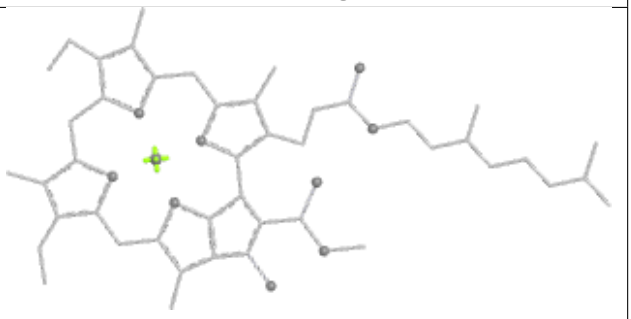
Bond lengths



Bond angles

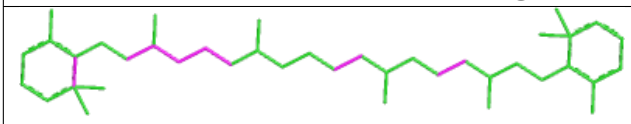


Torsions

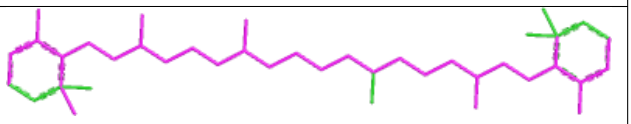


Rings

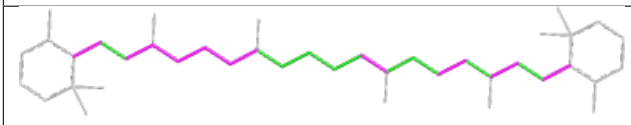
Ligand BCR G 4011



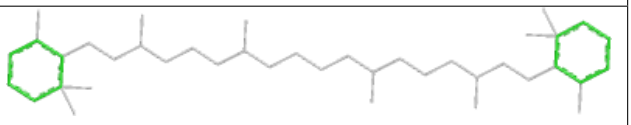
Bond lengths



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	T	1
9	k	1
9	K	1

All chain breaks are listed below:

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

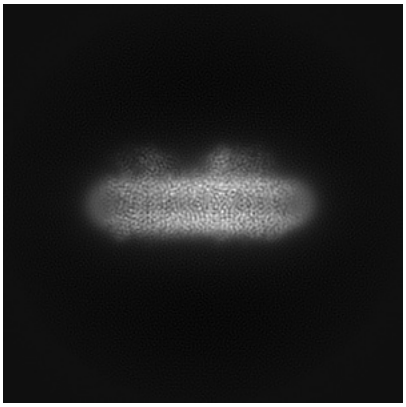
6 Map visualisation

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

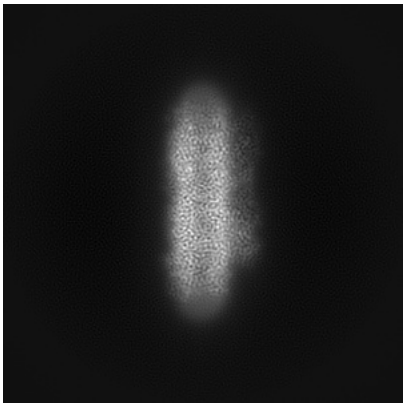
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

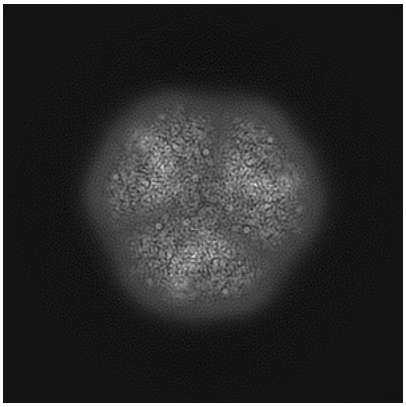
6.1.1 Primary map



X



Y

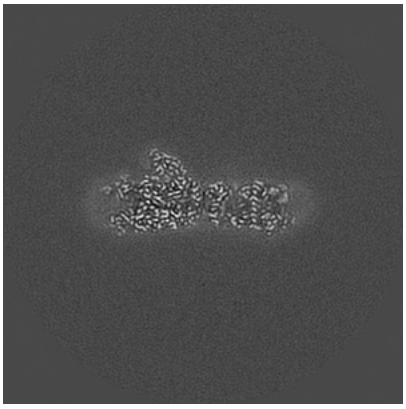


Z

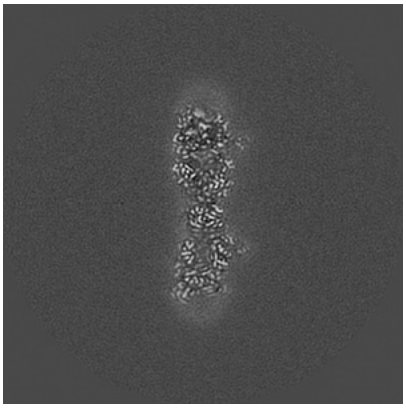
The images above show the map projected in three orthogonal directions.

6.2 Central slices

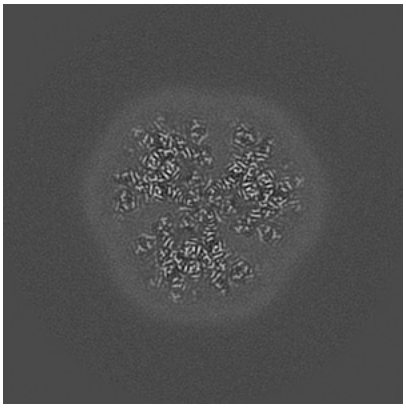
6.2.1 Primary map



X Index: 128



Y Index: 128

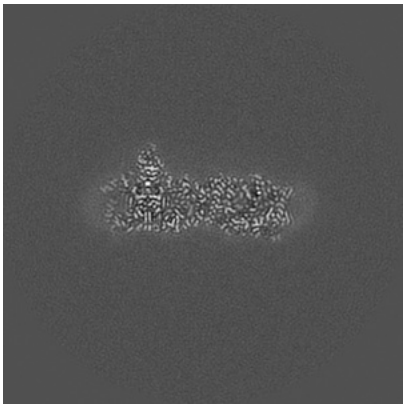


Z Index: 128

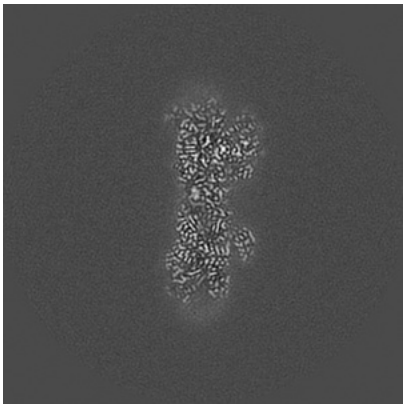
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

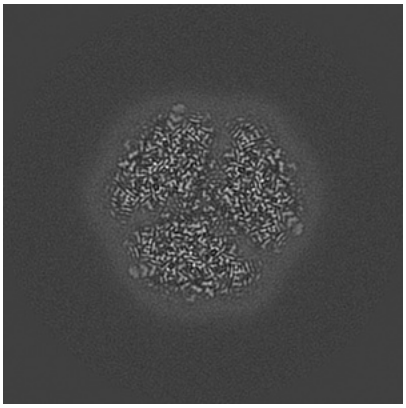
6.3.1 Primary map



X Index: 121



Y Index: 140

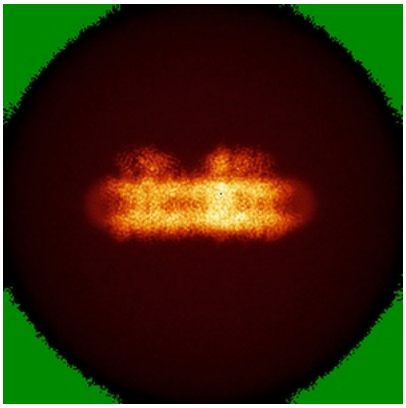


Z Index: 120

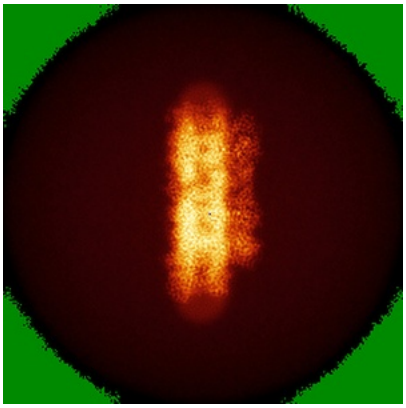
The images above show the largest variance slices of the map in three orthogonal directions.

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

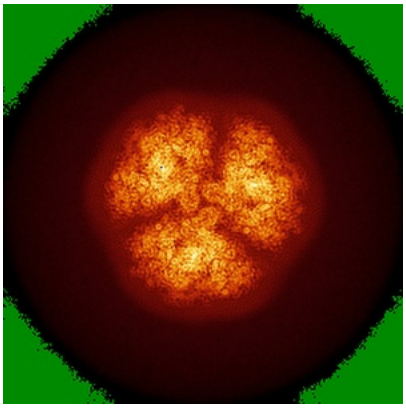
6.4.1 Primary map



X



Y

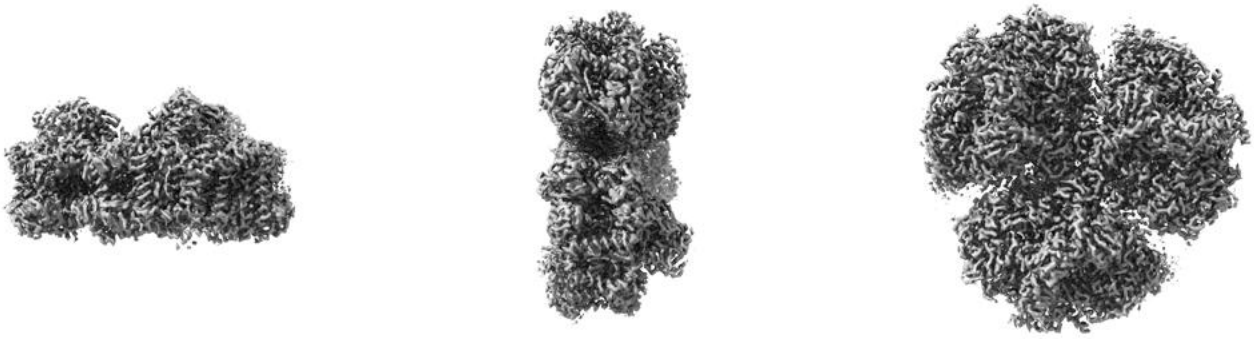


Z

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

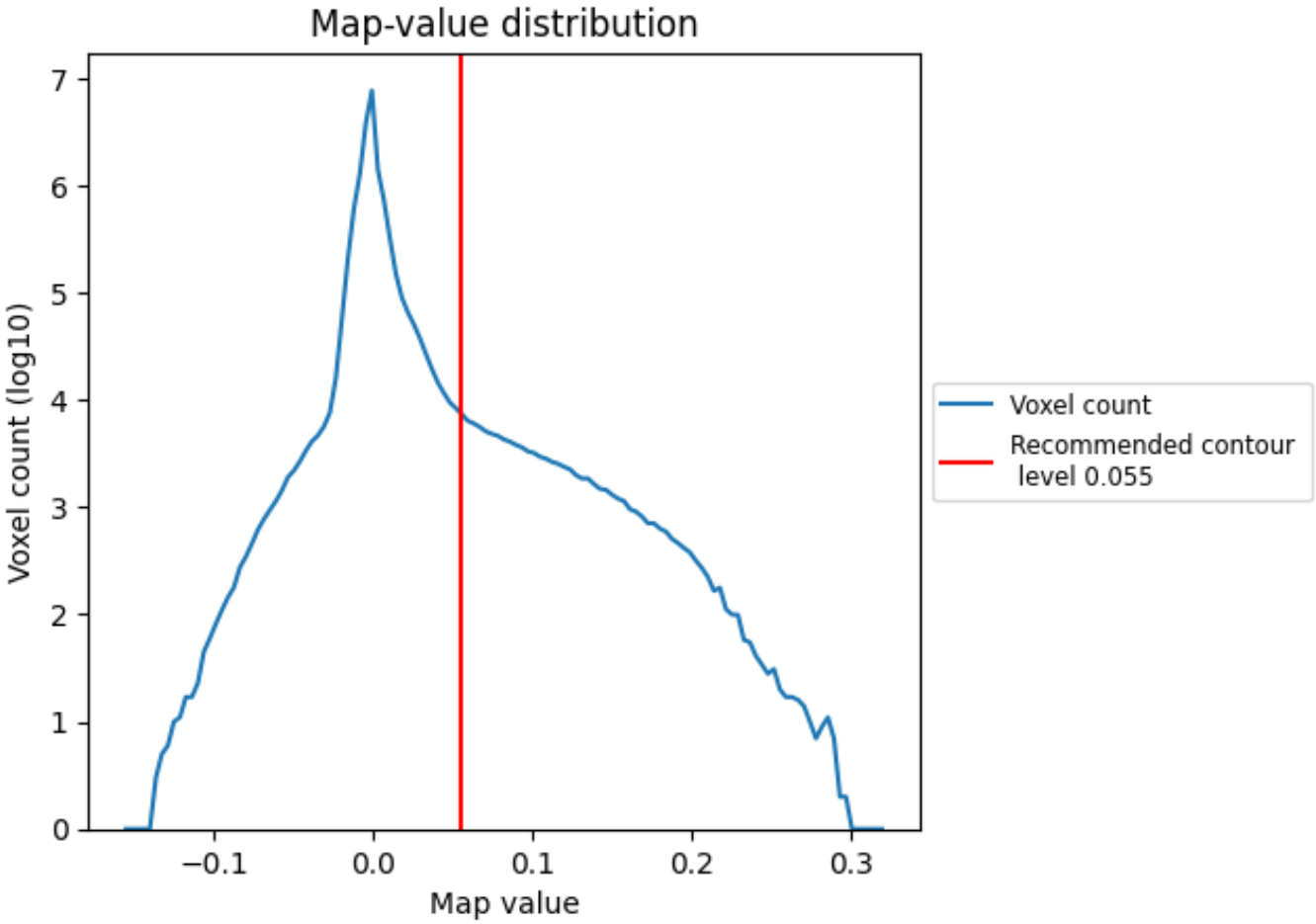
6.6 Mask visualisation (i)

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

7 Map analysis

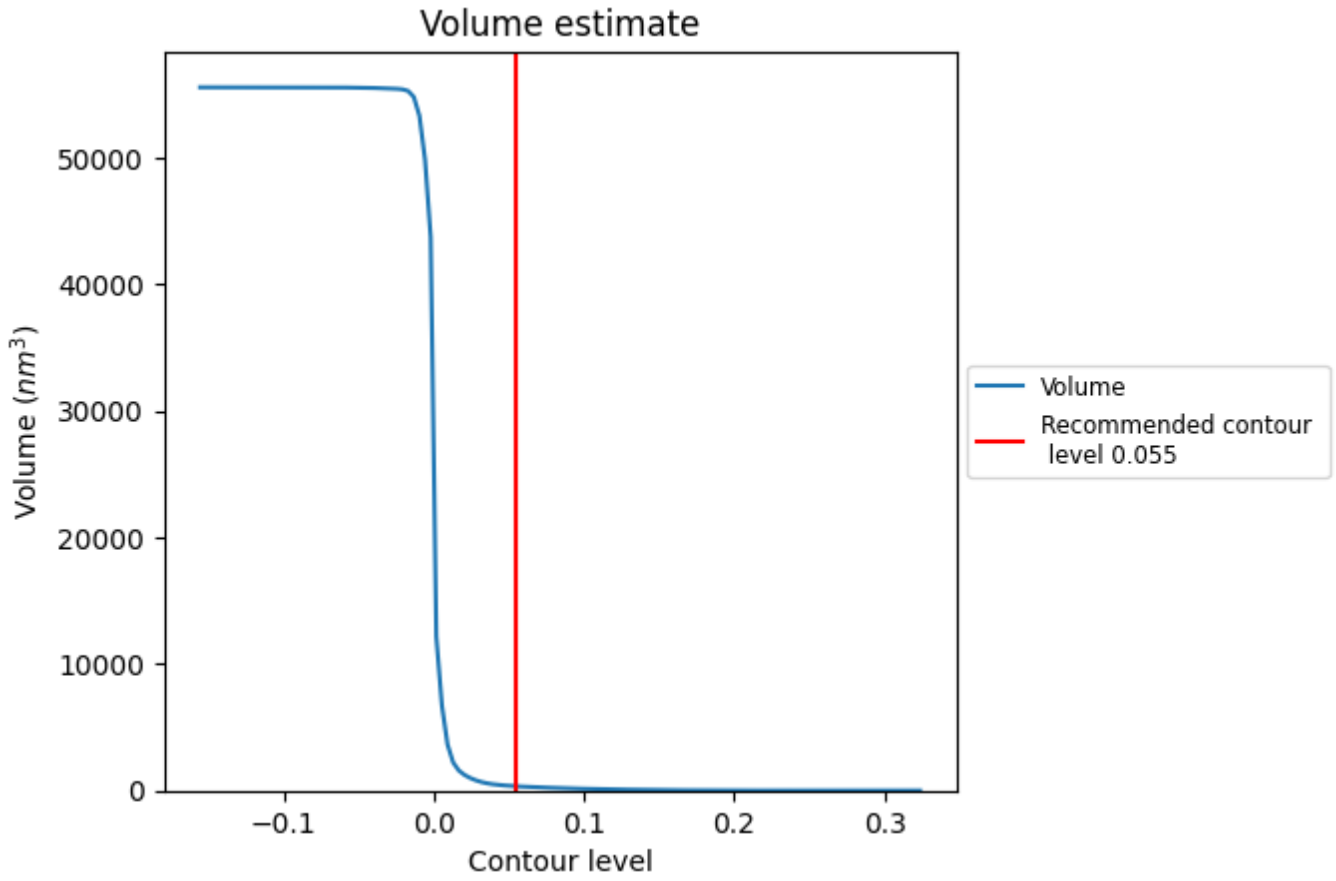
This section contains the results of statistical analysis of the map.

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.

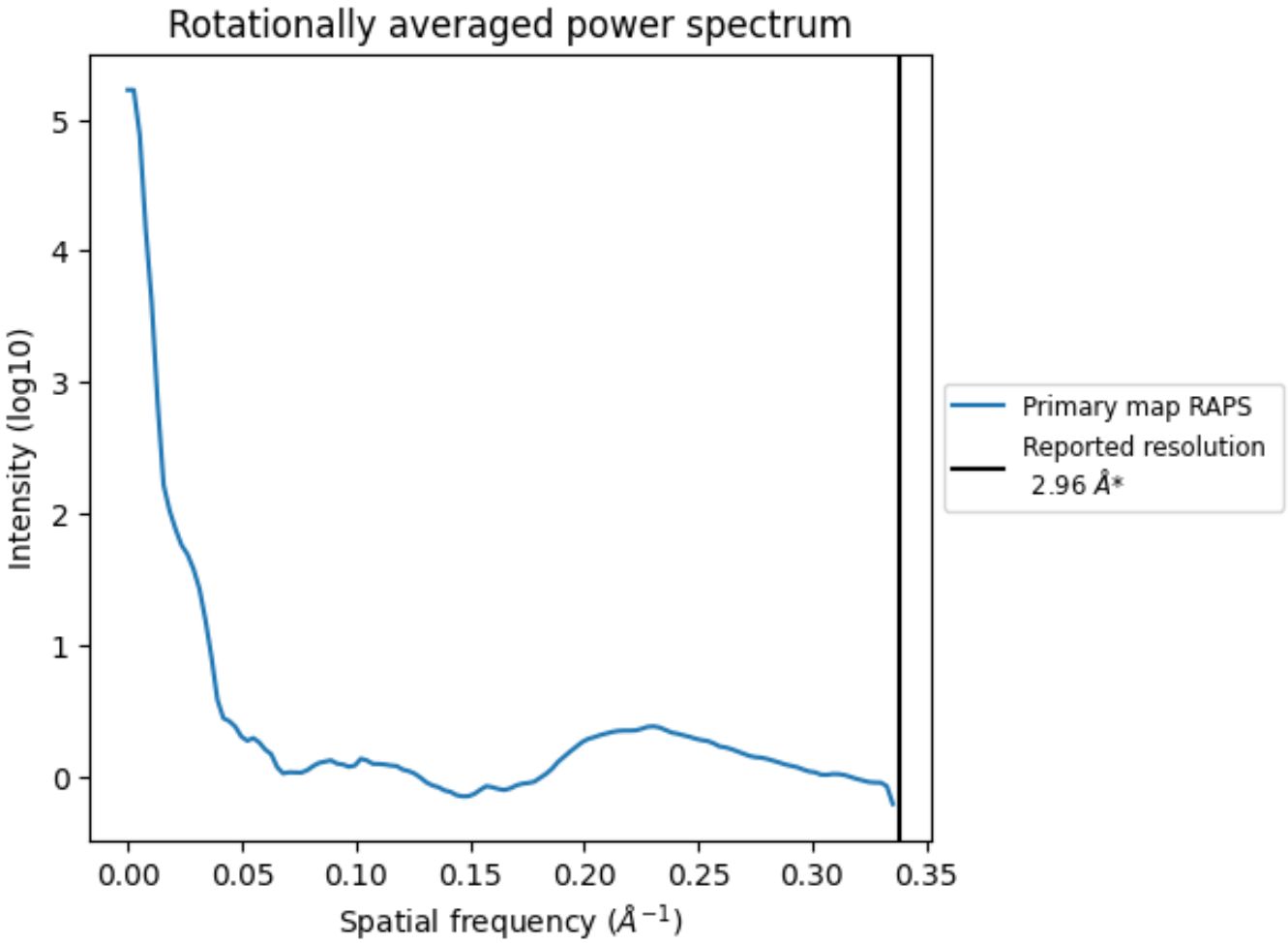
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)

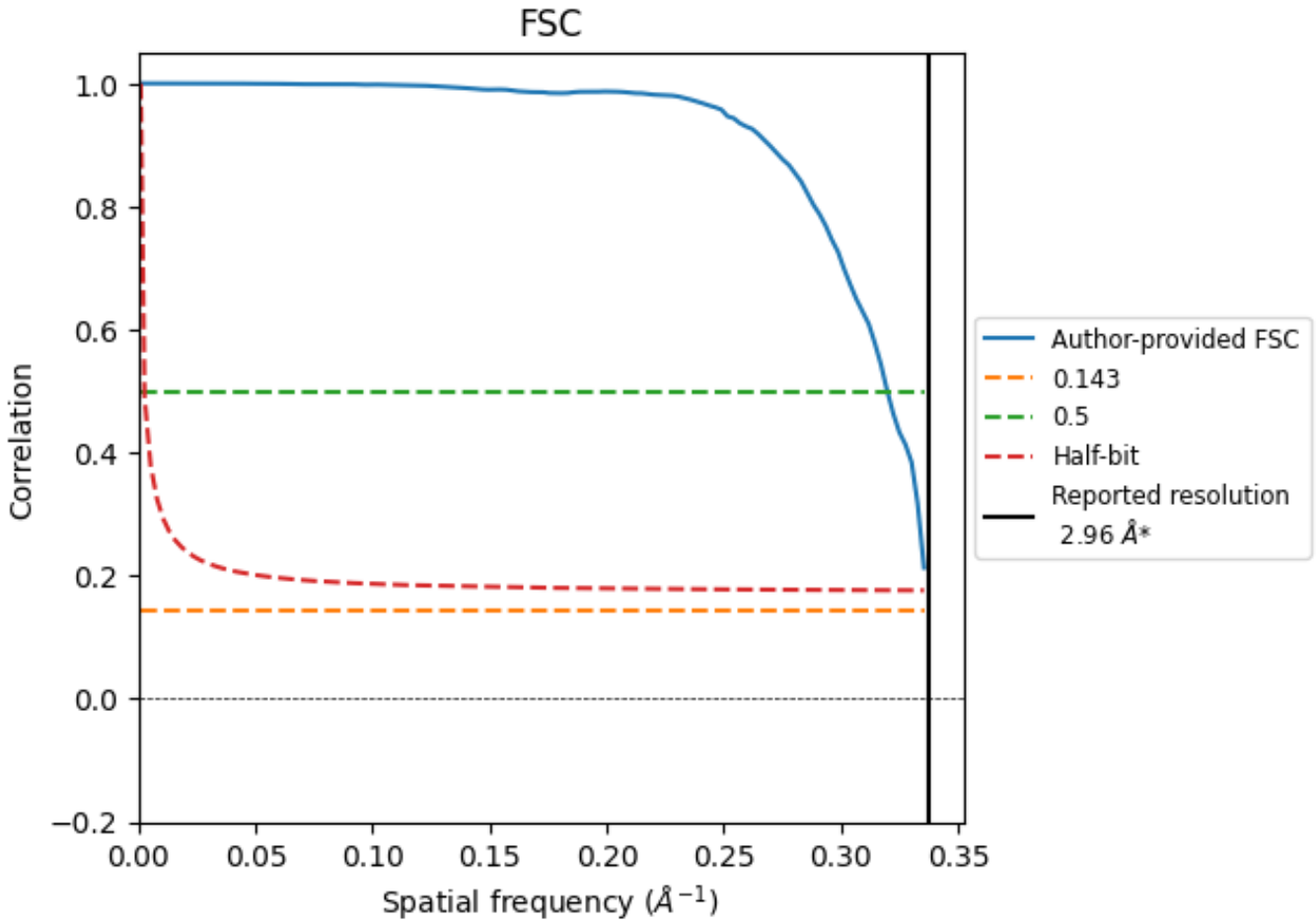


*Reported resolution corresponds to spatial frequency of 0.338 Å^{-1}

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 0.338 Å^{-1}

8.2 Resolution estimates (i)

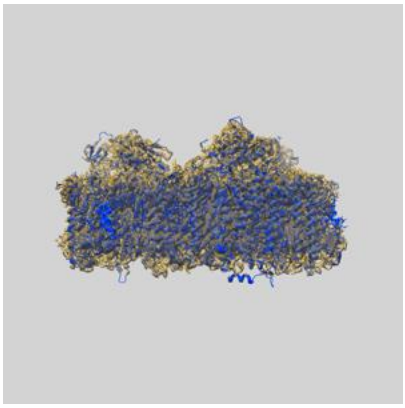
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	-	3.13	-
Unmasked-calculated*	-	-	-

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

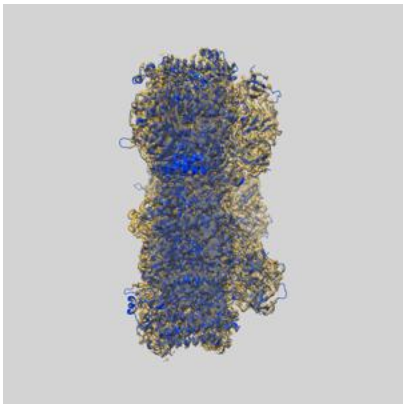
9 Map-model fit

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

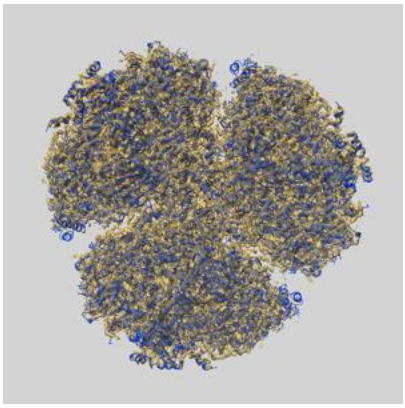
9.1 Map-model overlay



X



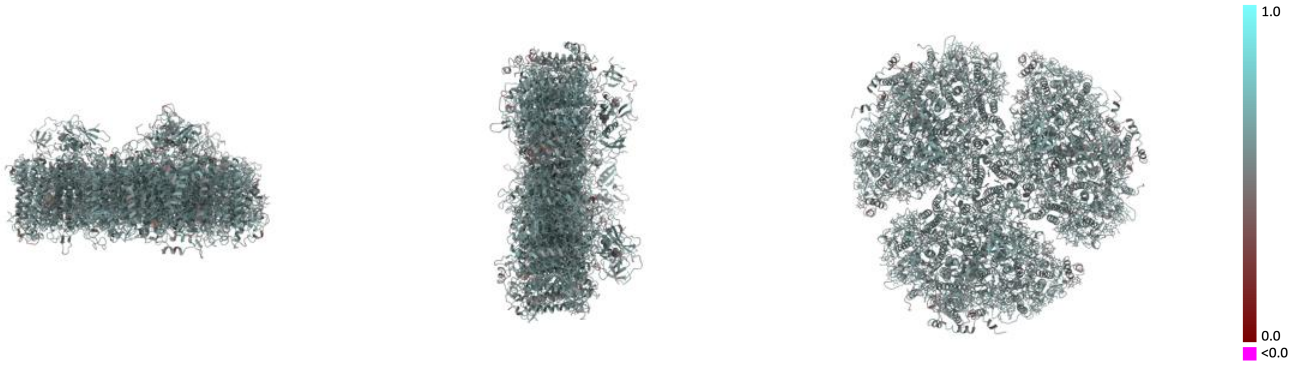
Y



Z

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

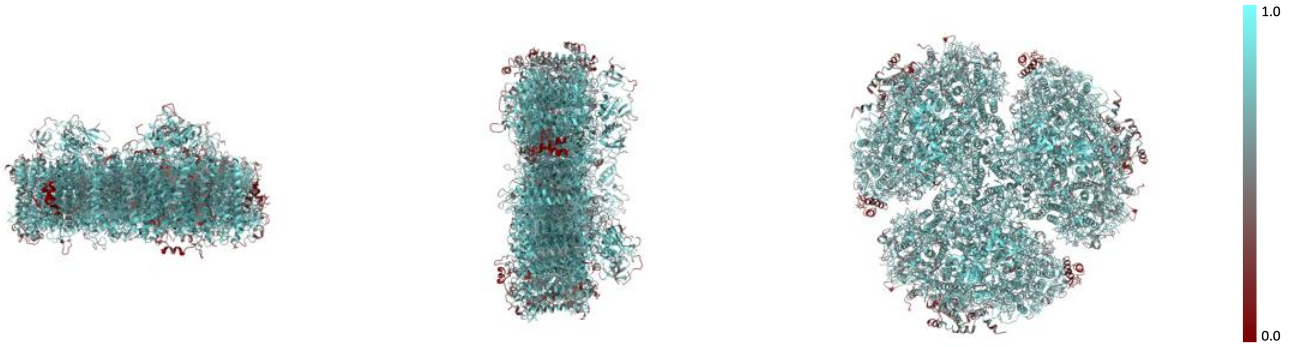
9.2 Q-score mapped to coordinate model (i)



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.

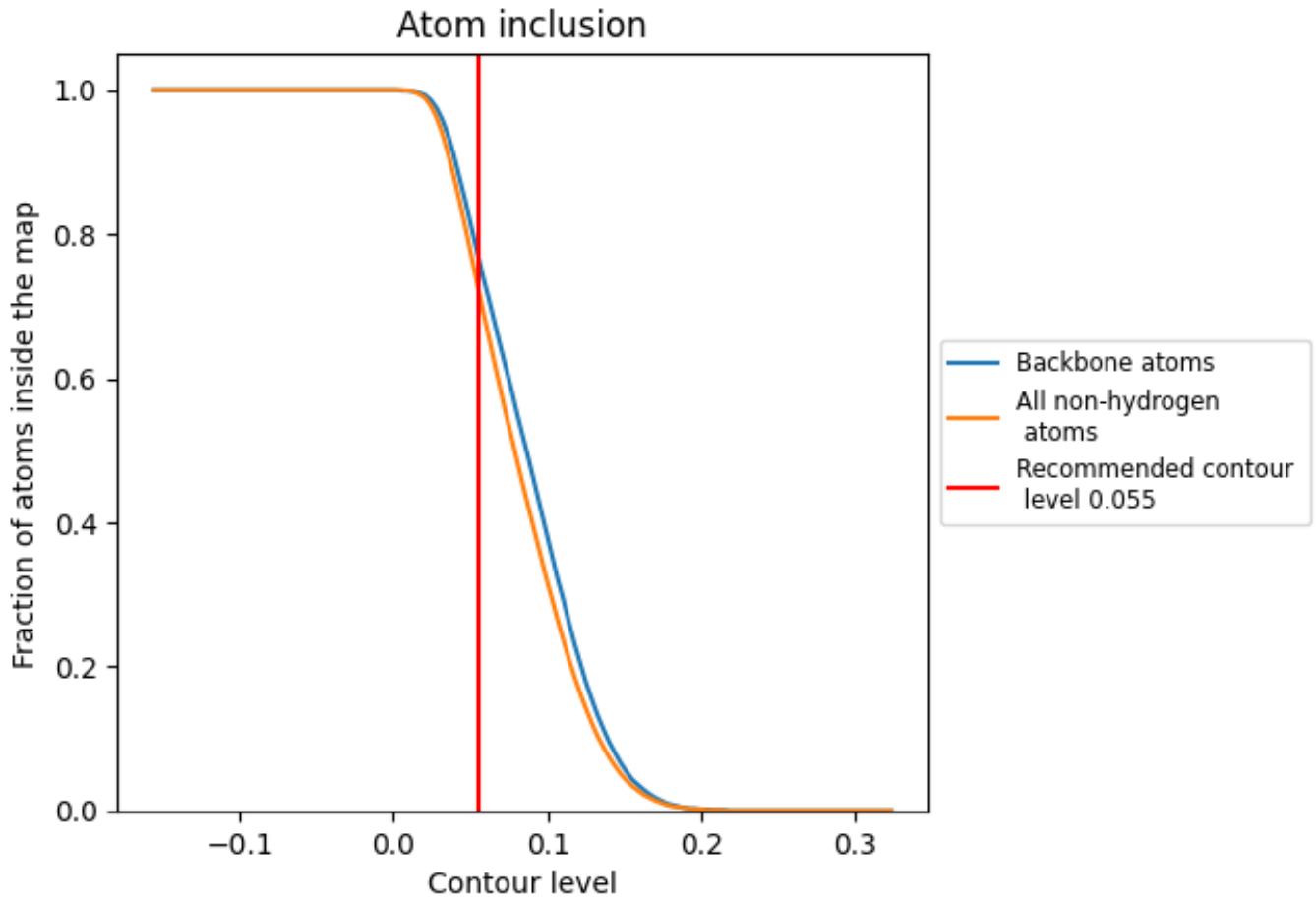
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.5650
A	0.7680	0.5740
B	0.7700	0.5740
C	0.7790	0.5640
D	0.6530	0.5490
E	0.5630	0.5200
F	0.3940	0.4990
G	0.7700	0.5750
H	0.7680	0.5770
I	0.7960	0.5720
J	0.4490	0.4770
K	0.0920	0.4640
L	0.7760	0.5720
M	0.7000	0.5480
N	0.7850	0.5550
O	0.6520	0.5470
P	0.5610	0.5160
Q	0.3970	0.5010
R	0.7830	0.5670
S	0.4580	0.4730
T	0.0710	0.4560
U	0.7790	0.5690
V	0.7110	0.5530
W	0.4910	0.4970
X	0.4810	0.4960
a	0.7690	0.5770
b	0.7650	0.5770
c	0.7870	0.5610
d	0.6450	0.5480
e	0.5400	0.5100
f	0.3960	0.4930
i	0.7920	0.5750
j	0.4410	0.4730
k	0.1050	0.4620
l	0.7700	0.5720



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
m	0.7000	0.5580
x	0.4780	0.4930