



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 20, 2017 – 02:15 AM EDT

PDB ID : 4L6V
Title : Crystal structure of a virus like photosystem I from the cyanobacterium Synechocystis PCC 6803
Authors : Mazor, Y.; Nataf, D.; Toporik, H.; Nelson, N.
Deposited on : unknown
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

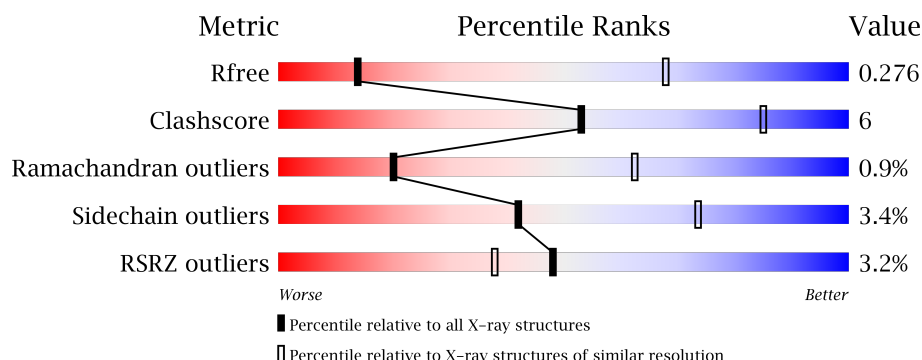
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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

Mol	Chain	Length	Quality of chain
1	1	751	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	A	751	<div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	a	751	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
2	2	731	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	731	<div> <div>87%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	b	731	 2% 96% .
3	3	81	 % 88% 9% ..
3	C	81	 84% 10% 5% .
3	c	81	 94% 5% .
4	4	141	 3% 91% . . .
4	D	141	 88% 8% ..
4	d	141	 % 94% . .
5	5	74	 5% 82% 7% . 8%
5	E	74	 5% 84% 7% . 8%
5	e	74	 14% 88% . 8%
6	6	125	 31% 94% 6%
6	F	125	 11% 90% 9% .
6	f	125	 33% 98% .
7	8	157	 % 91% 5% .
7	L	157	 88% 8% ..
7	l	157	 % 94% . .
8	7	31	 81% 16% .
8	M	31	 84% 13% .
8	m	31	 97% .
9	9	40	 70% 25% 5%
9	I	40	 3% 70% 25% 5%
9	i	40	 3% 85% 10% 5%
10	0	128	 8% 51% 10% . 38%
10	K	128	 % 45% 15% . 38%
10	k	128	 9% 55% 8% 38%

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
11	CLA	0	1401	X	-	-	X
11	CLA	0	1402	X	-	-	X
11	CLA	1	1011	X	-	-	-
11	CLA	1	1012	X	-	-	X
11	CLA	1	1022	X	-	-	-
11	CLA	1	1101	X	-	-	X
11	CLA	1	1102	X	-	-	X
11	CLA	1	1103	X	-	-	X
11	CLA	1	1104	X	-	-	X
11	CLA	1	1105	X	-	-	-
11	CLA	1	1106	X	-	-	X
11	CLA	1	1107	X	-	-	X
11	CLA	1	1108	X	-	-	-
11	CLA	1	1109	X	-	-	X
11	CLA	1	1110	X	-	-	-
11	CLA	1	1111	X	-	-	-
11	CLA	1	1112	X	-	-	X
11	CLA	1	1113	X	-	-	X
11	CLA	1	1114	X	-	-	-
11	CLA	1	1115	X	-	-	-
11	CLA	1	1116	X	-	-	-
11	CLA	1	1117	X	-	-	X
11	CLA	1	1118	X	-	-	X
11	CLA	1	1119	X	-	-	-
11	CLA	1	1120	X	-	-	-
11	CLA	1	1121	X	-	-	-
11	CLA	1	1122	X	-	-	-
11	CLA	1	1123	X	-	-	X
11	CLA	1	1124	X	-	-	-
11	CLA	1	1125	X	-	-	X
11	CLA	1	1126	X	-	-	X
11	CLA	1	1127	X	-	-	X
11	CLA	1	1128	X	-	-	X
11	CLA	1	1129	X	-	-	X
11	CLA	1	1130	X	-	-	-
11	CLA	1	1131	X	-	-	X
11	CLA	1	1132	X	-	-	-
11	CLA	1	1133	X	-	-	-
11	CLA	1	1134	X	-	-	-
11	CLA	1	1135	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	1	1136	X	-	-	-
11	CLA	1	1137	X	-	-	X
11	CLA	1	1138	X	-	-	-
11	CLA	1	1139	X	-	-	-
11	CLA	1	1140	X	-	-	X
11	CLA	1	1237	X	-	-	-
11	CLA	1	1801	X	-	-	-
11	CLA	2	1013	X	-	-	X
11	CLA	2	1021	X	-	-	X
11	CLA	2	1023	X	-	-	-
11	CLA	2	1201	X	-	-	-
11	CLA	2	1202	X	-	-	X
11	CLA	2	1203	X	-	-	-
11	CLA	2	1204	X	-	-	X
11	CLA	2	1205	X	-	-	-
11	CLA	2	1206	X	-	-	-
11	CLA	2	1207	X	-	-	X
11	CLA	2	1208	X	-	-	-
11	CLA	2	1209	X	-	-	-
11	CLA	2	1210	X	-	-	X
11	CLA	2	1211	X	-	-	X
11	CLA	2	1212	X	-	-	-
11	CLA	2	1213	X	-	-	X
11	CLA	2	1214	X	-	-	-
11	CLA	2	1215	X	-	-	-
11	CLA	2	1216	X	-	-	-
11	CLA	2	1217	X	-	-	-
11	CLA	2	1218	X	-	-	-
11	CLA	2	1219	X	-	-	-
11	CLA	2	1220	X	-	-	-
11	CLA	2	1221	X	-	-	-
11	CLA	2	1222	X	-	-	X
11	CLA	2	1223	X	-	-	X
11	CLA	2	1224	X	-	-	X
11	CLA	2	1225	X	-	-	X
11	CLA	2	1226	X	-	-	-
11	CLA	2	1227	X	-	-	X
11	CLA	2	1228	X	-	-	-
11	CLA	2	1229	X	-	-	-
11	CLA	2	1230	X	-	-	-
11	CLA	2	1231	X	-	-	-
11	CLA	2	1232	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	2	1234	X	-	-	X
11	CLA	2	1235	X	-	-	X
11	CLA	2	1236	X	-	-	-
11	CLA	2	1238	X	-	-	-
11	CLA	2	1239	X	-	-	-
11	CLA	2	1240	X	-	-	-
11	CLA	8	1501	X	-	-	-
11	CLA	8	1502	X	-	-	-
11	CLA	8	1503	X	-	-	X
11	CLA	A	1011	X	-	-	-
11	CLA	A	1012	X	-	-	X
11	CLA	A	1022	X	-	-	-
11	CLA	A	1101	X	-	-	-
11	CLA	A	1102	X	-	-	-
11	CLA	A	1103	X	-	-	X
11	CLA	A	1104	X	-	-	-
11	CLA	A	1105	X	-	-	-
11	CLA	A	1106	X	-	-	X
11	CLA	A	1107	X	-	-	-
11	CLA	A	1108	X	-	-	-
11	CLA	A	1109	X	-	-	-
11	CLA	A	1110	X	-	-	-
11	CLA	A	1111	X	-	-	X
11	CLA	A	1112	X	-	-	-
11	CLA	A	1113	X	-	-	-
11	CLA	A	1114	X	-	-	-
11	CLA	A	1115	X	-	-	-
11	CLA	A	1116	X	-	-	-
11	CLA	A	1117	X	-	-	X
11	CLA	A	1118	X	-	-	X
11	CLA	A	1119	X	-	-	-
11	CLA	A	1120	X	-	-	-
11	CLA	A	1121	X	-	-	-
11	CLA	A	1122	X	-	-	-
11	CLA	A	1123	X	-	-	-
11	CLA	A	1124	X	-	-	X
11	CLA	A	1125	X	-	-	X
11	CLA	A	1126	X	-	-	X
11	CLA	A	1127	X	-	-	X
11	CLA	A	1128	X	-	-	-
11	CLA	A	1129	X	-	-	-
11	CLA	A	1130	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	1131	X	-	-	-
11	CLA	A	1132	X	-	-	-
11	CLA	A	1133	X	-	-	-
11	CLA	A	1134	X	-	-	-
11	CLA	A	1135	X	-	-	-
11	CLA	A	1136	X	-	-	-
11	CLA	A	1137	X	-	-	-
11	CLA	A	1138	X	-	-	-
11	CLA	A	1139	X	-	-	X
11	CLA	A	1140	X	-	-	X
11	CLA	A	1237	X	-	-	-
11	CLA	A	1801	X	-	-	-
11	CLA	B	1013	X	-	-	-
11	CLA	B	1021	X	-	-	-
11	CLA	B	1023	X	-	-	-
11	CLA	B	1201	X	-	-	-
11	CLA	B	1202	X	-	-	X
11	CLA	B	1203	X	-	-	X
11	CLA	B	1204	X	-	-	-
11	CLA	B	1205	X	-	-	-
11	CLA	B	1206	X	-	-	X
11	CLA	B	1207	X	-	-	X
11	CLA	B	1208	X	-	-	-
11	CLA	B	1209	X	-	-	X
11	CLA	B	1210	X	-	-	X
11	CLA	B	1211	X	-	-	-
11	CLA	B	1212	X	-	-	-
11	CLA	B	1213	X	-	-	X
11	CLA	B	1214	X	-	-	-
11	CLA	B	1215	X	-	-	-
11	CLA	B	1216	X	-	-	-
11	CLA	B	1217	X	-	-	-
11	CLA	B	1218	X	-	-	-
11	CLA	B	1219	X	-	-	X
11	CLA	B	1220	X	-	-	-
11	CLA	B	1221	X	-	-	X
11	CLA	B	1222	X	-	-	X
11	CLA	B	1223	X	-	-	X
11	CLA	B	1224	X	-	-	-
11	CLA	B	1225	X	-	-	X
11	CLA	B	1226	X	-	-	X
11	CLA	B	1227	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	1228	X	-	-	X
11	CLA	B	1229	X	-	-	X
11	CLA	B	1230	X	-	-	-
11	CLA	B	1231	X	-	-	-
11	CLA	B	1232	X	-	-	-
11	CLA	B	1234	X	-	-	-
11	CLA	B	1235	X	-	-	-
11	CLA	B	1236	X	-	-	-
11	CLA	B	1238	X	-	-	X
11	CLA	B	1239	X	-	-	X
11	CLA	B	1240	X	-	-	X
11	CLA	K	1401	X	-	-	-
11	CLA	K	1402	X	-	-	-
11	CLA	L	1501	X	-	-	-
11	CLA	L	1502	X	-	-	-
11	CLA	L	1503	X	-	-	-
11	CLA	a	1011	X	-	-	X
11	CLA	a	1012	X	-	-	X
11	CLA	a	1022	X	-	-	-
11	CLA	a	1101	X	-	-	-
11	CLA	a	1102	X	-	-	-
11	CLA	a	1103	X	-	-	-
11	CLA	a	1104	X	-	-	-
11	CLA	a	1105	X	-	-	X
11	CLA	a	1106	X	-	-	-
11	CLA	a	1107	X	-	-	-
11	CLA	a	1108	X	-	-	-
11	CLA	a	1109	X	-	-	X
11	CLA	a	1110	X	-	-	-
11	CLA	a	1111	X	-	-	-
11	CLA	a	1112	X	-	-	-
11	CLA	a	1113	X	-	-	X
11	CLA	a	1114	X	-	-	-
11	CLA	a	1115	X	-	-	-
11	CLA	a	1116	X	-	-	-
11	CLA	a	1117	X	-	-	X
11	CLA	a	1118	X	-	-	X
11	CLA	a	1119	X	-	-	X
11	CLA	a	1120	X	-	-	-
11	CLA	a	1121	X	-	-	-
11	CLA	a	1122	X	-	-	-
11	CLA	a	1123	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	a	1124	X	-	-	X
11	CLA	a	1125	X	-	-	-
11	CLA	a	1126	X	-	-	X
11	CLA	a	1127	X	-	-	X
11	CLA	a	1128	X	-	-	X
11	CLA	a	1129	X	-	-	-
11	CLA	a	1130	X	-	-	-
11	CLA	a	1131	X	-	-	X
11	CLA	a	1132	X	-	-	X
11	CLA	a	1133	X	-	-	-
11	CLA	a	1134	X	-	-	X
11	CLA	a	1135	X	-	-	-
11	CLA	a	1136	X	-	-	-
11	CLA	a	1137	X	-	-	X
11	CLA	a	1138	X	-	-	-
11	CLA	a	1139	X	-	-	-
11	CLA	a	1140	X	-	-	X
11	CLA	a	1237	X	-	-	-
11	CLA	a	1801	X	-	-	-
11	CLA	b	1013	X	-	-	X
11	CLA	b	1021	X	-	-	-
11	CLA	b	1023	X	-	-	-
11	CLA	b	1201	X	-	-	-
11	CLA	b	1202	X	-	-	X
11	CLA	b	1203	X	-	-	X
11	CLA	b	1204	X	-	-	-
11	CLA	b	1205	X	-	-	-
11	CLA	b	1206	X	-	-	X
11	CLA	b	1207	X	-	-	-
11	CLA	b	1208	X	-	-	X
11	CLA	b	1209	X	-	-	-
11	CLA	b	1210	X	-	-	X
11	CLA	b	1211	X	-	-	-
11	CLA	b	1212	X	-	-	-
11	CLA	b	1213	X	-	-	-
11	CLA	b	1214	X	-	-	X
11	CLA	b	1215	X	-	-	-
11	CLA	b	1216	X	-	-	X
11	CLA	b	1217	X	-	-	-
11	CLA	b	1218	X	-	-	-
11	CLA	b	1219	X	-	-	X
11	CLA	b	1220	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	b	1221	X	-	-	X
11	CLA	b	1222	X	-	-	X
11	CLA	b	1223	X	-	-	X
11	CLA	b	1224	X	-	-	-
11	CLA	b	1225	X	-	-	X
11	CLA	b	1226	X	-	-	-
11	CLA	b	1227	X	-	-	-
11	CLA	b	1228	X	-	-	-
11	CLA	b	1229	X	-	-	X
11	CLA	b	1230	X	-	-	-
11	CLA	b	1231	X	-	-	-
11	CLA	b	1232	X	-	-	-
11	CLA	b	1234	X	-	-	X
11	CLA	b	1235	X	-	-	-
11	CLA	b	1236	X	-	-	-
11	CLA	b	1238	X	-	-	-
11	CLA	b	1239	X	-	-	-
11	CLA	b	1240	X	-	-	X
11	CLA	k	1401	X	-	-	-
11	CLA	k	1402	X	-	-	-
11	CLA	l	1501	X	-	-	X
11	CLA	l	1502	X	-	-	-
11	CLA	l	1503	X	-	-	-
12	PQN	1	2001	-	-	-	X
12	PQN	2	2002	-	-	-	X
12	PQN	A	2001	-	-	-	X
12	PQN	B	2002	-	-	-	X
12	PQN	a	2001	-	-	-	X
12	PQN	b	2002	-	-	-	X
13	SF4	3	3002	-	-	X	-
13	SF4	3	3003	-	-	X	-
13	SF4	A	3001	-	-	X	-
13	SF4	C	3002	-	-	X	-
13	SF4	C	3003	-	-	X	-
14	BCR	1	4001	-	-	-	X
14	BCR	1	4002	-	-	-	X
14	BCR	1	4003	-	-	-	X
14	BCR	1	4007	-	-	-	X
14	BCR	1	4008	-	-	-	X
14	BCR	2	4004	-	-	-	X
14	BCR	2	4005	-	-	-	X
14	BCR	2	4006	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	BCR	2	4010	-	-	-	X
14	BCR	2	4011	-	-	-	X
14	BCR	2	4014	-	-	-	X
14	BCR	2	4017	-	-	-	X
14	BCR	6	4013	-	-	-	X
14	BCR	6	4018	-	-	-	X
14	BCR	6	4020	-	-	-	X
14	BCR	7	4021	-	-	-	X
14	BCR	8	4019	-	-	-	X
14	BCR	8	4022	-	-	-	X
14	BCR	A	4001	-	-	-	X
14	BCR	A	4003	-	-	-	X
14	BCR	A	4008	-	-	-	X
14	BCR	B	4004	-	-	-	X
14	BCR	B	4005	-	-	-	X
14	BCR	B	4010	-	-	-	X
14	BCR	B	4011	-	-	-	X
14	BCR	B	4014	-	-	-	X
14	BCR	B	4017	-	-	-	X
14	BCR	F	4018	-	-	-	X
14	BCR	L	4019	-	-	-	X
14	BCR	L	4022	-	-	-	X
14	BCR	M	4021	-	-	-	X
14	BCR	a	4001	-	-	-	X
14	BCR	a	4002	-	-	-	X
14	BCR	a	4003	-	-	-	X
14	BCR	a	4007	-	-	-	X
14	BCR	a	4008	-	-	-	X
14	BCR	b	4004	-	-	-	X
14	BCR	b	4005	-	-	-	X
14	BCR	b	4006	-	-	-	X
14	BCR	b	4010	-	-	-	X
14	BCR	b	4011	-	-	-	X
14	BCR	b	4014	-	-	-	X
14	BCR	b	4017	-	-	-	X
14	BCR	f	4013	-	-	-	X
14	BCR	f	4018	-	-	-	X
14	BCR	f	4020	-	-	-	X
14	BCR	l	4019	-	-	-	X
14	BCR	l	4022	-	-	-	X
14	BCR	m	4021	-	-	-	X
15	LHG	1	5001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	LHG	1	5003	-	-	-	X
15	LHG	2	5004	-	-	-	X
15	LHG	A	5001	-	-	-	X
15	LHG	B	5004	-	-	-	X
15	LHG	a	5001	-	-	-	X
15	LHG	a	5003	-	-	-	X
15	LHG	b	5004	-	-	-	X
16	LMG	2	5002	-	-	-	X
16	LMG	B	5002	-	-	-	X
16	LMG	b	5002	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 68370 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	b	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			
2	2	728	Total	C	N	O	S	0	0	0
			5765	3796	966	988	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	c	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			
3	3	80	Total	C	N	O	S	0	0	0
			600	369	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			
4	4	138	Total	C	N	O	S	0	0	0
			1079	683	187	206	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	e	68	Total	C	N	O	0	0	0
			529	332	93	104			
5	5	68	Total	C	N	O	0	0	0
			529	332	93	104			

- Molecule 6 is a protein called Fusion protein of Photosystem I subunit III and subunit IX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	F	125	Total	C	N	O	0	0	0
			676	420	126	130			
6	f	125	Total	C	N	O	0	0	0
			685	429	126	130			
6	6	125	Total	C	N	O	0	0	0
			685	429	126	130			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	41	CYS	-	LINKER	UNP L8AII8
F	42	SER	-	LINKER	UNP L8AII8
F	43	CYS	-	LINKER	UNP L8AII8
F	53	ILE	LEU	engineered mutation	UNP L8AII8
f	41	CYS	-	LINKER	UNP L8AII8
f	42	SER	-	LINKER	UNP L8AII8
f	43	CYS	-	LINKER	UNP L8AII8
f	53	ILE	LEU	engineered mutation	UNP L8AII8
6	41	CYS	-	LINKER	UNP L8AII8
6	42	SER	-	LINKER	UNP L8AII8
6	43	CYS	-	LINKER	UNP L8AII8
6	53	ILE	LEU	engineered mutation	UNP L8AII8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	l	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			
7	8	151	Total	C	N	O	S	0	0	0
			1133	741	183	207	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	m	31	Total	C	N	O	0	0	0
			235	157	36	42			
8	7	31	Total	C	N	O	0	0	0
			235	157	36	42			

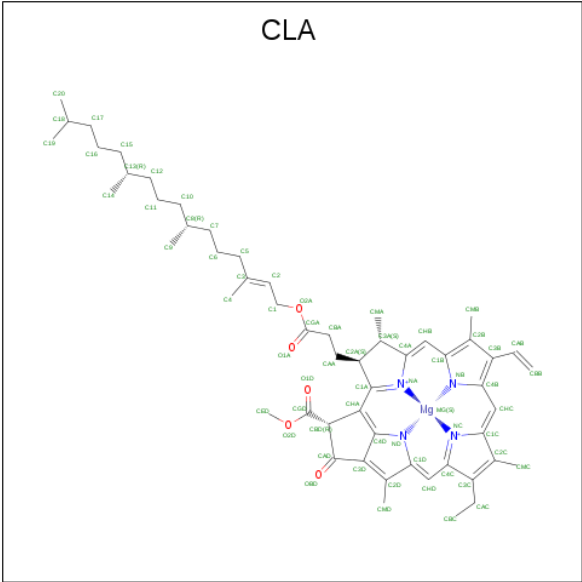
- Molecule 9 is a protein called Photosystem I subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	i	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	9	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			
9	I	38	Total	C	N	O	S	0	0	0
			297	202	42	50	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	k	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			
10	0	80	Total	C	N	O	S	0	0	0
			496	320	83	88	5			

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	a	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	b	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	l	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
11	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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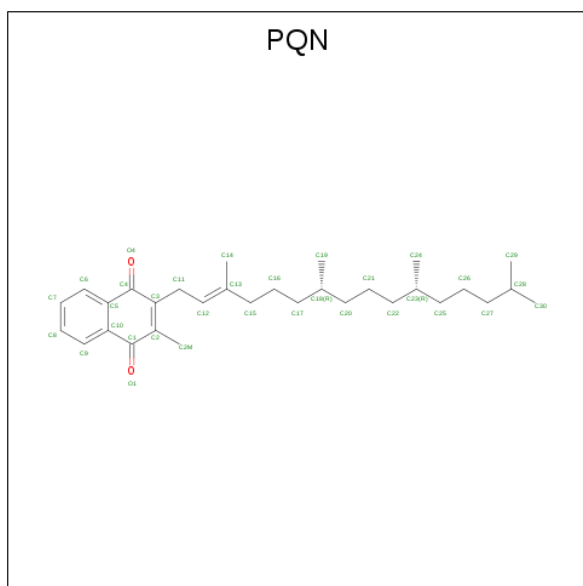
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	8	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	8	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	k	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	0	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 12 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



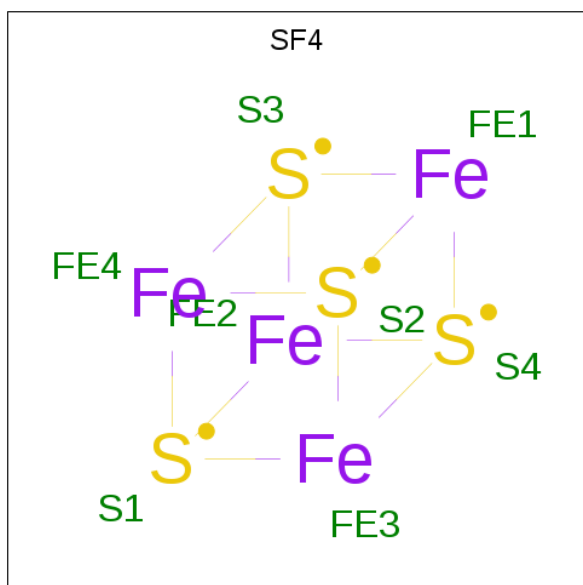
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

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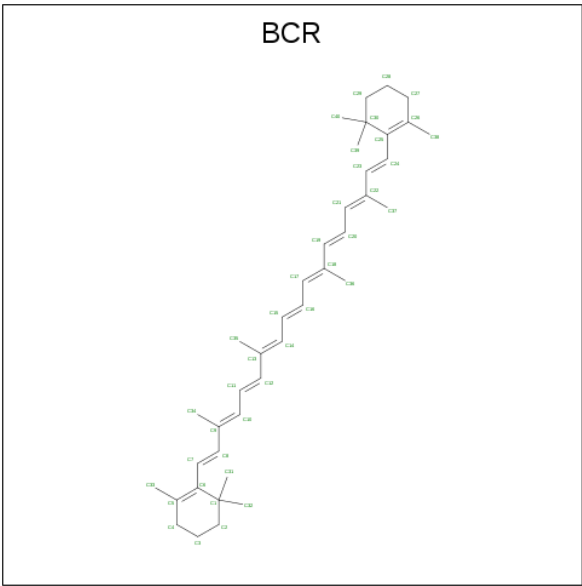
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	C	1	Total	Fe	S	0	0
			8	4	4		
13	a	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	c	1	Total	Fe	S	0	0
			8	4	4		
13	1	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		
13	3	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	F	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	L	1	Total C 40 40	0	0
14	M	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	a	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	b	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0
14	f	1	Total C 40 40	0	0

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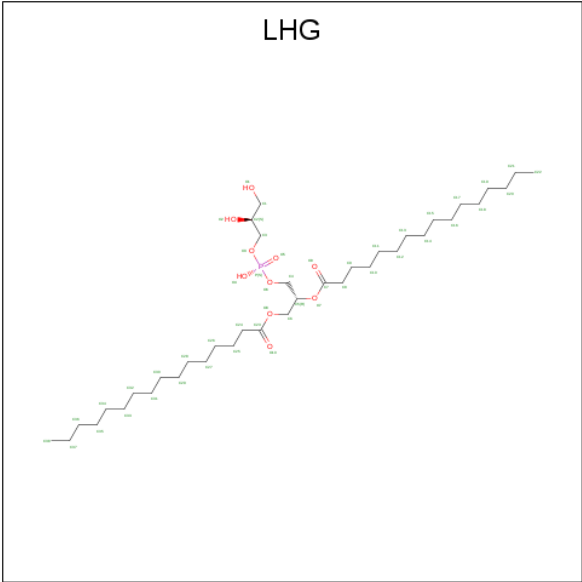
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	6	1	Total C 40 40	0	0
14	8	1	Total C 40 40	0	0

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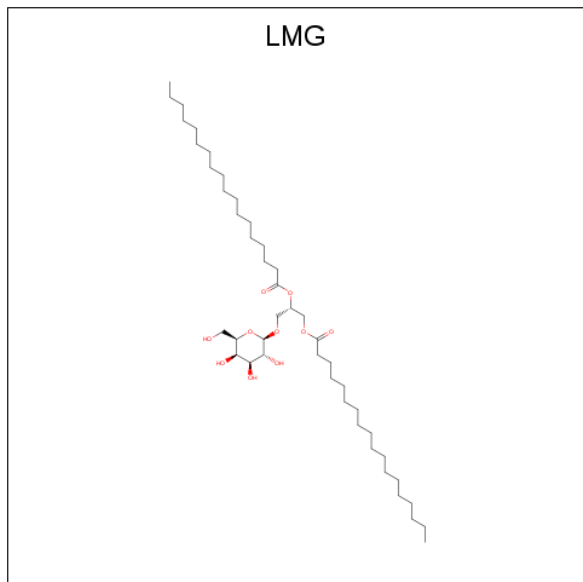
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O P 49 38 10 1	0	0
15	A	1	Total C O P 49 38 10 1	0	0
15	B	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	a	1	Total C O P 49 38 10 1	0	0
15	b	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	1	1	Total C O P 49 38 10 1	0	0
15	2	1	Total C O P 49 38 10 1	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

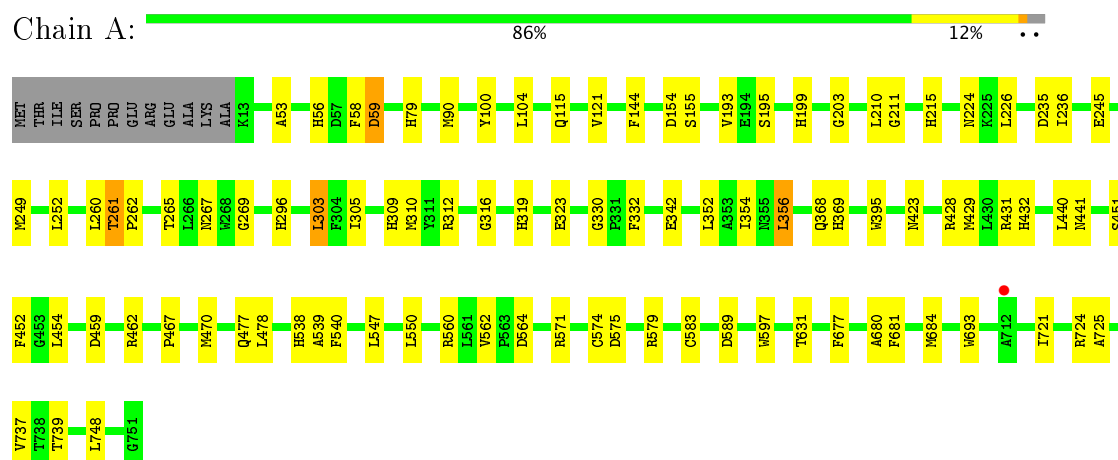


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			55	45	10		
16	b	1	Total	C	O	0	0
			55	45	10		
16	2	1	Total	C	O	0	0
			55	45	10		

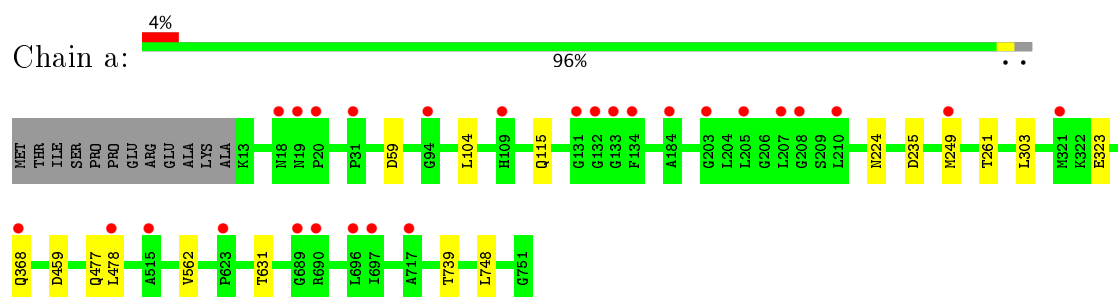
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

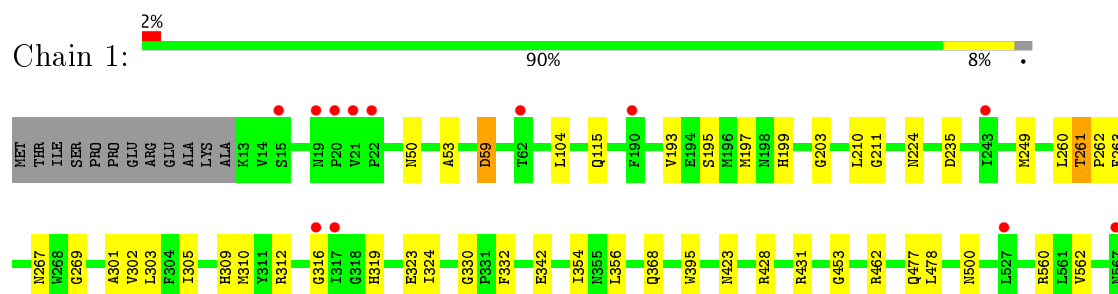
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

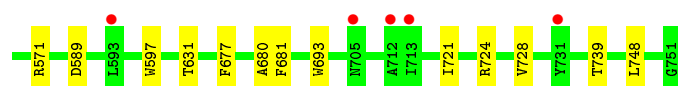


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



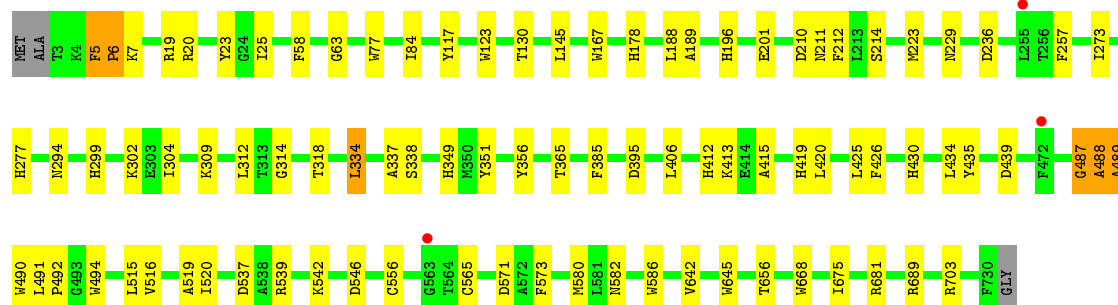
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





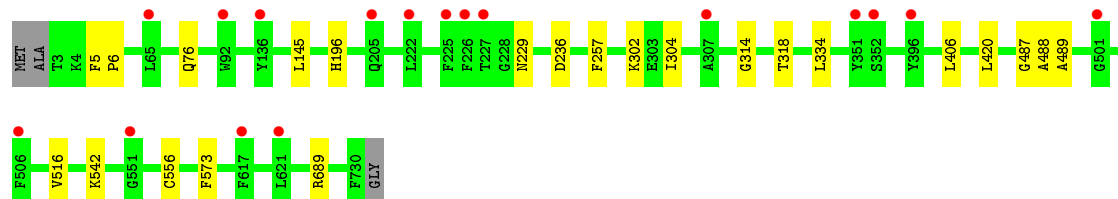
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 87% 11% .



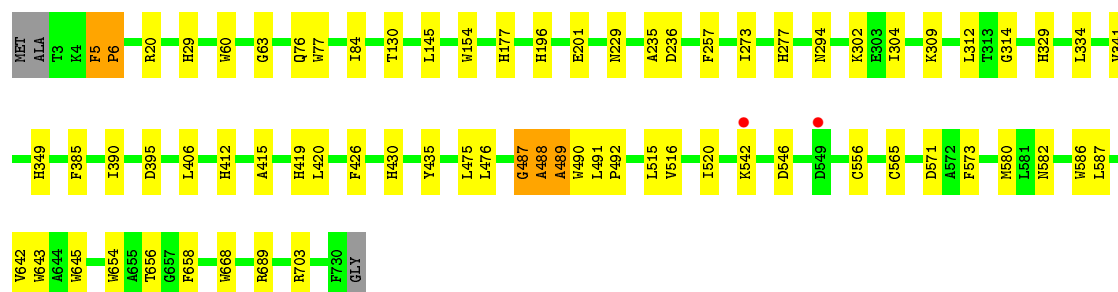
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 2% 96% .



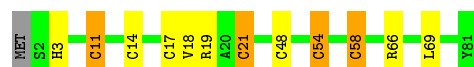
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2: 90% 9% .



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 84% 10% 5% .




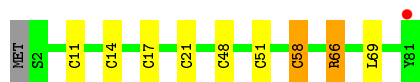
- Molecule 3: Photosystem I iron-sulfur center

Chain c:  94% 5%




- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  .% 88% 9%



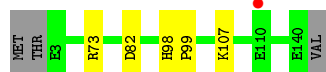
- Molecule 4: Photosystem I subunit II

Chain D:  88% 8%



- Molecule 4: Photosystem I subunit II

Chain d:  .% 94%




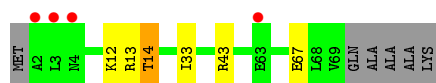
- Molecule 4: Photosystem I subunit II

Chain 4:  3% 91%




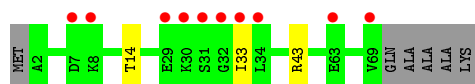
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  5% 84% 7% 8%

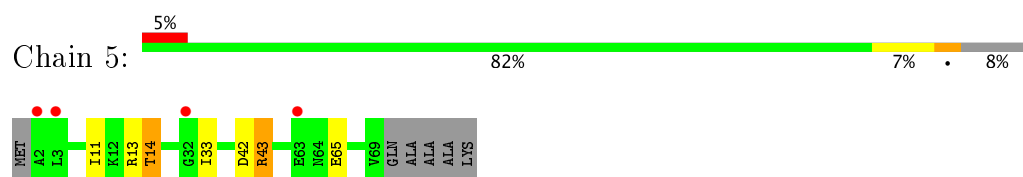


- Molecule 5: Photosystem I reaction center subunit IV

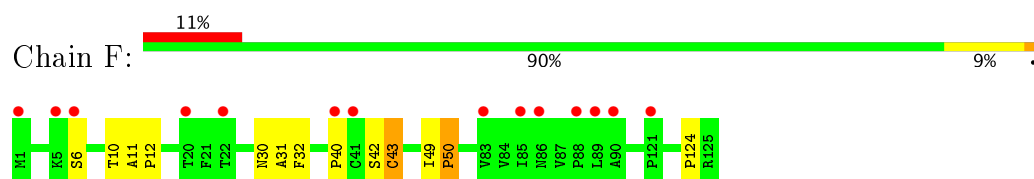
Chain e:  14% 88% 8%



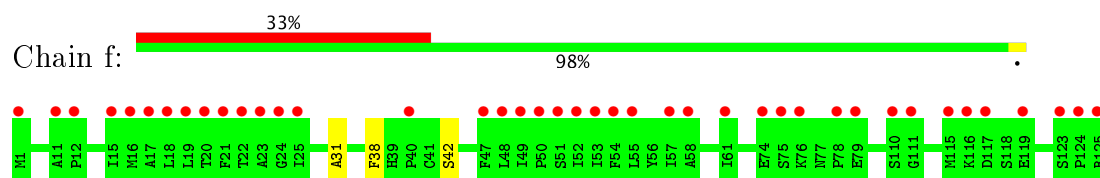
- Molecule 5: Photosystem I reaction center subunit IV



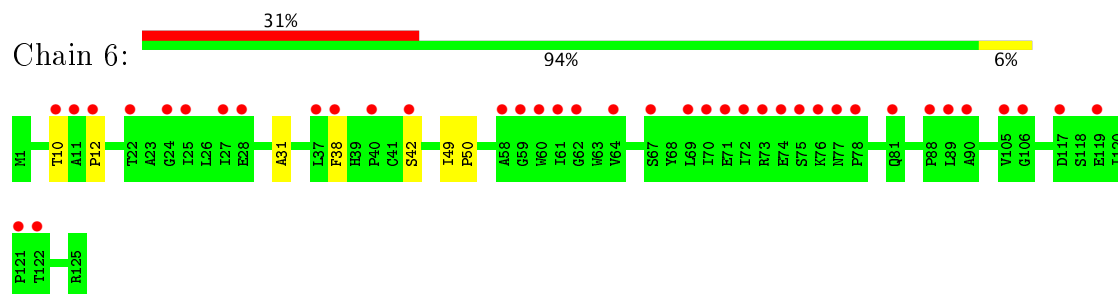
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



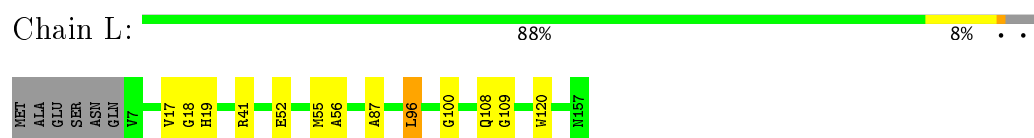
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



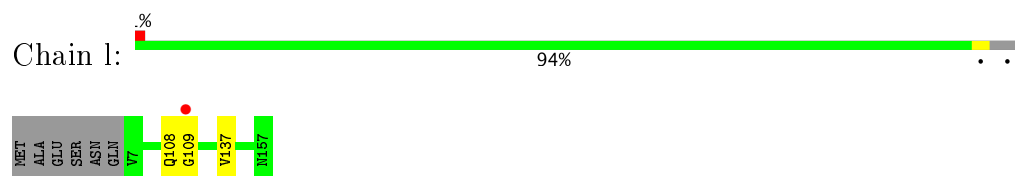
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



- Molecule 7: Photosystem I reaction center subunit XI



- Molecule 7: Photosystem I reaction center subunit XI



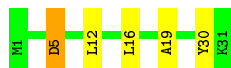
- Molecule 7: Photosystem I reaction center subunit XI





- Molecule 8: Photosystem I reaction center subunit XII

Chain M: 84% 13% .



- Molecule 8: Photosystem I reaction center subunit XII

Chain m: 97% .



- Molecule 8: Photosystem I reaction center subunit XII

Chain 7: 81% 16% .



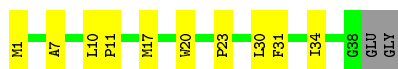
- Molecule 9: Photosystem I subunit III

Chain i: 3% 85% 10% 5%



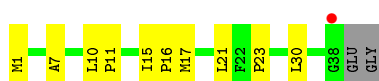
- Molecule 9: Photosystem I subunit III

Chain 9: 70% 25% 5%



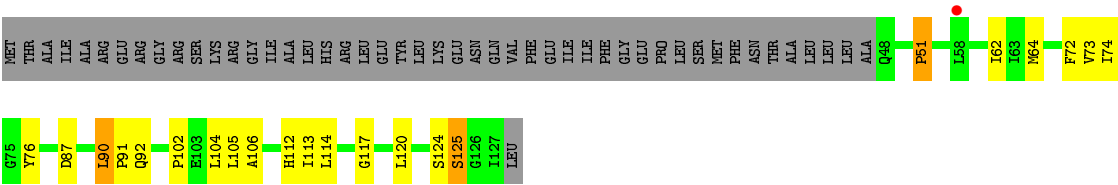
- Molecule 9: Photosystem I subunit III

Chain I: 3% 70% 25% 5%

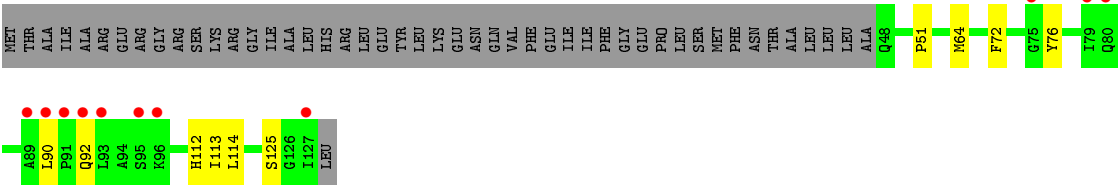


- Molecule 10: Photosystem I reaction center subunit VIII

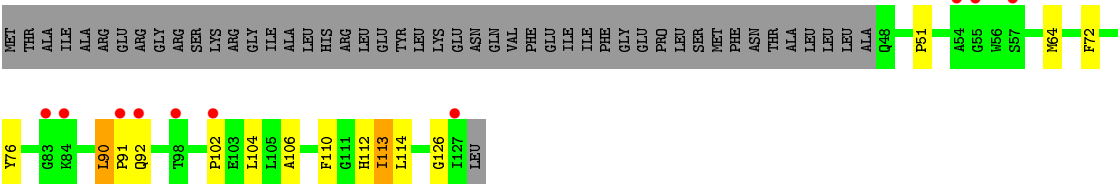
Chain K: % 45% 15% . 38%



● Molecule 10: Photosystem I reaction center subunit VIII



● Molecule 10: Photosystem I reaction center subunit VIII



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 133.68Å 219.85Å 90.00° 111.14° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 39.96 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-3.80) 71.5 (39.96-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032, PHENIX 1.8.2-1309	Depositor
R, R_{free}	0.253 , 0.297 0.263 , 0.276	Depositor DCC
R_{free} test set	4452 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	68370	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: LHG, SF4, CLA, PQN, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.22	0/5970	0.37	0/8138
1	A	0.23	0/5970	0.38	0/8138
1	a	0.22	0/5970	0.37	0/8138
2	2	0.23	0/5976	0.39	0/8173
2	B	0.24	0/5976	0.39	0/8173
2	b	0.23	0/5976	0.38	0/8173
3	3	0.28	0/610	0.44	0/826
3	C	0.24	0/610	0.46	0/826
3	c	0.25	0/610	0.43	0/826
4	4	0.23	0/1103	0.40	0/1487
4	D	0.23	0/1103	0.40	0/1487
4	d	0.23	0/1103	0.39	0/1487
5	5	0.23	0/538	0.45	0/729
5	E	0.24	0/538	0.43	0/729
5	e	0.23	0/538	0.42	0/729
6	6	0.23	0/700	0.43	0/976
6	F	0.24	0/690	0.47	0/963
6	f	0.23	0/700	0.43	0/976
7	8	0.23	0/1163	0.38	0/1580
7	L	0.23	0/1163	0.38	0/1580
7	l	0.23	0/1163	0.38	0/1580
8	7	0.26	0/238	0.38	0/323
8	M	0.26	0/238	0.39	0/323
8	m	0.25	0/238	0.38	0/323
9	9	0.25	0/308	0.42	0/421
9	I	0.24	0/308	0.41	0/421
9	i	0.25	0/308	0.43	0/421
10	0	0.22	0/504	0.48	0/688
10	K	0.24	0/504	0.45	0/688
10	k	0.23	0/504	0.45	0/688
All	All	0.23	0/51320	0.39	0/70010

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
2	2	0	1
2	B	0	1
2	b	0	1
4	4	0	1
4	D	0	1
4	d	0	1
6	F	0	1
10	k	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	5	PHE	Peptide
4	4	98	HIS	Peptide
2	B	5	PHE	Peptide
4	D	98	HIS	Peptide
6	F	40	PRO	Mainchain
2	b	5	PHE	Peptide
4	d	98	HIS	Peptide
10	k	125	SER	Peptide

5.2 Too-close contacts ⓘ

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	1	5772	0	5621	48	0
1	A	5772	0	5621	94	0
1	a	5772	0	5621	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2	5765	0	5546	48	0
2	B	5765	0	5546	64	0
2	b	5765	0	5545	0	0
3	3	600	0	588	22	0
3	C	600	0	586	25	0
3	c	600	0	587	0	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	9	0
4	d	1079	0	1073	0	0
5	5	529	0	506	4	0
5	E	529	0	506	2	0
5	e	529	0	506	0	0
6	6	685	0	411	3	0
6	F	676	0	395	11	0
6	f	685	0	411	0	0
7	8	1133	0	1108	5	0
7	L	1133	0	1108	9	0
7	l	1133	0	1108	0	0
8	7	235	0	253	7	0
8	M	235	0	253	7	0
8	m	235	0	253	0	0
9	9	297	0	295	10	0
9	I	297	0	295	7	0
9	i	297	0	295	0	0
10	0	496	0	439	4	0
10	K	496	0	439	12	0
10	k	496	0	439	0	0
11	0	115	0	111	4	0
11	1	2546	0	2430	89	0
11	2	2313	0	2213	84	0
11	8	176	0	177	8	0
11	A	2546	0	2435	159	0
11	B	2313	0	2213	127	0
11	K	115	0	111	8	0
11	L	176	0	177	8	0
11	a	2546	0	2434	0	0
11	b	2313	0	2213	0	0
11	k	115	0	111	0	0
11	l	176	0	177	0	0
12	1	33	0	45	1	0
12	2	33	0	45	3	0
12	A	33	0	45	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	B	33	0	45	4	0
12	a	33	0	46	0	0
12	b	33	0	45	0	0
13	1	8	0	0	1	0
13	3	16	0	0	21	0
13	A	8	0	0	4	0
13	C	16	0	0	22	0
13	a	8	0	0	0	0
13	c	16	0	0	0	0
14	1	200	0	242	23	0
14	2	320	0	391	40	0
14	6	120	0	147	20	0
14	7	40	0	49	6	0
14	8	80	0	97	15	0
14	A	200	0	244	35	0
14	B	320	0	390	62	0
14	F	120	0	146	23	0
14	L	80	0	97	22	0
14	M	40	0	49	7	0
14	a	200	0	243	0	0
14	b	320	0	389	0	0
14	f	120	0	147	0	0
14	l	80	0	97	0	0
14	m	40	0	49	0	0
15	1	98	0	148	16	0
15	2	49	0	74	7	0
15	A	98	0	148	15	0
15	B	49	0	74	8	0
15	a	98	0	148	0	0
15	b	49	0	74	0	0
16	2	55	0	86	1	0
16	B	55	0	86	1	0
16	b	55	0	86	0	0
All	All	68370	0	66274	831	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (831) 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)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:A:56:HIS:CG	11:A:1103:CLA:HBB2	3.55	1.62
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61
3:C:58:CYS:SG	13:C:3003:SF4:FE1	1.08	1.57
3:C:11:CYS:SG	13:C:3003:SF4:FE3	0.82	1.54
3:C:14:CYS:SG	13:C:3003:SF4:FE2	1.31	1.44
1:A:56:HIS:CD2	11:A:1103:CLA:HBB2	2.63	1.40
1:A:56:HIS:CG	11:A:1103:CLA:CBB	3.92	1.36
3:C:54:CYS:SG	13:C:3002:SF4:FE3	1.22	1.29
3:3:58:CYS:SG	13:3:3003:SF4:FE1	1.23	1.29
3:3:14:CYS:SG	13:3:3003:SF4:FE2	1.29	1.23
3:C:48:CYS:SG	13:C:3002:SF4:S3	2.39	1.20
3:C:21:CYS:SG	13:C:3002:SF4:S1	2.57	1.06
3:3:51:CYS:SG	13:3:3002:SF4:FE1	1.45	1.06
3:3:58:CYS:SG	13:3:3003:SF4:S3	2.58	1.02
3:C:14:CYS:HG	13:C:3003:SF4:FE2	1.15	1.02
1:A:583:CYS:HG	13:A:3001:SF4:FE2	0.73	0.97
3:C:14:CYS:SG	13:C:3003:SF4:S4	3.10	0.96
3:C:54:CYS:HG	13:C:3002:SF4:FE3	0.67	0.93
2:2:586:TRP:CZ2	11:2:1021:CLA:H201	2.05	0.92
1:A:56:HIS:CD2	11:A:1103:CLA:CBB	3.27	0.92
3:3:48:CYS:HG	13:3:3002:SF4:FE4	0.83	0.91
3:3:51:CYS:HG	13:3:3002:SF4:FE1	0.65	0.91
11:B:1222:CLA:HBA1	11:B:1223:CLA:OBD	2.44	0.90
3:3:17:CYS:HG	13:3:3003:SF4:FE4	0.64	0.89
3:C:48:CYS:HG	13:C:3002:SF4:FE4	1.51	0.88
1:A:56:HIS:CB	11:A:1103:CLA:HBB2	4.57	0.88
14:B:4004:BCR:H23C	14:B:4004:BCR:H403	1.58	0.85
3:3:11:CYS:HG	13:3:3003:SF4:FE3	0.88	0.85
3:3:48:CYS:SG	13:3:3002:SF4:S1	2.75	0.84
14:F:4018:BCR:H14C	9:I:23:PRO:CG	2.08	0.83
3:3:17:CYS:SG	13:3:3003:SF4:FE4	1.71	0.82
11:A:1127:CLA:HHC	11:A:1127:CLA:HBB1	4.33	0.81
11:A:1123:CLA:HBB1	11:A:1123:CLA:HHC	1.63	0.81
3:C:48:CYS:SG	13:C:3002:SF4:S1	2.79	0.80
14:L:4019:BCR:HC8	14:L:4019:BCR:H321	1.62	0.80
11:A:1134:CLA:HHC	11:A:1134:CLA:HBB1	1.63	0.80
3:3:58:CYS:SG	13:3:3003:SF4:S2	2.80	0.80
1:1:395:TRP:CD1	11:1:1126:CLA:HAB	2.17	0.80
1:A:56:HIS:ND1	11:A:1103:CLA:CBB	4.21	0.79
1:A:574:CYS:SG	13:A:3001:SF4:S3	2.87	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1103:CLA:H51	11:A:1111:CLA:H12	2.31	0.79
11:A:1801:CLA:C1C	15:A:5003:LHG:HC31	2.38	0.79
11:A:1801:CLA:HHC	11:A:1801:CLA:HBB1	1.65	0.79
11:B:1227:CLA:HBC3	11:B:1227:CLA:HHD	1.65	0.78
14:2:4004:BCR:H403	14:2:4004:BCR:H23C	1.65	0.78
1:A:583:CYS:SG	13:A:3001:SF4:FE2	1.75	0.78
11:A:1140:CLA:HHC	11:A:1140:CLA:HBB1	1.67	0.77
3:C:58:CYS:SG	13:C:3003:SF4:S2	2.69	0.77
11:1:1107:CLA:HHC	11:1:1107:CLA:HBB1	1.67	0.77
3:3:11:CYS:SG	13:3:3003:SF4:S2	2.81	0.77
6:F:10:THR:CB	14:F:4013:BCR:H401	3.98	0.77
1:A:395:TRP:CD1	11:A:1126:CLA:HAB	2.20	0.77
11:1:1131:CLA:HAB	11:1:1132:CLA:HBB1	1.66	0.76
7:8:96:LEU:HG	14:8:4019:BCR:H24C	1.67	0.76
11:2:1231:CLA:HHC	11:2:1231:CLA:HBB1	1.65	0.76
1:A:354:ILE:HD11	14:A:4007:BCR:HC7	1.66	0.76
14:A:4001:BCR:H331	14:A:4002:BCR:H24C	1.66	0.76
14:B:4014:BCR:HC21	11:B:1229:CLA:HBB2	1.68	0.76
3:3:21:CYS:SG	13:3:3002:SF4:S1	2.78	0.75
11:A:1237:CLA:HHC	11:A:1237:CLA:HBB1	1.92	0.75
11:A:1128:CLA:HBB1	11:A:1128:CLA:HHC	3.40	0.75
14:B:4014:BCR:HC21	11:B:1229:CLA:CBB	2.17	0.74
1:A:193:VAL:CG1	11:A:1123:CLA:HHD	2.17	0.74
14:8:4019:BCR:H321	14:8:4019:BCR:HC8	1.69	0.74
11:A:1116:CLA:HHC	11:A:1116:CLA:HBB1	2.67	0.74
11:A:1129:CLA:HHC	11:A:1129:CLA:HBB1	1.70	0.74
11:B:1229:CLA:HHC	11:B:1229:CLA:HBB1	1.69	0.74
11:A:1125:CLA:HBB1	11:A:1125:CLA:HHC	4.18	0.74
14:A:4001:BCR:C33	14:A:4002:BCR:H24C	2.54	0.74
6:F:12:PRO:HG2	14:F:4013:BCR:H401	1.70	0.74
11:B:1214:CLA:HHC	11:B:1214:CLA:HBB1	2.25	0.74
11:A:1110:CLA:HHC	11:A:1110:CLA:HBB1	1.70	0.73
11:1:1125:CLA:HHD	11:1:1125:CLA:HBC2	1.70	0.73
1:A:56:HIS:CB	11:A:1103:CLA:CBB	4.84	0.73
11:A:1111:CLA:HBB1	11:A:1111:CLA:HHC	2.34	0.73
14:F:4018:BCR:H402	14:F:4020:BCR:H353	1.86	0.73
11:B:1021:CLA:HHC	11:B:1021:CLA:HBB1	4.13	0.73
14:2:4011:BCR:H23C	11:2:1230:CLA:HMC2	1.70	0.73
3:3:21:CYS:SG	13:3:3002:SF4:S3	2.80	0.73
11:K:1402:CLA:HHC	11:K:1402:CLA:HBB1	1.81	0.72
2:2:426:PHE:O	2:2:430:HIS:ND1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:656:THR:HA	11:B:1023:CLA:HAB	1.72	0.72
11:B:1229:CLA:H201	11:B:1235:CLA:C15	2.20	0.72
2:B:426:PHE:CE2	11:B:1235:CLA:HAB	3.29	0.72
11:1:1128:CLA:HBB1	11:1:1128:CLA:HHC	1.72	0.71
1:1:571:ARG:NH1	15:1:5001:LHG:O10	2.23	0.71
6:F:12:PRO:HB3	14:F:4013:BCR:H19C	6.28	0.71
14:F:4013:BCR:H392	14:F:4013:BCR:H23C	1.72	0.71
14:6:4013:BCR:H392	14:6:4013:BCR:H23C	1.72	0.71
14:6:4018:BCR:H14C	9:9:23:PRO:CG	2.21	0.71
11:A:1126:CLA:H42	14:B:4011:BCR:HC7	1.73	0.71
1:A:571:ARG:NH1	15:A:5001:LHG:O10	2.51	0.71
14:2:4009:BCR:H353	15:2:5004:LHG:H202	1.72	0.70
11:1:1106:CLA:H191	11:1:1109:CLA:H91	1.73	0.70
11:A:1101:CLA:H202	11:A:1126:CLA:H203	1.73	0.70
1:1:330:GLY:HA3	15:1:5003:LHG:HC32	1.72	0.70
1:A:330:GLY:HA3	15:A:5003:LHG:HC32	1.73	0.70
11:2:1220:CLA:HHD	11:2:1220:CLA:HBC2	1.73	0.70
11:A:1136:CLA:HHC	11:A:1136:CLA:HBB1	1.74	0.70
3:C:58:CYS:SG	13:C:3003:SF4:S3	2.05	0.70
2:2:309:LYS:O	15:2:5004:LHG:HC31	1.93	0.69
14:B:4010:BCR:HC41	11:B:1223:CLA:HMA3	1.94	0.69
14:1:4008:BCR:C8	11:1:1124:CLA:HAB	2.21	0.69
2:B:415:ALA:O	2:B:419:HIS:ND1	2.33	0.69
15:1:5001:LHG:H202	11:1:1128:CLA:H202	1.75	0.69
14:B:4006:BCR:H392	14:B:4006:BCR:H23C	1.97	0.69
11:1:1127:CLA:H71	11:1:1127:CLA:HMD2	1.75	0.68
2:B:309:LYS:O	15:B:5004:LHG:HC31	2.12	0.68
11:B:1238:CLA:H142	14:F:4020:BCR:HC8	1.75	0.68
11:L:1501:CLA:H43	14:L:4022:BCR:H14C	1.73	0.68
11:1:1104:CLA:HHC	11:1:1104:CLA:HBB1	1.74	0.68
11:1:1127:CLA:C7	11:1:1127:CLA:HMD2	2.24	0.68
11:1:1115:CLA:CHD	11:0:1401:CLA:HBA1	2.24	0.68
11:1:1012:CLA:C1B	11:2:1021:CLA:H203	2.24	0.68
14:A:4008:BCR:C8	11:A:1124:CLA:HAB	2.24	0.67
11:1:1110:CLA:HBB1	11:1:1110:CLA:HHC	1.76	0.67
11:1:1131:CLA:HAB	11:1:1132:CLA:CHB	2.25	0.67
4:D:82:ASP:N	4:D:82:ASP:OD1	2.28	0.67
7:L:96:LEU:HG	14:L:4019:BCR:H24C	1.80	0.67
11:1:1012:CLA:C2B	11:2:1021:CLA:H203	2.25	0.67
2:2:426:PHE:CE2	11:2:1235:CLA:HAB	2.29	0.67
11:B:1238:CLA:C14	14:F:4020:BCR:HC8	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4008:BCR:HC8	11:A:1124:CLA:HAB	1.83	0.67
1:A:681:PHE:HA	11:B:1013:CLA:HAB	1.75	0.67
2:B:23:TYR:CE2	16:B:5002:LMG:HC71	2.31	0.66
2:2:426:PHE:CD2	11:2:1235:CLA:HAB	2.31	0.66
14:B:4005:BCR:HC7	11:B:1209:CLA:HMC1	1.78	0.66
14:A:4003:BCR:H23C	14:A:4003:BCR:H403	1.78	0.66
11:B:1223:CLA:HHD	11:B:1223:CLA:HBC3	1.98	0.66
11:A:1104:CLA:HMD1	11:A:1106:CLA:H202	1.77	0.66
14:B:4009:BCR:H23C	11:B:1227:CLA:HBC2	1.77	0.66
1:A:560:ARG:O	4:D:61:ARG:NH1	2.86	0.66
14:F:4018:BCR:H14C	9:I:23:PRO:HG3	1.77	0.66
14:B:4004:BCR:H14C	11:B:1217:CLA:HBB1	3.27	0.65
14:B:4009:BCR:H23C	11:B:1227:CLA:CBC	2.26	0.65
14:A:4007:BCR:H19C	11:A:1122:CLA:H43	1.76	0.65
2:B:426:PHE:O	2:B:430:HIS:ND1	2.37	0.65
6:F:12:PRO:CG	14:F:4013:BCR:H401	2.27	0.65
11:8:1501:CLA:HBA2	14:8:4022:BCR:H363	1.77	0.65
3:C:48:CYS:SG	13:C:3002:SF4:S2	2.95	0.65
2:B:546:ASP:OD2	3:C:66:ARG:NH1	2.29	0.65
15:1:5003:LHG:H302	11:1:1137:CLA:H102	1.79	0.65
8:M:16:LEU:CD2	14:M:4021:BCR:H19C	2.27	0.65
13:A:3001:SF4:S2	2:B:565:CYS:SG	2.95	0.64
14:B:4011:BCR:H23C	11:B:1230:CLA:HMC2	1.79	0.64
14:B:4017:BCR:HC7	11:B:1205:CLA:C10	3.64	0.64
14:1:4001:BCR:C33	14:1:4002:BCR:H24C	2.27	0.64
1:A:56:HIS:HB3	11:A:1103:CLA:CBB	4.61	0.64
1:1:312:ARG:NH2	1:1:316:GLY:O	2.29	0.64
11:B:1222:CLA:CBA	11:B:1223:CLA:OBD	3.05	0.64
14:A:4001:BCR:H333	14:A:4002:BCR:H24C	2.97	0.64
14:B:4010:BCR:H14C	11:B:1222:CLA:HMA1	2.17	0.64
16:2:5002:LMG:H202	11:2:1201:CLA:HBC1	1.80	0.64
3:3:14:CYS:SG	13:3:3003:SF4:S4	2.95	0.64
11:B:1222:CLA:CMB	11:B:1223:CLA:H202	2.28	0.64
11:B:1206:CLA:H43	14:F:4018:BCR:H342	2.56	0.63
10:K:102:PRO:O	10:K:106:ALA:N	2.30	0.63
14:2:4009:BCR:H23C	11:2:1227:CLA:HBC1	1.79	0.63
2:B:656:THR:CA	11:B:1023:CLA:HAB	2.28	0.63
11:A:1137:CLA:HAB	11:A:1129:CLA:CBB	2.29	0.63
11:A:1132:CLA:H201	14:L:4022:BCR:H343	2.19	0.62
1:A:597:TRP:HH2	11:A:1022:CLA:HAB	1.64	0.62
11:2:1212:CLA:HHC	11:2:1212:CLA:HBB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:TRP:CH2	11:A:1022:CLA:HAB	2.34	0.62
1:1:597:TRP:CH2	11:1:1022:CLA:HAB	2.34	0.62
11:A:1138:CLA:HHD	14:B:4014:BCR:C38	2.30	0.62
11:1:1022:CLA:H172	14:2:4017:BCR:H343	1.82	0.62
11:2:1212:CLA:HAB	11:2:1211:CLA:HMC1	1.82	0.62
13:1:3001:SF4:S2	2:2:565:CYS:SG	2.97	0.62
11:1:1112:CLA:CMC	11:1:1113:CLA:HAB	2.30	0.61
14:6:4018:BCR:H14C	9:9:23:PRO:HG3	1.82	0.61
11:2:1206:CLA:H43	14:6:4018:BCR:H342	1.81	0.61
11:A:1012:CLA:CHB	11:B:1021:CLA:H202	2.36	0.61
11:A:1125:CLA:CBC	11:A:1125:CLA:HHD	2.31	0.61
8:M:16:LEU:HD23	14:M:4021:BCR:H19C	1.87	0.61
11:A:1115:CLA:HHD	11:A:1115:CLA:HBC3	1.83	0.61
11:2:1206:CLA:H201	9:9:23:PRO:HA	1.83	0.61
14:A:4007:BCR:H352	11:A:1119:CLA:H71	2.32	0.61
11:1:1106:CLA:HBB1	11:1:1106:CLA:HHC	1.82	0.61
1:1:677:PHE:CG	14:2:4011:BCR:H363	2.35	0.61
1:A:677:PHE:CD1	14:B:4011:BCR:H363	2.35	0.61
11:1:1801:CLA:C1C	15:1:5003:LHG:HC31	2.31	0.60
11:1:1137:CLA:HAB	11:1:1129:CLA:CBB	2.32	0.60
2:2:520:ILE:HD13	11:2:1234:CLA:HAB	1.83	0.60
14:2:4017:BCR:H342	11:2:1205:CLA:C10	2.32	0.60
6:6:10:THR:CB	14:6:4013:BCR:H401	2.31	0.60
11:A:1131:CLA:H192	11:B:1023:CLA:H201	3.09	0.60
11:B:1225:CLA:C16	11:B:1211:CLA:HAB	2.44	0.60
11:L:1501:CLA:C4	14:L:4022:BCR:H14C	2.32	0.60
11:A:1119:CLA:HBC2	11:A:1119:CLA:HHD	1.82	0.60
1:1:597:TRP:HH2	11:1:1022:CLA:HAB	1.67	0.59
11:A:1126:CLA:C4	14:B:4011:BCR:HC7	2.54	0.59
2:2:312:LEU:HD23	15:2:5004:LHG:HC61	1.85	0.59
2:B:488:ALA:O	2:B:490:TRP:N	2.35	0.59
14:1:4008:BCR:HC8	11:1:1124:CLA:HAB	1.84	0.59
11:B:1210:CLA:HBC2	11:B:1210:CLA:HHD	1.85	0.59
7:L:41:ARG:NH2	7:L:52:GLU:OE2	2.35	0.59
11:2:1214:CLA:H92	11:2:1231:CLA:O1A	2.03	0.59
14:2:4010:BCR:H14C	11:2:1222:CLA:HMA1	1.85	0.59
2:B:188:LEU:HD21	14:B:4004:BCR:H331	1.85	0.59
14:A:4002:BCR:H14C	11:A:1112:CLA:HBB1	2.18	0.59
14:1:4007:BCR:H341	11:1:1123:CLA:HAB	1.86	0.58
2:2:312:LEU:HD22	15:2:5004:LHG:HC42	1.85	0.58
1:1:302:VAL:HG22	14:1:4001:BCR:H352	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:1205:CLA:CGA	11:B:1205:CLA:C1A	2.82	0.58
11:B:1202:CLA:H202	11:B:1210:CLA:HMD1	1.84	0.58
3:C:21:CYS:SG	13:C:3002:SF4:S3	2.84	0.58
11:2:1231:CLA:C4C	11:2:1232:CLA:HAB	2.34	0.58
11:2:1205:CLA:HAB	11:2:1206:CLA:HAA2	1.85	0.58
2:B:63:GLY:HA3	11:B:1204:CLA:HAB	1.85	0.58
14:2:4014:BCR:HC21	11:2:1229:CLA:CBB	2.34	0.58
4:D:61:ARG:NH2	4:D:63:GLU:OE1	2.36	0.58
3:C:14:CYS:SG	13:C:3003:SF4:S3	3.20	0.58
11:2:1205:CLA:C1A	11:2:1205:CLA:CGA	2.81	0.58
11:A:1022:CLA:H172	14:B:4017:BCR:H343	1.85	0.58
8:7:16:LEU:HD23	14:7:4021:BCR:H19C	1.84	0.58
2:B:299:HIS:NE2	11:B:1219:CLA:OBD	2.48	0.58
2:B:426:PHE:HE2	11:B:1235:CLA:HAB	2.93	0.58
11:1:1133:CLA:HBB1	11:1:1133:CLA:HHC	1.86	0.57
14:2:4014:BCR:HC21	11:2:1229:CLA:HBB1	1.86	0.57
14:B:4005:BCR:H321	14:B:4005:BCR:HC8	1.86	0.57
11:2:1204:CLA:H2	14:6:4018:BCR:HC32	1.86	0.57
2:2:488:ALA:O	2:2:490:TRP:N	2.37	0.57
14:A:4007:BCR:HC41	11:A:1119:CLA:H191	1.86	0.57
14:2:4009:BCR:H23C	11:2:1227:CLA:CBC	2.34	0.57
11:A:1126:CLA:C4C	14:B:4011:BCR:HC42	2.34	0.57
14:F:4020:BCR:H333	7:L:87:ALA:HB3	2.25	0.57
14:1:4003:BCR:H321	14:1:4003:BCR:HC8	1.86	0.57
8:7:16:LEU:CD2	14:7:4021:BCR:H19C	2.35	0.57
14:2:4005:BCR:H321	14:2:4005:BCR:HC8	1.86	0.57
11:A:1138:CLA:HHC	11:A:1138:CLA:HBB1	1.87	0.57
11:2:1240:CLA:HHC	11:2:1240:CLA:HBB1	1.87	0.57
11:1:1106:CLA:H191	11:1:1109:CLA:C9	2.33	0.57
11:1:1115:CLA:C1D	11:0:1401:CLA:HBA1	2.35	0.56
14:6:4020:BCR:HC22	9:9:20:TRP:CD1	2.40	0.56
11:A:1131:CLA:H203	11:B:1023:CLA:H201	1.85	0.56
14:1:4008:BCR:H331	14:1:4008:BCR:C8	2.35	0.56
1:1:50:ASN:ND2	15:1:5001:LHG:HC12	2.21	0.56
5:5:13:ARG:NH1	5:5:65:GLU:OE2	2.39	0.56
14:B:4010:BCR:C19	11:B:1223:CLA:H111	5.12	0.56
14:2:4014:BCR:H333	11:2:1230:CLA:H51	1.87	0.56
11:8:1501:CLA:C4	14:8:4022:BCR:H14C	2.35	0.56
11:B:1224:CLA:HBC2	11:B:1224:CLA:HHD	1.86	0.56
14:B:4010:BCR:H23C	14:B:4010:BCR:H392	1.93	0.56
5:5:42:ASP:OD2	5:5:43:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ILE:O	2:B:277:HIS:ND1	2.39	0.56
12:2:2002:PQN:H302	11:2:1239:CLA:C1	2.36	0.55
11:B:1201:CLA:HMB2	14:M:4021:BCR:H333	1.88	0.55
3:3:11:CYS:SG	13:3:3003:SF4:S4	3.04	0.55
11:A:1114:CLA:HHC	11:A:1114:CLA:HBB1	1.89	0.55
1:A:395:TRP:NE1	11:A:1126:CLA:HAB	2.22	0.55
14:A:4003:BCR:H23C	14:A:4003:BCR:C40	2.36	0.55
11:L:1501:CLA:H41	14:L:4022:BCR:H14C	2.14	0.55
1:1:199:HIS:O	1:1:203:GLY:N	2.40	0.55
11:2:1227:CLA:HHD	11:2:1227:CLA:HBC3	1.88	0.55
14:1:4001:BCR:HC42	11:1:1113:CLA:HBB1	1.87	0.55
1:A:211:GLY:CA	14:A:4002:BCR:H363	2.38	0.55
1:A:677:PHE:CG	14:B:4011:BCR:H363	2.59	0.55
11:B:1220:CLA:HBC2	11:B:1220:CLA:HHD	2.01	0.55
10:K:120:LEU:HD13	11:K:1401:CLA:H11	2.39	0.55
2:2:645:TRP:CZ3	14:2:4017:BCR:HC21	2.41	0.55
1:A:560:ARG:NH2	4:D:15:THR:O	2.70	0.55
15:B:5004:LHG:HC82	15:B:5004:LHG:H262	1.88	0.55
11:A:1104:CLA:CMD	11:A:1106:CLA:H202	2.37	0.55
11:B:1208:CLA:HHC	11:B:1208:CLA:HBB1	2.90	0.55
2:B:5:PHE:CG	2:B:6:PRO:CD	2.90	0.55
3:C:54:CYS:SG	13:C:3002:SF4:S4	2.99	0.55
14:A:4008:BCR:H342	11:A:1124:CLA:CHC	2.37	0.54
11:1:1106:CLA:C9	11:1:1128:CLA:H203	2.38	0.54
11:1:1801:CLA:HBB1	11:1:1121:CLA:HAB	1.89	0.54
1:A:193:VAL:HG11	11:A:1123:CLA:HHD	1.89	0.54
11:0:1402:CLA:HBB1	11:0:1402:CLA:HHC	1.90	0.54
14:2:4017:BCR:H331	14:2:4017:BCR:C8	2.38	0.54
11:A:1801:CLA:HAB	11:A:1122:CLA:HHB	3.58	0.54
11:1:1101:CLA:H203	11:1:1140:CLA:H152	1.90	0.54
11:B:1228:CLA:HBB1	11:B:1228:CLA:HHC	3.84	0.54
14:B:4009:BCR:H321	14:B:4009:BCR:HC8	2.08	0.54
2:2:63:GLY:HA3	11:2:1204:CLA:HAB	1.90	0.54
1:A:571:ARG:HD2	15:A:5001:LHG:HC42	1.89	0.54
11:B:1221:CLA:CMB	11:B:1223:CLA:H8	2.43	0.54
2:B:130:THR:OG1	2:B:201:GLU:OE1	2.26	0.54
8:M:12:LEU:HD13	14:M:4021:BCR:H372	1.89	0.54
11:B:1238:CLA:O1A	14:L:4019:BCR:H363	2.08	0.54
2:B:349:HIS:ND1	11:B:1214:CLA:OBD	2.37	0.53
11:B:1222:CLA:HMB2	11:B:1223:CLA:H202	1.90	0.53
14:B:4017:BCR:H342	11:B:1205:CLA:C10	3.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:PHE:CE1	14:B:4005:BCR:H373	2.51	0.53
11:A:1101:CLA:C20	11:A:1126:CLA:H203	2.38	0.53
14:B:4010:BCR:C19	11:B:1223:CLA:H93	2.71	0.53
14:1:4002:BCR:HC41	11:1:1103:CLA:H142	1.91	0.53
11:1:1137:CLA:HAB	11:1:1129:CLA:HBB2	1.91	0.53
14:A:4008:BCR:H353	11:A:1119:CLA:H62	1.90	0.53
2:B:656:THR:N	11:B:1023:CLA:HAB	2.26	0.53
1:A:574:CYS:HB3	1:A:583:CYS:HA	1.90	0.53
11:B:1225:CLA:H162	11:B:1211:CLA:HAB	2.12	0.53
2:2:5:PHE:CG	2:2:6:PRO:CD	2.92	0.53
1:1:263:PHE:CE2	14:1:4001:BCR:H343	2.43	0.53
2:2:546:ASP:OD2	3:3:66:ARG:NH1	2.41	0.53
12:A:2001:PQN:H243	11:B:1013:CLA:H202	3.32	0.53
2:B:210:ASP:OD1	2:B:211:ASN:ND2	2.38	0.53
11:A:1112:CLA:CMC	11:A:1113:CLA:HAB	2.74	0.53
11:L:1501:CLA:H202	11:L:1503:CLA:C1	3.89	0.53
1:A:332:PHE:HB2	15:A:5003:LHG:HC41	1.91	0.52
1:A:90:MET:HE1	11:A:1106:CLA:HBA2	2.54	0.52
3:3:11:CYS:SG	13:3:3003:SF4:S1	3.07	0.52
1:A:681:PHE:CA	11:B:1013:CLA:HAB	2.39	0.52
8:M:16:LEU:HD21	14:M:4021:BCR:H19C	1.90	0.52
11:A:1106:CLA:HBB1	11:A:1106:CLA:HHC	2.72	0.52
11:B:1204:CLA:H93	14:F:4018:BCR:HC31	3.06	0.52
14:B:4006:BCR:H372	11:B:1225:CLA:H142	1.92	0.52
3:C:54:CYS:SG	13:C:3002:SF4:S2	3.08	0.52
7:L:55:MET:HB3	14:L:4022:BCR:H19C	1.92	0.52
11:A:1110:CLA:HAB	11:A:1118:CLA:H61	2.45	0.52
14:B:4010:BCR:H19C	11:B:1223:CLA:H111	4.82	0.52
2:2:349:HIS:ND1	11:2:1214:CLA:OBD	2.42	0.52
14:B:4017:BCR:H362	11:B:1023:CLA:H143	2.13	0.52
14:B:4009:BCR:C13	15:B:5004:LHG:H202	2.39	0.52
10:0:102:PRO:O	10:0:106:ALA:N	2.41	0.52
11:1:1801:CLA:HMA3	15:1:5003:LHG:HC62	1.92	0.52
1:1:560:ARG:NH2	4:4:15:THR:O	2.44	0.51
9:9:7:ALA:N	8:7:5:ASP:OD1	2.41	0.51
11:8:1503:CLA:HBC1	14:8:4022:BCR:H341	1.91	0.51
11:A:1112:CLA:HMC1	11:A:1113:CLA:HAB	2.53	0.51
11:B:1238:CLA:C2	14:L:4019:BCR:H363	3.31	0.51
11:B:1212:CLA:HAB	11:B:1211:CLA:HMC3	1.92	0.51
2:B:520:ILE:HD13	11:B:1234:CLA:HAB	1.92	0.51
2:B:413:LYS:NZ	6:F:124:PRO:O	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:ASN:O	6:F:32:PHE:N	2.43	0.51
15:B:5004:LHG:HC62	11:B:1220:CLA:HBB1	2.05	0.51
1:A:441:ASN:ND2	11:A:1237:CLA:OBD	3.30	0.51
14:B:4011:BCR:H392	14:B:4011:BCR:H23C	1.92	0.51
3:3:48:CYS:SG	13:3:3002:SF4:S3	2.99	0.51
2:B:337:ALA:HB2	14:B:4010:BCR:H372	1.93	0.51
1:1:193:VAL:CG1	11:1:1123:CLA:HHD	2.41	0.51
11:A:1125:CLA:HED1	11:A:1133:CLA:HAB	2.35	0.51
3:C:11:CYS:SG	13:C:3003:SF4:S4	2.63	0.51
14:2:4014:BCR:H23C	14:2:4014:BCR:H382	1.91	0.51
1:1:395:TRP:HD1	11:1:1126:CLA:HAB	1.71	0.51
2:2:668:TRP:CZ2	12:2:2002:PQN:H2M3	2.46	0.51
14:6:4020:BCR:HC22	9:9:20:TRP:NE1	2.26	0.51
14:A:4008:BCR:C8	14:A:4008:BCR:H331	2.41	0.51
2:B:571:ASP:OD1	2:B:703:ARG:NH2	2.44	0.51
14:2:4017:BCR:H362	11:2:1023:CLA:H111	1.93	0.51
7:8:41:ARG:NH2	7:8:52:GLU:OE2	2.41	0.51
1:A:725:ALA:HB2	15:A:5001:LHG:HC62	1.91	0.51
1:A:56:HIS:CE1	11:A:1103:CLA:CBB	3.84	0.51
5:E:12:LYS:NZ	5:E:67:GLU:OE1	2.39	0.51
11:A:1119:CLA:HBB1	11:A:1119:CLA:HHC	2.36	0.51
11:A:1012:CLA:H42	14:B:4011:BCR:H362	2.59	0.50
11:1:1112:CLA:HMC1	11:1:1113:CLA:HAB	1.92	0.50
14:2:4009:BCR:H353	15:2:5004:LHG:C20	2.40	0.50
11:8:1501:CLA:H41	14:8:4022:BCR:H14C	1.93	0.50
2:B:487:GLY:O	2:B:489:ALA:N	2.44	0.50
3:3:48:CYS:SG	13:3:3002:SF4:S2	3.08	0.50
11:L:1501:CLA:HBA2	14:L:4022:BCR:H363	1.94	0.50
11:L:1501:CLA:H202	11:L:1503:CLA:C2	2.86	0.50
11:2:1238:CLA:O1A	14:8:4019:BCR:H363	2.12	0.50
1:A:267:ASN:O	1:A:269:GLY:N	2.46	0.50
1:A:684:MET:HE2	1:A:693:TRP:CH2	2.46	0.50
11:B:1013:CLA:CGA	11:B:1013:CLA:H3A	2.42	0.50
14:A:4003:BCR:H353	11:A:1111:CLA:C15	2.42	0.50
1:A:538:HIS:ND1	11:A:1135:CLA:HAB	2.94	0.50
3:C:11:CYS:SG	13:C:3003:SF4:S2	2.17	0.50
6:F:12:PRO:CB	14:F:4013:BCR:H19C	6.16	0.50
11:B:1212:CLA:HBB1	11:B:1212:CLA:HHC	3.24	0.50
11:1:1011:CLA:HMB3	11:1:1012:CLA:HMD1	1.94	0.50
11:B:1226:CLA:HHC	11:B:1226:CLA:HBB1	1.94	0.50
3:C:11:CYS:SG	13:C:3003:SF4:S1	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:1130:CLA:HHC	11:1:1130:CLA:HBB1	1.94	0.49
11:1:1133:CLA:HHC	11:1:1133:CLA:CBB	2.42	0.49
1:1:354:ILE:HD11	14:1:4007:BCR:HC7	1.94	0.49
1:1:332:PHE:O	1:1:428:ARG:NH2	2.45	0.49
1:1:681:PHE:HA	11:2:1013:CLA:HAB	1.93	0.49
1:1:589:ASP:OD1	1:1:724:ARG:NH1	2.44	0.49
2:2:415:ALA:O	2:2:419:HIS:ND1	2.43	0.49
11:1:1127:CLA:H72	11:1:1127:CLA:HMD2	1.93	0.49
1:1:677:PHE:CD1	14:2:4011:BCR:H363	2.47	0.49
11:A:1138:CLA:HHD	14:B:4014:BCR:H381	1.94	0.49
1:A:199:HIS:O	1:A:203:GLY:N	2.44	0.49
11:1:1022:CLA:H203	11:2:1206:CLA:H51	1.94	0.49
11:1:1237:CLA:H3A	14:6:4020:BCR:H401	1.94	0.49
11:A:1106:CLA:CHC	11:A:1107:CLA:HMD2	2.42	0.49
11:B:1212:CLA:HAB	11:B:1211:CLA:CMC	2.43	0.49
7:8:137:VAL:HG23	14:8:4022:BCR:H403	1.93	0.49
11:B:1221:CLA:HMB2	11:B:1223:CLA:H8	2.17	0.49
11:2:1212:CLA:HHC	11:2:1212:CLA:CBB	2.43	0.49
6:6:12:PRO:CG	14:6:4013:BCR:H403	2.43	0.49
14:1:4007:BCR:H352	11:1:1119:CLA:H71	1.94	0.49
14:8:4019:BCR:H23C	14:8:4019:BCR:H392	1.94	0.49
11:A:1125:CLA:HBC3	11:A:1125:CLA:HHD	1.94	0.49
1:A:454:LEU:HD23	11:A:1132:CLA:HAB	1.95	0.49
10:K:90:LEU:CB	10:K:91:PRO:CD	2.91	0.49
2:2:312:LEU:CD2	15:2:5004:LHG:HC42	2.43	0.49
10:K:117:GLY:HA3	11:K:1401:CLA:C3B	2.64	0.49
1:1:267:ASN:O	1:1:269:GLY:N	2.45	0.48
14:2:4014:BCR:HC41	11:2:1229:CLA:CBB	2.43	0.48
2:B:334:LEU:HB3	14:B:4010:BCR:H401	3.41	0.48
11:A:1022:CLA:C17	14:B:4017:BCR:H343	2.43	0.48
11:1:1119:CLA:HMB2	11:1:1123:CLA:HMA3	1.95	0.48
14:2:4011:BCR:H321	14:2:4011:BCR:HC8	1.95	0.48
11:8:1501:CLA:H202	11:8:1503:CLA:H2	1.95	0.48
11:1:1106:CLA:H91	11:1:1106:CLA:H111	1.72	0.48
2:2:587:LEU:CD1	11:2:1234:CLA:HBB2	2.44	0.48
1:A:540:PHE:HE2	11:A:1022:CLA:HAB	2.41	0.48
11:2:1238:CLA:HBB1	11:2:1238:CLA:HHC	1.96	0.48
1:A:352:LEU:HD11	11:A:1128:CLA:HBB1	1.94	0.48
11:B:1223:CLA:HED1	11:B:1231:CLA:HAB	1.94	0.48
14:B:4017:BCR:H331	14:B:4017:BCR:C8	2.44	0.48
1:A:540:PHE:CE2	11:A:1022:CLA:HAB	3.03	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HB2	11:A:1112:CLA:CHC	2.44	0.48
14:A:4007:BCR:H24C	11:A:1137:CLA:C9	2.43	0.48
1:1:195:SER:O	1:1:199:HIS:ND1	2.36	0.48
14:2:4005:BCR:H343	11:2:1209:CLA:HMC1	1.95	0.48
2:2:587:LEU:HD12	11:2:1234:CLA:HBB2	1.94	0.48
11:A:1131:CLA:HAB	11:A:1132:CLA:HMB2	1.95	0.48
11:1:1125:CLA:HHD	11:1:1125:CLA:CBC	2.42	0.48
15:A:5003:LHG:H02	15:A:5003:LHG:P	2.72	0.48
11:1:1128:CLA:H172	14:2:4011:BCR:H342	1.96	0.48
14:B:4017:BCR:H331	14:B:4017:BCR:HC8	1.95	0.48
11:1:1106:CLA:H93	11:1:1128:CLA:H203	1.96	0.48
14:2:4010:BCR:H23C	14:2:4010:BCR:H392	1.95	0.48
11:A:1121:CLA:HHC	11:A:1121:CLA:HBB1	1.95	0.48
2:B:586:TRP:CE2	11:B:1021:CLA:H191	2.49	0.48
11:1:1107:CLA:H12	14:6:4013:BCR:H14C	1.96	0.48
11:A:1102:CLA:HAB	11:A:1104:CLA:CAD	2.44	0.48
1:1:681:PHE:N	11:2:1013:CLA:HAB	2.29	0.47
14:B:4004:BCR:H351	14:B:4004:BCR:H15C	1.60	0.47
14:B:4017:BCR:H15C	14:B:4017:BCR:H351	1.61	0.47
1:1:680:ALA:C	11:2:1013:CLA:HAB	2.34	0.47
14:A:4007:BCR:H15C	14:A:4007:BCR:H351	1.64	0.47
1:A:121:VAL:HB	11:B:1230:CLA:HMD1	1.95	0.47
14:1:4001:BCR:H332	14:1:4002:BCR:H24C	1.96	0.47
14:1:4007:BCR:H372	15:1:5003:LHG:H262	1.95	0.47
1:A:423:ASN:OD1	1:A:431:ARG:NH2	2.47	0.47
14:B:4009:BCR:H353	15:B:5004:LHG:H223	2.23	0.47
1:1:423:ASN:OD1	1:1:431:ARG:NH2	2.48	0.47
2:2:586:TRP:CE2	11:2:1021:CLA:H201	2.48	0.47
14:A:4003:BCR:H402	11:A:1103:CLA:H72	2.39	0.47
1:A:429:MET:HA	1:A:432:HIS:CE1	2.50	0.47
14:B:4014:BCR:H15C	14:B:4014:BCR:H351	1.56	0.47
11:A:1138:CLA:HHD	14:B:4014:BCR:H383	1.96	0.47
2:B:539:ARG:NH2	4:D:127:GLU:OE1	2.41	0.47
14:2:4010:BCR:H363	11:2:1222:CLA:C2B	2.44	0.47
11:B:1238:CLA:H2	14:L:4019:BCR:H363	3.26	0.47
6:F:42:SER:O	6:F:43:CYS:CB	2.63	0.47
11:1:1117:CLA:HAB	11:1:1117:CLA:C11	2.45	0.47
7:8:96:LEU:CG	14:8:4019:BCR:H24C	2.43	0.47
11:B:1207:CLA:HBB1	11:B:1207:CLA:HHC	2.47	0.47
11:B:1208:CLA:CBB	11:B:1208:CLA:HHC	2.98	0.47
14:B:4005:BCR:H343	11:B:1209:CLA:CMC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4002:BCR:H15C	14:A:4002:BCR:H351	1.65	0.47
2:B:586:TRP:CD2	11:B:1021:CLA:H191	2.50	0.47
14:1:4001:BCR:H331	14:1:4002:BCR:H24C	1.96	0.47
14:2:4010:BCR:H351	14:2:4010:BCR:H15C	1.54	0.47
14:6:4018:BCR:H382	14:6:4018:BCR:H23C	1.96	0.47
14:B:4009:BCR:C14	15:B:5004:LHG:H202	2.45	0.47
11:2:1229:CLA:CAB	11:2:1230:CLA:HMB2	2.44	0.47
11:2:1238:CLA:H193	14:6:4018:BCR:H362	1.95	0.47
14:2:4006:BCR:H15C	14:2:4006:BCR:H351	1.72	0.47
14:2:4017:BCR:H15C	14:2:4017:BCR:H351	1.65	0.47
11:A:1137:CLA:HMB1	11:A:1137:CLA:HBB1	1.96	0.47
1:A:195:SER:O	1:A:199:HIS:ND1	2.44	0.47
11:B:1205:CLA:HAB	11:B:1206:CLA:HAA2	1.97	0.47
11:2:1013:CLA:CGA	11:2:1013:CLA:H3A	2.44	0.47
11:2:1223:CLA:HBB1	11:2:1231:CLA:HMA2	1.96	0.47
12:A:2001:PQN:C24	11:B:1013:CLA:H202	2.91	0.47
2:B:312:LEU:HD22	15:B:5004:LHG:HC42	2.17	0.47
8:7:26:SER:HB3	14:7:4021:BCR:HC41	1.97	0.47
11:A:1112:CLA:HBB1	11:A:1112:CLA:HHC	2.16	0.47
11:A:1136:CLA:HHC	11:A:1136:CLA:CBB	2.44	0.47
14:A:4007:BCR:HC41	11:A:1119:CLA:C19	2.45	0.47
11:B:1201:CLA:HAB	11:B:1203:CLA:CAD	2.84	0.47
11:2:1231:CLA:NC	11:2:1232:CLA:HAB	2.30	0.46
11:A:1114:CLA:CBB	11:A:1114:CLA:HHC	2.45	0.46
11:A:1133:CLA:HHC	11:A:1133:CLA:HBB1	4.19	0.46
11:1:1115:CLA:CBB	11:1:1115:CLA:HHC	2.45	0.46
11:2:1212:CLA:HAB	11:2:1211:CLA:CMC	2.45	0.46
11:A:1011:CLA:HBB1	11:A:1011:CLA:HMB1	1.97	0.46
1:A:589:ASP:OD1	1:A:724:ARG:NH1	2.55	0.46
11:A:1012:CLA:HMB3	11:B:1021:CLA:H203	1.96	0.46
11:B:1217:CLA:HBB1	11:B:1217:CLA:HHC	4.00	0.46
2:B:668:TRP:CZ2	12:B:2002:PQN:H2M3	2.50	0.46
11:1:1112:CLA:HBB1	11:1:1112:CLA:HHC	1.97	0.46
14:A:4001:BCR:H15C	14:A:4001:BCR:H351	1.54	0.46
2:B:642:VAL:HG22	11:B:1206:CLA:HHD	1.97	0.46
10:0:90:LEU:CB	10:0:91:PRO:CD	2.93	0.46
1:1:210:LEU:HB2	1:1:301:ALA:HB1	1.98	0.46
1:1:693:TRP:CZ2	12:1:2001:PQN:H2M3	2.50	0.46
14:F:4018:BCR:H14C	9:I:23:PRO:HG2	1.96	0.46
1:1:342:GLU:OE1	1:1:342:GLU:N	2.45	0.46
14:1:4001:BCR:H24C	10:0:110:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4014:BCR:H15C	14:2:4014:BCR:H351	1.65	0.46
11:A:1138:CLA:HHC	11:A:1138:CLA:CBB	2.44	0.46
2:B:668:TRP:CH2	12:B:2002:PQN:H2M3	2.50	0.46
2:2:5:PHE:HB2	9:9:34:ILE:HA	1.98	0.46
11:1:1105:CLA:C2	14:6:4013:BCR:H342	2.46	0.46
1:A:330:GLY:N	15:A:5003:LHG:HC2	2.52	0.46
2:B:211:ASN:O	2:B:214:SER:OG	2.29	0.46
11:A:1125:CLA:HBC2	11:A:1125:CLA:HHD	1.99	0.46
14:B:4010:BCR:H332	11:B:1223:CLA:HED2	1.97	0.46
2:B:582:ASN:ND2	2:B:586:TRP:CZ2	2.83	0.46
11:B:1023:CLA:H193	14:F:4018:BCR:H19C	1.97	0.46
14:F:4020:BCR:HC42	7:L:87:ALA:HB1	1.96	0.46
11:A:1101:CLA:H8	11:A:1101:CLA:H52	2.75	0.46
1:A:369:HIS:ND1	11:A:1116:CLA:OBD	2.67	0.46
14:A:4003:BCR:C23	14:A:4003:BCR:H403	2.43	0.46
1:1:356:LEU:HD11	11:1:1128:CLA:CBB	2.46	0.46
11:8:1503:CLA:HMB1	11:8:1503:CLA:HBB1	1.97	0.46
11:1:1117:CLA:HAB	11:1:1117:CLA:H111	1.97	0.46
9:9:31:PHE:HB2	14:8:4019:BCR:H14C	1.97	0.46
14:B:4009:BCR:H23C	11:B:1227:CLA:HBC1	1.99	0.46
2:B:117:TYR:HA	2:B:365:THR:HG22	2.09	0.46
14:F:4018:BCR:H24C	14:F:4018:BCR:H371	1.65	0.46
11:1:1101:CLA:HAB	11:1:1102:CLA:C2C	2.46	0.45
14:6:4013:BCR:H351	14:6:4013:BCR:H15C	1.62	0.45
11:A:1012:CLA:H43	14:B:4011:BCR:H362	1.97	0.45
11:A:1125:CLA:HAB	11:A:1133:CLA:HMA2	1.98	0.45
11:B:1210:CLA:HBB1	11:B:1210:CLA:HHC	2.09	0.45
10:K:62:ILE:HD12	11:K:1402:CLA:HMA1	1.98	0.45
11:1:1134:CLA:HBB1	11:1:1134:CLA:HHC	1.97	0.45
1:1:721:ILE:HG21	15:1:5001:LHG:HC42	1.97	0.45
2:2:668:TRP:CH2	12:2:2002:PQN:H2M3	2.51	0.45
1:A:79:HIS:CD2	11:A:1103:CLA:HMA1	2.82	0.45
1:A:53:ALA:HB2	15:A:5001:LHG:HC82	1.98	0.45
2:B:434:LEU:HD23	11:B:1230:CLA:HBB1	1.97	0.45
11:1:1237:CLA:HBA1	11:1:1237:CLA:CHA	2.45	0.45
11:A:1103:CLA:H51	11:A:1111:CLA:C1	2.94	0.45
11:A:1107:CLA:HAB	11:B:1230:CLA:HMD2	1.98	0.45
2:B:435:TYR:CE2	2:B:515:LEU:HB3	2.52	0.45
11:A:1117:CLA:H111	11:A:1117:CLA:HAB	3.44	0.45
11:A:1131:CLA:HAB	11:A:1132:CLA:HBB	1.98	0.45
2:B:519:ALA:HB1	11:B:1021:CLA:C19	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4017:BCR:H331	14:2:4017:BCR:HC8	1.99	0.45
14:A:4003:BCR:H402	14:A:4003:BCR:H23C	2.28	0.45
11:A:1102:CLA:HMA2	11:A:1109:CLA:HMD2	1.99	0.45
1:A:193:VAL:HG13	11:A:1123:CLA:HHD	1.98	0.45
11:A:1104:CLA:H3A	11:A:1128:CLA:HAB	1.99	0.45
11:B:1231:CLA:HHC	11:B:1231:CLA:HBB1	1.99	0.45
8:M:5:ASP:OD1	9:I:7:ALA:N	3.55	0.45
1:1:203:GLY:HA2	11:1:1118:CLA:HBC1	1.97	0.45
1:1:395:TRP:NE1	11:1:1126:CLA:HAB	2.32	0.45
1:A:79:HIS:CG	11:A:1103:CLA:HMA1	2.91	0.45
11:B:1222:CLA:HMB1	11:B:1223:CLA:H202	1.98	0.45
2:B:7:LYS:NZ	8:M:30:TYR:O	2.48	0.45
11:1:1101:CLA:H201	11:1:1012:CLA:H203	1.99	0.45
14:1:4008:BCR:H331	14:1:4008:BCR:HC8	1.98	0.45
2:2:130:THR:OG1	2:2:201:GLU:OE1	2.34	0.45
2:2:5:PHE:HB3	2:2:20:ARG:NH1	2.32	0.45
14:2:4017:BCR:H371	14:2:4017:BCR:H24C	1.78	0.45
2:2:487:GLY:O	2:2:489:ALA:N	2.50	0.45
1:A:721:ILE:HG21	15:A:5001:LHG:HC42	1.99	0.45
15:A:5003:LHG:H301	15:A:5003:LHG:H171	3.08	0.45
1:A:737:VAL:HG22	14:B:4011:BCR:H321	1.99	0.45
12:A:2001:PQN:H251	11:B:1013:CLA:H202	1.99	0.45
11:B:1215:CLA:CGA	11:B:1215:CLA:H3A	2.46	0.45
11:B:1228:CLA:CBB	11:B:1228:CLA:HHC	3.51	0.45
7:L:17:VAL:O	7:L:19:HIS:N	2.49	0.45
14:1:4007:BCR:C34	11:1:1123:CLA:HAB	2.45	0.45
14:6:4018:BCR:H351	14:6:4018:BCR:H15C	1.62	0.45
14:A:4003:BCR:H351	14:A:4003:BCR:H15C	1.64	0.45
1:A:681:PHE:N	11:B:1013:CLA:HAB	2.42	0.45
14:2:4009:BCR:H321	14:2:4009:BCR:HC8	1.99	0.45
14:2:4011:BCR:H15C	14:2:4011:BCR:H351	1.77	0.45
11:8:1501:CLA:HBB1	11:8:1501:CLA:HHC	1.98	0.45
11:A:1137:CLA:HAB	11:A:1129:CLA:HBB2	1.97	0.45
11:L:1501:CLA:H202	11:L:1503:CLA:H2	2.31	0.44
1:1:59:ASP:N	1:1:59:ASP:OD1	2.50	0.44
11:A:1105:CLA:HHC	11:A:1105:CLA:CBB	2.84	0.44
14:L:4019:BCR:H331	14:L:4019:BCR:HC7	1.58	0.44
11:L:1501:CLA:CBA	14:L:4022:BCR:H363	2.46	0.44
4:4:3:GLU:HB3	4:4:4:LEU:H	1.61	0.44
1:A:59:ASP:N	1:A:59:ASP:OD1	2.49	0.44
2:B:25:ILE:HG12	14:L:4019:BCR:HC41	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:4005:BCR:H351	14:2:4005:BCR:H15C	1.77	0.44
1:A:100:TYR:HA	1:A:144:PHE:CE2	2.53	0.44
11:A:1102:CLA:H203	11:A:1106:CLA:C14	2.48	0.44
11:B:1212:CLA:CBB	11:B:1212:CLA:HHC	3.15	0.44
14:B:4005:BCR:H351	14:B:4005:BCR:H15C	1.64	0.44
14:1:4007:BCR:H15C	14:1:4007:BCR:H351	1.56	0.44
11:2:1240:CLA:HHC	11:2:1240:CLA:CBB	2.47	0.44
5:5:13:ARG:O	5:5:14:THR:HB	2.18	0.44
6:6:49:ILE:CB	6:6:50:PRO:HD3	2.47	0.44
1:A:680:ALA:C	11:B:1013:CLA:HAB	2.74	0.44
14:B:4006:BCR:H351	14:B:4006:BCR:H15C	1.61	0.44
9:I:10:LEU:HB2	9:I:11:PRO:HD3	2.02	0.44
11:2:1023:CLA:CGA	11:2:1023:CLA:H3A	2.47	0.44
11:A:1104:CLA:HBB	11:A:1128:CLA:HAB	1.99	0.44
1:A:203:GLY:HA2	11:A:1118:CLA:HBC1	1.98	0.44
11:B:1238:CLA:C1	14:L:4019:BCR:H363	2.69	0.44
2:2:312:LEU:HB2	15:2:5004:LHG:HC42	1.99	0.44
8:7:9:LEU:HD12	14:7:4021:BCR:H401	1.99	0.44
11:8:1501:CLA:H43	14:8:4022:BCR:H14C	1.99	0.44
11:A:1127:CLA:HMD2	11:A:1127:CLA:H71	2.00	0.44
2:B:338:SER:HB3	11:B:1221:CLA:H42	2.26	0.44
2:2:582:ASN:ND2	2:2:586:TRP:CZ2	2.86	0.44
11:A:1102:CLA:H142	11:A:1107:CLA:H202	2.00	0.44
1:A:356:LEU:HD11	11:A:1128:CLA:CBB	2.63	0.44
6:F:11:ALA:N	6:F:12:PRO:HD2	2.33	0.44
11:A:1104:CLA:HHD	11:A:1104:CLA:HBC3	2.00	0.44
11:A:1108:CLA:HBB1	11:A:1108:CLA:HHC	4.41	0.44
1:A:226:LEU:HD21	1:A:252:LEU:HD11	2.00	0.44
3:C:17:CYS:HB2	3:C:54:CYS:HB3	2.80	0.44
14:F:4018:BCR:H351	14:F:4018:BCR:H15C	1.63	0.44
6:F:49:ILE:CB	6:F:50:PRO:HD3	3.38	0.44
1:1:728:VAL:CG1	15:1:5001:LHG:H301	2.47	0.43
11:2:1205:CLA:CHA	11:2:1205:CLA:CGA	2.96	0.43
11:2:1210:CLA:H203	11:2:1225:CLA:C3D	2.48	0.43
14:A:4003:BCR:H23C	11:A:1103:CLA:H72	2.00	0.43
14:A:4001:BCR:H14C	11:A:1118:CLA:HBB1	2.75	0.43
1:A:440:LEU:HD23	1:A:547:LEU:HA	2.09	0.43
12:B:2002:PQN:H291	14:L:4019:BCR:HC8	3.20	0.43
14:F:4018:BCR:H14C	9:I:23:PRO:CB	2.48	0.43
1:1:500:ASN:ND2	11:1:1115:CLA:OBD	2.51	0.43
14:6:4020:BCR:H15C	14:6:4020:BCR:H351	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:8:17:VAL:O	7:8:19:HIS:N	2.48	0.43
11:A:1115:CLA:HBB1	11:A:1115:CLA:HHC	2.00	0.43
11:A:1133:CLA:CBB	11:A:1133:CLA:HHC	3.68	0.43
2:B:77:TRP:HA	2:B:84:ILE:HG21	2.00	0.43
11:1:1128:CLA:H201	11:1:1140:CLA:H2	2.00	0.43
11:A:1107:CLA:CBA	11:A:1107:CLA:HBD	2.66	0.43
11:A:1136:CLA:C1A	11:A:1136:CLA:CGA	2.96	0.43
1:A:354:ILE:CD1	14:A:4007:BCR:HC7	2.42	0.43
11:B:1238:CLA:H193	14:F:4018:BCR:H362	2.00	0.43
2:B:385:PHE:CZ	14:B:4010:BCR:H373	2.87	0.43
8:M:19:ALA:HB2	14:M:4021:BCR:H15C	2.26	0.43
14:1:4003:BCR:H371	11:1:1127:CLA:H62	2.01	0.43
11:1:1126:CLA:C4C	14:2:4011:BCR:HC42	2.48	0.43
14:A:4002:BCR:C14	11:A:1112:CLA:HBB1	2.48	0.43
1:A:342:GLU:N	1:A:342:GLU:OE1	2.55	0.43
11:B:1201:CLA:HHC	11:B:1203:CLA:OBD	2.45	0.43
2:B:412:HIS:O	2:B:412:HIS:ND1	2.52	0.43
11:A:1118:CLA:H3A	10:K:105:LEU:HD12	2.01	0.43
2:2:273:ILE:O	2:2:277:HIS:ND1	2.50	0.43
9:9:10:LEU:HB2	9:9:11:PRO:HD3	2.01	0.43
1:A:296:HIS:HE1	11:A:1117:CLA:C2B	2.31	0.43
11:B:1207:CLA:CBB	11:B:1207:CLA:HHC	2.71	0.43
4:D:98:HIS:CG	4:D:99:PRO:CD	3.01	0.43
11:B:1204:CLA:H92	14:M:4021:BCR:C14	2.48	0.43
11:1:1119:CLA:HMB1	11:1:1123:CLA:HED2	1.99	0.43
11:2:1207:CLA:HHC	11:2:1207:CLA:CBB	2.48	0.43
11:A:1125:CLA:CBB	11:A:1125:CLA:HHC	3.66	0.43
2:B:5:PHE:HB3	2:B:20:ARG:NH1	2.36	0.43
14:F:4020:BCR:H333	7:L:87:ALA:CB	3.07	0.43
11:A:1119:CLA:OBD	11:A:1121:CLA:HHD	2.41	0.43
11:A:1801:CLA:CHC	15:A:5003:LHG:HC31	2.85	0.43
11:B:1223:CLA:HBD	11:B:1223:CLA:HAA2	2.13	0.43
11:A:1237:CLA:HHD	14:B:4017:BCR:H383	2.00	0.43
1:A:210:LEU:HD11	14:A:4001:BCR:HC8	2.01	0.43
11:2:1239:CLA:HBB1	11:2:1239:CLA:HHC	2.00	0.43
1:A:550:LEU:HD11	11:A:1119:CLA:H202	3.41	0.43
1:A:303:LEU:HD22	11:A:1119:CLA:HMC1	2.01	0.43
11:A:1237:CLA:CBB	11:A:1237:CLA:HHC	2.48	0.43
1:A:330:GLY:HA3	15:A:5003:LHG:HC2	2.69	0.43
1:1:571:ARG:NE	15:1:5001:LHG:O5	2.51	0.43
1:A:564:ASP:N	1:A:564:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:LEU:N	2:B:492:PRO:CD	2.83	0.43
15:1:5001:LHG:C20	11:1:1128:CLA:H202	2.47	0.42
11:A:1104:CLA:HAB	11:A:1127:CLA:HMC2	2.69	0.42
1:A:261:THR:O	1:A:265:THR:N	2.48	0.42
1:A:269:GLY:HA3	10:K:51:PRO:HG3	2.01	0.42
14:A:4002:BCR:HC41	11:A:1103:CLA:H142	2.01	0.42
2:B:642:VAL:CG2	11:B:1206:CLA:HHD	2.49	0.42
11:2:1021:CLA:HBA1	11:2:1021:CLA:H3A	1.78	0.42
14:8:4022:BCR:H15C	14:8:4022:BCR:H351	1.66	0.42
1:A:312:ARG:NH2	1:A:316:GLY:O	2.52	0.42
11:B:1021:CLA:H3A	11:B:1021:CLA:HBA2	1.91	0.42
12:B:2002:PQN:H291	14:L:4019:BCR:H342	2.00	0.42
2:B:294:ASN:OD1	2:B:294:ASN:N	2.52	0.42
11:1:1103:CLA:H3A	11:1:1103:CLA:CGA	2.49	0.42
1:1:263:PHE:CZ	14:1:4001:BCR:H343	2.54	0.42
2:2:656:THR:HA	11:2:1023:CLA:HAB	2.01	0.42
11:2:1206:CLA:CMB	11:2:1207:CLA:C1C	2.97	0.42
5:E:13:ARG:O	5:E:14:THR:HB	2.18	0.42
10:0:110:PHE:HA	10:0:113:ILE:HG22	2.00	0.42
11:1:1134:CLA:O1A	11:0:1401:CLA:O1D	2.36	0.42
11:2:1207:CLA:H2A	11:2:1207:CLA:O2A	2.20	0.42
11:A:1801:CLA:NC	15:A:5003:LHG:HC31	2.93	0.42
10:K:120:LEU:HD13	11:K:1401:CLA:C1	2.97	0.42
11:2:1208:CLA:HHC	11:2:1208:CLA:CBB	2.50	0.42
2:2:177:HIS:CG	11:2:1210:CLA:HMC2	2.54	0.42
2:2:412:HIS:O	2:2:412:HIS:ND1	2.53	0.42
2:2:77:TRP:HA	2:2:84:ILE:HG21	2.01	0.42
14:8:4022:BCR:H371	14:8:4022:BCR:H24C	1.78	0.42
6:F:6:SER:O	6:F:10:THR:N	3.91	0.42
1:1:260:LEU:O	1:1:261:THR:OG1	2.31	0.42
11:2:1202:CLA:H141	11:2:1202:CLA:C17	2.49	0.42
2:2:385:PHE:CE2	14:2:4010:BCR:H373	2.55	0.42
2:2:435:TYR:CE2	2:2:515:LEU:HB3	2.55	0.42
4:4:77:LYS:HB2	4:4:78:PRO:HD3	2.00	0.42
11:B:1209:CLA:HHC	11:B:1209:CLA:CBB	2.57	0.42
14:B:4010:BCR:C20	11:B:1223:CLA:H91	3.84	0.42
1:1:262:PRO:O	1:1:267:ASN:N	2.49	0.42
1:1:305:ILE:O	1:1:309:HIS:ND1	2.53	0.42
2:2:294:ASN:N	2:2:294:ASN:OD1	2.52	0.42
2:2:642:VAL:HG12	2:2:643:TRP:N	2.35	0.42
1:A:211:GLY:HA2	14:A:4002:BCR:H363	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LEU:HB3	11:B:1229:CLA:CED	2.48	0.42
2:B:167:TRP:CZ2	11:B:1208:CLA:HMA1	2.54	0.42
2:B:178:HIS:ND1	11:B:1221:CLA:O1D	2.53	0.42
14:B:4010:BCR:H351	14:B:4010:BCR:H15C	1.62	0.42
4:D:27:LYS:HG3	4:D:88:VAL:HG13	2.02	0.42
11:2:1207:CLA:HBB1	11:2:1207:CLA:HHC	2.01	0.42
1:A:395:TRP:HE1	11:A:1126:CLA:HAB	1.85	0.42
1:A:467:PRO:HA	1:A:470:MET:HG2	2.02	0.42
14:B:4010:BCR:HC21	11:B:1223:CLA:CMA	2.49	0.42
7:L:100:GLY:HA3	7:L:120:TRP:CD1	2.55	0.42
1:1:211:GLY:CA	14:1:4002:BCR:H363	2.50	0.42
1:1:681:PHE:CA	11:2:1013:CLA:HAB	2.49	0.42
11:2:1202:CLA:H142	11:2:1202:CLA:CAD	2.49	0.42
2:2:341:VAL:HG13	11:2:1222:CLA:HED1	2.01	0.42
4:4:98:HIS:CG	4:4:99:PRO:CD	3.03	0.42
11:1:1237:CLA:C10	14:8:4019:BCR:H361	2.50	0.42
11:A:1011:CLA:HBA2	11:A:1011:CLA:H3A	1.89	0.42
1:A:226:LEU:HD12	1:A:236:ILE:HG23	2.01	0.42
14:A:4003:BCR:C40	14:A:4003:BCR:C23	2.98	0.42
11:B:1201:CLA:HAC1	14:L:4019:BCR:HC32	2.01	0.42
14:B:4010:BCR:H332	11:B:1223:CLA:CED	2.50	0.42
2:B:212:PHE:CB	11:B:1211:CLA:HMD3	2.50	0.42
14:L:4019:BCR:HC8	14:L:4019:BCR:C32	2.46	0.42
11:1:1130:CLA:HHC	11:1:1130:CLA:CBB	2.50	0.42
11:2:1238:CLA:CBB	11:2:1238:CLA:HHC	2.49	0.42
11:A:1108:CLA:CBB	11:A:1108:CLA:HHC	3.89	0.42
11:B:1205:CLA:HAB	11:B:1206:CLA:O1A	3.77	0.42
2:B:189:ALA:HA	11:B:1212:CLA:HAB	2.02	0.42
11:A:1801:CLA:HBC2	11:A:1801:CLA:HMC1	2.00	0.41
11:B:1209:CLA:HHC	11:B:1209:CLA:HBB1	2.16	0.41
14:L:4022:BCR:H351	14:L:4022:BCR:H15C	1.75	0.41
14:F:4020:BCR:H351	14:F:4020:BCR:H15C	1.83	0.41
10:K:124:SER:O	10:K:125:SER:C	2.84	0.41
1:1:319:HIS:HB3	1:1:324:ILE:HD11	2.02	0.41
11:A:1118:CLA:H3A	10:K:105:LEU:CD1	2.50	0.41
1:A:262:PRO:O	1:A:267:ASN:N	2.58	0.41
11:A:1801:CLA:C2C	15:A:5003:LHG:HC31	2.51	0.41
11:1:1110:CLA:HAB	11:1:1118:CLA:H61	2.02	0.41
14:1:4007:BCR:H363	11:1:1122:CLA:H143	2.01	0.41
11:1:1106:CLA:H91	11:1:1128:CLA:H203	2.01	0.41
12:A:2001:PQN:H201	11:A:1101:CLA:H12	2.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1103:CLA:HBB1	11:A:1104:CLA:HBA1	4.61	0.41
11:A:1119:CLA:HMB2	11:A:1123:CLA:HMA3	2.02	0.41
1:A:305:ILE:O	1:A:309:HIS:ND1	2.55	0.41
1:A:681:PHE:HA	11:B:1013:CLA:CAB	2.58	0.41
11:B:1222:CLA:CAD	11:B:1234:CLA:HBB1	2.49	0.41
2:B:123:TRP:HA	2:B:356:TYR:CD1	2.56	0.41
9:I:15:ILE:HB	9:I:16:PRO:HD3	2.03	0.41
14:L:4019:BCR:C8	14:L:4019:BCR:H321	2.43	0.41
2:2:571:ASP:OD1	2:2:703:ARG:NH2	2.52	0.41
4:4:82:ASP:N	4:4:82:ASP:OD1	2.52	0.41
1:A:58:PHE:CD2	11:A:1103:CLA:HMC2	2.55	0.41
11:A:1138:CLA:C1A	11:A:1138:CLA:CGA	3.05	0.41
1:A:332:PHE:O	1:A:428:ARG:NH2	2.69	0.41
2:B:312:LEU:HB2	15:B:5004:LHG:HC42	2.21	0.41
1:1:721:ILE:CG2	15:1:5001:LHG:HC42	2.50	0.41
14:2:4004:BCR:H15C	14:2:4004:BCR:H351	1.67	0.41
2:2:491:LEU:N	2:2:492:PRO:CD	2.84	0.41
8:7:19:ALA:HB2	14:7:4021:BCR:C15	2.50	0.41
14:B:4005:BCR:H343	11:B:1209:CLA:HMC3	2.02	0.41
11:1:1137:CLA:HBB1	11:1:1137:CLA:HMB1	2.01	0.41
11:2:1201:CLA:HMB2	14:7:4021:BCR:H333	2.01	0.41
14:B:4010:BCR:C20	11:B:1223:CLA:C9	3.57	0.41
2:B:494:TRP:CE2	11:B:1231:CLA:HED2	3.33	0.41
4:D:77:LYS:HB2	4:D:78:PRO:HD3	2.02	0.41
10:K:73:VAL:HG13	10:K:74:ILE:N	2.36	0.41
2:2:60:TRP:HA	11:2:1204:CLA:HBB2	2.02	0.41
14:2:4014:BCR:HC41	11:2:1229:CLA:HBB2	2.02	0.41
14:2:4017:BCR:H352	11:2:1239:CLA:HBA2	2.03	0.41
11:A:1137:CLA:HAB	11:A:1129:CLA:HBB1	2.01	0.41
11:B:1220:CLA:HHB	11:B:1240:CLA:HAB	2.93	0.41
10:K:120:LEU:CD1	11:K:1401:CLA:H11	2.97	0.41
1:1:453:GLY:C	11:1:1132:CLA:HAB	2.41	0.41
1:1:53:ALA:HB2	15:1:5001:LHG:HC91	2.03	0.41
2:2:154:TRP:CD1	8:7:28:GLU:HG3	2.56	0.41
11:2:1238:CLA:C19	14:6:4018:BCR:H362	2.51	0.41
11:A:1103:CLA:H111	11:A:1103:CLA:H71	2.20	0.41
11:A:1119:CLA:CBB	11:A:1119:CLA:HHC	2.73	0.41
1:A:310:MET:O	1:A:319:HIS:N	2.72	0.41
14:A:4007:BCR:H341	11:A:1123:CLA:HAB	3.30	0.41
2:B:645:TRP:CZ3	14:B:4017:BCR:HC21	2.56	0.41
2:B:413:LYS:NZ	2:B:537:ASP:OD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:310:MET:O	1:1:319:HIS:N	2.54	0.41
11:2:1202:CLA:H141	11:2:1202:CLA:H171	2.03	0.41
2:2:329:HIS:CE1	2:2:390:ILE:HG21	2.56	0.41
2:2:520:ILE:HG21	11:2:1234:CLA:HAB	2.03	0.41
11:A:1121:CLA:HHC	11:A:1121:CLA:CBB	2.53	0.41
1:A:575:ASP:OD2	1:A:579:ARG:NH1	2.53	0.41
14:B:4005:BCR:HC7	11:B:1209:CLA:CMC	2.47	0.41
11:1:1801:CLA:CMA	15:1:5003:LHG:HC62	2.51	0.41
11:2:1239:CLA:HHC	11:2:1239:CLA:CBB	2.51	0.41
11:A:1107:CLA:HBA1	11:A:1107:CLA:HBD	2.04	0.41
1:A:260:LEU:O	1:A:261:THR:OG1	2.32	0.41
11:B:1229:CLA:CAB	11:B:1230:CLA:HMB2	2.58	0.41
11:1:1106:CLA:CBB	11:1:1106:CLA:HHC	2.49	0.40
11:1:1107:CLA:C1	14:6:4013:BCR:H14C	2.51	0.40
11:1:1012:CLA:CHB	11:2:1021:CLA:H203	2.51	0.40
11:1:1022:CLA:H203	11:2:1206:CLA:H62	2.03	0.40
14:6:4018:BCR:H14C	9:9:23:PRO:HG2	2.00	0.40
1:A:154:ASP:OD1	1:A:155:SER:N	2.55	0.40
11:B:1207:CLA:O2A	11:B:1207:CLA:H2A	2.20	0.40
1:1:197:MET:HE3	11:1:1119:CLA:HMB3	2.02	0.40
14:2:4010:BCR:HC21	11:2:1223:CLA:CMA	2.51	0.40
2:2:476:LEU:HD12	11:2:1231:CLA:HED3	2.03	0.40
5:5:11:ILE:N	5:5:11:ILE:HD12	2.36	0.40
11:A:1112:CLA:HBC2	11:A:1112:CLA:HHH	2.03	0.40
1:A:539:ALA:HB1	11:A:1136:CLA:HMB3	2.03	0.40
1:A:684:MET:HE2	1:A:693:TRP:CZ2	2.56	0.40
2:B:19:ARG:HG2	2:B:23:TYR:CD1	2.56	0.40
2:B:656:THR:HA	11:B:1023:CLA:CAB	2.46	0.40
4:D:10:LYS:HG3	4:D:49:ILE:HD11	2.03	0.40
7:L:56:ALA:HA	14:L:4022:BCR:H15C	2.03	0.40
11:1:1111:CLA:CGA	11:1:1111:CLA:H3A	2.51	0.40
11:1:1801:CLA:H3A	11:1:1801:CLA:HBA2	1.93	0.40
11:2:1231:CLA:C4C	11:2:1232:CLA:CAB	2.99	0.40
11:A:1103:CLA:NC	11:A:1128:CLA:HMB3	2.51	0.40
1:A:451:SER:OG	1:A:452:PHE:N	2.55	0.40
11:B:1223:CLA:H111	11:B:1223:CLA:H93	3.77	0.40
11:K:1402:CLA:C1A	11:K:1402:CLA:CGA	3.00	0.40
11:K:1402:CLA:CBB	11:K:1402:CLA:HHC	2.49	0.40
11:1:1134:CLA:CBB	11:1:1134:CLA:HHC	2.50	0.40
1:1:728:VAL:HG13	15:1:5001:LHG:H301	2.04	0.40
2:2:29:HIS:ND1	11:2:1203:CLA:O1A	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:654:TRP:CH2	2:2:658:PHE:CZ	3.10	0.40
1:A:684:MET:HE2	12:A:2001:PQN:H2M3	2.03	0.40
11:B:1219:CLA:C1A	11:B:1219:CLA:CGA	4.44	0.40
2:B:223:MET:SD	2:B:223:MET:N	2.94	0.40
1:A:441:ASN:ND2	2:B:675:ILE:HG12	2.36	0.40
3:C:17:CYS:SG	3:C:18:VAL:N	3.19	0.40
2:2:475:LEU:HD13	11:2:1231:CLA:HHD	2.03	0.40
11:A:1011:CLA:HMB3	11:A:1012:CLA:HMD1	2.03	0.40
1:A:395:TRP:HD1	11:A:1126:CLA:HAB	1.79	0.40
11:A:1801:CLA:HBB1	11:A:1121:CLA:CAB	3.73	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 X-ray entries followed by that with respect to entries of similar resolution.

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	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	44	81
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	44	81
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	44	81
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	18	61
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	22	65
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	22	65
3	3	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	121 (89%)	14 (10%)	1 (1%)	25	68
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	25	68
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	25	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	12	53
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	12	53
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	12	53
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	11	52
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	7	45
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	11	52
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	14	56
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	9	49
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	14	56
8	7	29/31 (94%)	29 (100%)	0	0	100	100
8	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
8	m	29/31 (94%)	29 (100%)	0	0	100	100
9	9	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	i	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
10	0	78/128 (61%)	65 (83%)	9 (12%)	4 (5%)	2	29
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	1	25
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	4	36
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	20	62

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
2	B	6	PRO
4	D	99	PRO
6	F	43	CYS
1	a	261	THR
2	b	6	PRO
4	d	99	PRO
1	1	261	THR
2	2	6	PRO
4	4	99	PRO
6	6	42	SER
10	K	92	GLN
10	K	125	SER

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Mol	Chain	Res	Type
10	k	92	GLN
10	0	92	GLN
2	B	488	ALA
2	B	489	ALA
5	E	14	THR
7	L	108	GLN
2	b	488	ALA
5	e	14	THR
6	f	42	SER
2	2	488	ALA
2	2	489	ALA
5	5	14	THR
7	8	108	GLN
10	K	90	LEU
10	k	90	LEU
10	0	90	LEU
10	0	126	GLY
2	B	556	CYS
6	F	31	ALA
2	b	489	ALA
2	b	556	CYS
7	l	108	GLN
2	2	314	GLY
2	2	487	GLY
2	2	556	CYS
1	A	115	GLN
2	B	314	GLY
2	B	487	GLY
7	L	109	GLY
1	a	115	GLN
2	b	487	GLY
6	f	31	ALA
1	1	115	GLN
6	6	31	ALA
10	k	51	PRO
6	F	50	PRO
2	2	235	ALA
2	b	314	GLY
7	l	109	GLY
7	8	109	GLY
10	K	51	PRO
10	K	87	ASP

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Mol	Chain	Res	Type
10	0	51	PRO
7	L	18	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	1	588/603 (98%)	573 (97%)	15 (3%)	51	78
1	A	588/603 (98%)	570 (97%)	18 (3%)	45	75
1	a	588/603 (98%)	573 (97%)	15 (3%)	51	78
2	2	582/583 (100%)	565 (97%)	17 (3%)	48	76
2	B	582/583 (100%)	562 (97%)	20 (3%)	42	73
2	b	582/583 (100%)	566 (97%)	16 (3%)	50	77
3	3	68/69 (99%)	65 (96%)	3 (4%)	33	68
3	C	68/69 (99%)	61 (90%)	7 (10%)	8	38
3	c	68/69 (99%)	64 (94%)	4 (6%)	23	60
4	4	113/116 (97%)	109 (96%)	4 (4%)	41	73
4	D	113/116 (97%)	111 (98%)	2 (2%)	64	85
4	d	113/116 (97%)	110 (97%)	3 (3%)	50	77
5	5	56/60 (93%)	54 (96%)	2 (4%)	40	72
5	E	56/60 (93%)	54 (96%)	2 (4%)	40	72
5	e	56/60 (93%)	54 (96%)	2 (4%)	40	72
6	6	21/106 (20%)	20 (95%)	1 (5%)	30	66
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	30	66
7	8	113/118 (96%)	113 (100%)	0	100	100
7	L	113/118 (96%)	112 (99%)	1 (1%)	82	92
7	l	113/118 (96%)	112 (99%)	1 (1%)	82	92
8	7	24/25 (96%)	23 (96%)	1 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	M	24/25 (96%)	23 (96%)	1 (4%)	34	68
8	m	24/25 (96%)	23 (96%)	1 (4%)	34	68
9	9	31/32 (97%)	28 (90%)	3 (10%)	9	40
9	I	31/32 (97%)	27 (87%)	4 (13%)	5	29
9	i	31/32 (97%)	27 (87%)	4 (13%)	5	29
10	0	37/100 (37%)	30 (81%)	7 (19%)	2	13
10	K	37/100 (37%)	30 (81%)	7 (19%)	2	13
10	k	37/100 (37%)	31 (84%)	6 (16%)	3	20
All	All	4897/5436 (90%)	4729 (97%)	168 (3%)	42	73

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	104	LEU
1	A	224	ASN
1	A	235	ASP
1	A	245	GLU
1	A	249	MET
1	A	303	LEU
1	A	323	GLU
1	A	356	LEU
1	A	368	GLN
1	A	459	ASP
1	A	462	ARG
1	A	477	GLN
1	A	478	LEU
1	A	562	VAL
1	A	631	THR
1	A	739	THR
1	A	748	LEU
2	B	145	LEU
2	B	196	HIS
2	B	229	ASN
2	B	236	ASP
2	B	257	PHE
2	B	302	LYS
2	B	304	ILE
2	B	318	THR

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Mol	Chain	Res	Type
2	B	334	LEU
2	B	351	TYR
2	B	395	ASP
2	B	406	LEU
2	B	420	LEU
2	B	439	ASP
2	B	516	VAL
2	B	542	LYS
2	B	573	PHE
2	B	580	MET
2	B	681	ARG
2	B	689	ARG
3	C	3	HIS
3	C	11	CYS
3	C	19	ARG
3	C	21	CYS
3	C	54	CYS
3	C	58	CYS
3	C	69	LEU
4	D	73	ARG
4	D	82	ASP
5	E	33	ILE
5	E	43	ARG
7	L	96	LEU
8	M	5	ASP
1	a	59	ASP
1	a	104	LEU
1	a	224	ASN
1	a	235	ASP
1	a	249	MET
1	a	303	LEU
1	a	323	GLU
1	a	368	GLN
1	a	459	ASP
1	a	477	GLN
1	a	478	LEU
1	a	562	VAL
1	a	631	THR
1	a	739	THR
1	a	748	LEU
2	b	76	GLN
2	b	145	LEU

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Mol	Chain	Res	Type
2	b	196	HIS
2	b	229	ASN
2	b	236	ASP
2	b	257	PHE
2	b	302	LYS
2	b	304	ILE
2	b	318	THR
2	b	334	LEU
2	b	406	LEU
2	b	420	LEU
2	b	516	VAL
2	b	542	LYS
2	b	573	PHE
2	b	689	ARG
3	c	21	CYS
3	c	58	CYS
3	c	66	ARG
3	c	69	LEU
4	d	73	ARG
4	d	82	ASP
4	d	107	LYS
5	e	33	ILE
5	e	43	ARG
6	f	38	PHE
9	i	1	MET
9	i	17	MET
9	i	21	LEU
9	i	30	LEU
7	l	137	VAL
8	m	5	ASP
1	1	59	ASP
1	1	104	LEU
1	1	224	ASN
1	1	235	ASP
1	1	249	MET
1	1	303	LEU
1	1	323	GLU
1	1	368	GLN
1	1	462	ARG
1	1	477	GLN
1	1	478	LEU
1	1	562	VAL

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Mol	Chain	Res	Type
1	1	631	THR
1	1	739	THR
1	1	748	LEU
2	2	76	GLN
2	2	145	LEU
2	2	196	HIS
2	2	229	ASN
2	2	236	ASP
2	2	257	PHE
2	2	302	LYS
2	2	304	ILE
2	2	334	LEU
2	2	395	ASP
2	2	406	LEU
2	2	420	LEU
2	2	516	VAL
2	2	542	LYS
2	2	573	PHE
2	2	580	MET
2	2	689	ARG
3	3	58	CYS
3	3	66	ARG
3	3	69	LEU
4	4	3	GLU
4	4	73	ARG
4	4	82	ASP
4	4	107	LYS
5	5	33	ILE
5	5	43	ARG
6	6	38	PHE
9	9	1	MET
9	9	17	MET
9	9	30	LEU
8	7	5	ASP
10	K	64	MET
10	K	72	PHE
10	K	76	TYR
10	K	104	LEU
10	K	112	HIS
10	K	113	ILE
10	K	114	LEU
9	I	1	MET

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Mol	Chain	Res	Type
9	I	17	MET
9	I	21	LEU
9	I	30	LEU
10	k	64	MET
10	k	72	PHE
10	k	76	TYR
10	k	112	HIS
10	k	113	ILE
10	k	114	LEU
10	0	64	MET
10	0	72	PHE
10	0	76	TYR
10	0	104	LEU
10	0	112	HIS
10	0	113	ILE
10	0	114	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS
1	A	432	HIS
1	A	608	HIS
2	B	34	HIS
2	B	373	HIS
2	B	437	HIS
2	B	582	ASN
1	a	224	ASN
1	a	296	HIS
1	a	432	HIS
2	b	34	HIS
2	b	437	HIS
2	b	582	ASN
1	1	76	HIS
1	1	224	ASN
1	1	296	HIS
1	1	432	HIS
1	1	488	HIS
1	1	608	HIS
2	2	34	HIS
2	2	317	HIS
2	2	373	HIS

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Mol	Chain	Res	Type
2	2	437	HIS
2	2	582	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

357 ligands are modelled in this entry.

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	$\# Z > 2$
11	CLA	0	1401	-	56,73,73	1.85	12 (21%)	65,113,113	2.18	16 (24%)
11	CLA	0	1402	-	41,58,73	2.24	13 (31%)	47,95,113	2.28	11 (23%)
11	CLA	1	1011	-	56,73,73	1.82	13 (23%)	65,113,113	2.53	18 (27%)
11	CLA	1	1012	-	56,73,73	1.88	12 (21%)	65,113,113	2.37	19 (29%)
11	CLA	1	1022	-	56,73,73	1.86	13 (23%)	65,113,113	2.14	14 (21%)
11	CLA	1	1101	-	56,73,73	1.84	12 (21%)	65,113,113	2.13	17 (26%)
11	CLA	1	1102	-	56,73,73	1.88	12 (21%)	65,113,113	1.99	11 (16%)
11	CLA	1	1103	-	56,73,73	1.85	12 (21%)	65,113,113	2.11	18 (27%)
11	CLA	1	1104	-	56,73,73	1.86	12 (21%)	65,113,113	2.12	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1105	-	39,56,73	2.23	12 (30%)	45,92,113	2.40	13 (28%)
11	CLA	1	1106	1	56,73,73	1.89	12 (21%)	65,113,113	2.04	15 (23%)
11	CLA	1	1107	-	56,73,73	1.89	12 (21%)	65,113,113	2.14	15 (23%)
11	CLA	1	1108	-	33,53,73	2.29	12 (36%)	37,89,113	2.33	9 (24%)
11	CLA	1	1109	-	56,73,73	1.88	12 (21%)	65,113,113	2.12	14 (21%)
11	CLA	1	1110	-	45,62,73	2.06	12 (26%)	51,99,113	2.48	15 (29%)
11	CLA	1	1111	-	51,68,73	1.93	11 (21%)	59,107,113	2.14	17 (28%)
11	CLA	1	1112	-	33,53,73	2.27	11 (33%)	37,89,113	2.35	11 (29%)
11	CLA	1	1113	-	33,53,73	2.27	12 (36%)	37,89,113	2.32	9 (24%)
11	CLA	1	1114	-	37,54,73	2.39	13 (35%)	43,90,113	2.33	13 (30%)
11	CLA	1	1115	-	37,54,73	2.36	13 (35%)	43,90,113	2.45	13 (30%)
11	CLA	1	1116	-	45,62,73	2.09	12 (26%)	51,99,113	2.31	16 (31%)
11	CLA	1	1117	-	56,73,73	1.87	12 (21%)	65,113,113	2.07	17 (26%)
11	CLA	1	1118	-	52,69,73	1.93	12 (23%)	60,108,113	2.12	17 (28%)
11	CLA	1	1119	-	56,73,73	1.87	12 (21%)	65,113,113	2.11	16 (24%)
11	CLA	1	1120	-	37,54,73	2.39	13 (35%)	43,90,113	2.39	13 (30%)
11	CLA	1	1121	-	37,54,73	2.37	12 (32%)	43,90,113	2.35	12 (27%)
11	CLA	1	1122	-	50,67,73	2.00	13 (26%)	57,105,113	2.25	15 (26%)
11	CLA	1	1123	-	56,73,73	1.85	13 (23%)	65,113,113	2.15	14 (21%)
11	CLA	1	1124	-	46,63,73	2.05	13 (28%)	53,101,113	2.25	14 (26%)
11	CLA	1	1125	-	43,60,73	2.10	13 (30%)	49,97,113	2.38	16 (32%)
11	CLA	1	1126	-	56,73,73	1.87	13 (23%)	65,113,113	2.12	17 (26%)
11	CLA	1	1127	-	56,73,73	1.89	12 (21%)	65,113,113	1.98	14 (21%)
11	CLA	1	1128	-	56,73,73	1.86	12 (21%)	65,113,113	2.05	15 (23%)
11	CLA	1	1129	-	37,54,73	2.39	13 (35%)	43,90,113	2.38	12 (27%)
11	CLA	1	1130	-	37,54,73	2.40	13 (35%)	43,90,113	2.27	11 (25%)
11	CLA	1	1131	-	56,73,73	1.86	13 (23%)	65,113,113	2.10	16 (24%)
11	CLA	1	1132	-	56,73,73	1.85	12 (21%)	65,113,113	2.00	13 (20%)
11	CLA	1	1133	-	37,54,73	2.39	12 (32%)	43,90,113	2.41	14 (32%)
11	CLA	1	1134	-	37,54,73	2.39	12 (32%)	43,90,113	2.37	13 (30%)
11	CLA	1	1135	-	42,59,73	2.16	13 (30%)	48,96,113	2.48	15 (31%)
11	CLA	1	1136	-	37,54,73	2.39	12 (32%)	43,90,113	2.25	12 (27%)
11	CLA	1	1137	-	56,73,73	1.89	13 (23%)	65,113,113	2.29	18 (27%)
11	CLA	1	1138	-	37,54,73	2.38	12 (32%)	43,90,113	2.20	13 (30%)
11	CLA	1	1139	-	41,58,73	2.18	13 (31%)	47,95,113	2.40	16 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1140	-	56,73,73	1.88	13 (23%)	65,113,113	2.17	17 (26%)
11	CLA	1	1237	-	46,63,73	2.02	12 (26%)	53,101,113	2.26	17 (32%)
11	CLA	1	1801	15	43,60,73	2.16	13 (30%)	49,97,113	2.47	16 (32%)
12	PQN	1	2001	-	34,34,34	1.45	2 (5%)	43,45,45	1.05	2 (4%)
13	SF4	1	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	1	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.51	27 (48%)
14	BCR	1	4002	-	41,41,41	2.73	6 (14%)	56,56,56	6.91	23 (41%)
14	BCR	1	4003	-	41,41,41	2.80	6 (14%)	56,56,56	6.35	28 (50%)
14	BCR	1	4007	-	41,41,41	2.73	6 (14%)	56,56,56	6.63	26 (46%)
14	BCR	1	4008	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	28 (50%)
15	LHG	1	5001	-	48,48,48	0.93	2 (4%)	49,54,54	1.13	3 (6%)
15	LHG	1	5003	11	48,48,48	0.94	2 (4%)	49,54,54	1.08	3 (6%)
11	CLA	2	1013	-	56,73,73	1.87	12 (21%)	65,113,113	2.09	17 (26%)
11	CLA	2	1021	-	56,73,73	1.85	12 (21%)	65,113,113	2.29	19 (29%)
11	CLA	2	1023	-	56,73,73	1.85	12 (21%)	65,113,113	2.23	17 (26%)
11	CLA	2	1201	-	45,62,73	2.11	12 (26%)	51,99,113	2.24	14 (27%)
11	CLA	2	1202	-	56,73,73	1.88	12 (21%)	65,113,113	2.06	17 (26%)
11	CLA	2	1203	-	56,73,73	1.84	12 (21%)	65,113,113	2.07	16 (24%)
11	CLA	2	1204	-	56,73,73	1.87	12 (21%)	65,113,113	2.03	14 (21%)
11	CLA	2	1205	-	46,63,73	2.04	13 (28%)	53,101,113	2.38	13 (24%)
11	CLA	2	1206	2	56,73,73	1.83	12 (21%)	65,113,113	2.13	13 (20%)
11	CLA	2	1207	-	56,73,73	1.86	12 (21%)	65,113,113	2.17	16 (24%)
11	CLA	2	1208	-	33,53,73	2.29	11 (33%)	37,89,113	2.28	9 (24%)
11	CLA	2	1209	-	33,53,73	2.26	11 (33%)	37,89,113	2.40	12 (32%)
11	CLA	2	1210	-	56,73,73	1.84	12 (21%)	65,113,113	2.11	19 (29%)
11	CLA	2	1211	-	37,54,73	2.40	11 (29%)	43,90,113	2.35	13 (30%)
11	CLA	2	1212	-	33,53,73	2.28	12 (36%)	37,89,113	2.42	12 (32%)
11	CLA	2	1213	-	56,73,73	1.94	13 (23%)	65,113,113	2.27	15 (23%)
11	CLA	2	1214	-	50,67,73	1.96	12 (24%)	57,105,113	2.16	16 (28%)
11	CLA	2	1215	-	56,73,73	1.88	12 (21%)	65,113,113	2.28	18 (27%)
11	CLA	2	1216	-	56,73,73	1.86	12 (21%)	65,113,113	2.19	15 (23%)
11	CLA	2	1217	-	38,55,73	2.22	12 (31%)	44,91,113	2.53	16 (36%)
11	CLA	2	1218	-	33,53,73	2.25	11 (33%)	37,89,113	2.24	11 (29%)
11	CLA	2	1219	-	46,63,73	2.11	13 (28%)	53,101,113	2.29	15 (28%)
11	CLA	2	1220	-	37,54,73	2.37	12 (32%)	43,90,113	2.33	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	2	1221	-	45,62,73	2.07	13 (28%)	51,99,113	2.35	15 (29%)
11	CLA	2	1222	-	47,64,73	2.04	13 (27%)	54,102,113	2.33	16 (29%)
11	CLA	2	1223	-	56,73,73	1.87	12 (21%)	65,113,113	2.06	17 (26%)
11	CLA	2	1224	-	46,63,73	2.04	13 (28%)	53,101,113	2.40	16 (30%)
11	CLA	2	1225	-	56,73,73	1.85	11 (19%)	65,113,113	2.05	15 (23%)
11	CLA	2	1226	-	56,73,73	1.88	11 (19%)	65,113,113	2.16	15 (23%)
11	CLA	2	1227	-	33,53,73	2.25	11 (33%)	37,89,113	2.42	10 (27%)
11	CLA	2	1228	-	41,58,73	2.19	13 (31%)	47,95,113	2.39	14 (29%)
11	CLA	2	1229	-	56,73,73	1.85	13 (23%)	65,113,113	2.05	14 (21%)
11	CLA	2	1230	-	49,66,73	2.03	12 (24%)	56,104,113	2.29	18 (32%)
11	CLA	2	1231	-	33,53,73	2.26	12 (36%)	37,89,113	2.43	14 (37%)
11	CLA	2	1232	-	33,53,73	2.25	12 (36%)	37,89,113	2.27	9 (24%)
11	CLA	2	1234	-	51,68,73	1.92	12 (23%)	59,107,113	2.21	14 (23%)
11	CLA	2	1235	-	51,68,73	1.96	13 (25%)	59,107,113	2.16	19 (32%)
11	CLA	2	1236	-	38,55,73	2.24	12 (31%)	44,91,113	2.52	14 (31%)
11	CLA	2	1238	-	56,73,73	1.88	13 (23%)	65,113,113	2.01	12 (18%)
11	CLA	2	1239	-	37,54,73	2.41	13 (35%)	43,90,113	2.41	13 (30%)
11	CLA	2	1240	15	33,53,73	2.28	11 (33%)	37,89,113	2.32	10 (27%)
12	PQN	2	2002	-	34,34,34	1.43	2 (5%)	43,45,45	1.04	5 (11%)
14	BCR	2	4004	-	41,41,41	2.73	6 (14%)	56,56,56	6.43	29 (51%)
14	BCR	2	4005	-	41,41,41	2.75	6 (14%)	56,56,56	6.34	21 (37%)
14	BCR	2	4006	-	41,41,41	2.74	6 (14%)	56,56,56	6.79	28 (50%)
14	BCR	2	4009	-	41,41,41	2.73	6 (14%)	56,56,56	6.72	24 (42%)
14	BCR	2	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.36	27 (48%)
14	BCR	2	4011	-	41,41,41	2.81	6 (14%)	56,56,56	6.74	26 (46%)
14	BCR	2	4014	-	41,41,41	2.82	6 (14%)	56,56,56	6.40	24 (42%)
14	BCR	2	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.50	28 (50%)
16	LMG	2	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.09	4 (6%)
15	LHG	2	5004	11	48,48,48	0.94	2 (4%)	49,54,54	1.10	3 (6%)
13	SF4	3	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
13	SF4	3	3003	-	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	6	4013	-	41,41,41	2.71	6 (14%)	56,56,56	6.59	24 (42%)
14	BCR	6	4018	-	41,41,41	2.89	7 (17%)	56,56,56	6.26	26 (46%)
14	BCR	6	4020	-	41,41,41	2.87	7 (17%)	56,56,56	6.50	23 (41%)
14	BCR	7	4021	-	41,41,41	2.79	6 (14%)	56,56,56	6.57	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	8	1501	-	56,73,73	1.84	12 (21%)	65,113,113	2.19	16 (24%)
11	CLA	8	1502	-	37,54,73	2.37	12 (32%)	43,90,113	2.43	14 (32%)
11	CLA	8	1503	-	56,73,73	1.90	13 (23%)	65,113,113	2.06	14 (21%)
14	BCR	8	4019	-	41,41,41	2.77	6 (14%)	56,56,56	6.61	24 (42%)
14	BCR	8	4022	-	41,41,41	2.80	6 (14%)	56,56,56	6.46	31 (55%)
11	CLA	A	1011	-	56,73,73	1.83	12 (21%)	65,113,113	2.14	16 (24%)
11	CLA	A	1012	-	56,73,73	1.87	13 (23%)	65,113,113	2.44	19 (29%)
11	CLA	A	1022	-	56,73,73	1.85	12 (21%)	65,113,113	2.10	16 (24%)
11	CLA	A	1101	-	56,73,73	1.85	12 (21%)	65,113,113	2.01	15 (23%)
11	CLA	A	1102	11	56,73,73	1.88	13 (23%)	65,113,113	2.14	17 (26%)
11	CLA	A	1103	-	56,73,73	1.87	11 (19%)	65,113,113	1.96	17 (26%)
11	CLA	A	1104	-	56,73,73	1.85	12 (21%)	65,113,113	2.18	18 (27%)
11	CLA	A	1105	-	39,56,73	2.22	13 (33%)	45,92,113	2.38	14 (31%)
11	CLA	A	1106	1	56,73,73	1.86	12 (21%)	65,113,113	2.08	13 (20%)
11	CLA	A	1107	1	56,73,73	1.86	11 (19%)	65,113,113	2.13	16 (24%)
11	CLA	A	1108	-	33,53,73	2.27	11 (33%)	37,89,113	2.30	11 (29%)
11	CLA	A	1109	11	56,73,73	1.90	12 (21%)	65,113,113	2.06	15 (23%)
11	CLA	A	1110	-	45,62,73	2.10	12 (26%)	51,99,113	2.46	15 (29%)
11	CLA	A	1111	-	51,68,73	1.92	12 (23%)	59,107,113	2.11	16 (27%)
11	CLA	A	1112	-	33,53,73	2.25	11 (33%)	37,89,113	2.31	11 (29%)
11	CLA	A	1113	-	33,53,73	2.27	12 (36%)	37,89,113	2.35	13 (35%)
11	CLA	A	1114	-	37,54,73	2.38	12 (32%)	43,90,113	2.30	12 (27%)
11	CLA	A	1115	-	37,54,73	2.41	13 (35%)	43,90,113	2.26	13 (30%)
11	CLA	A	1116	-	45,62,73	2.09	12 (26%)	51,99,113	2.29	16 (31%)
11	CLA	A	1117	-	56,73,73	1.94	12 (21%)	65,113,113	2.05	14 (21%)
11	CLA	A	1118	-	52,69,73	1.92	12 (23%)	60,108,113	2.16	17 (28%)
11	CLA	A	1119	-	56,73,73	1.84	12 (21%)	65,113,113	2.02	17 (26%)
11	CLA	A	1120	-	37,54,73	2.38	13 (35%)	43,90,113	2.30	14 (32%)
11	CLA	A	1121	-	37,54,73	2.38	13 (35%)	43,90,113	2.28	12 (27%)
11	CLA	A	1122	-	50,67,73	1.98	11 (22%)	57,105,113	2.31	17 (29%)
11	CLA	A	1123	-	56,73,73	1.80	12 (21%)	65,113,113	2.18	18 (27%)
11	CLA	A	1124	-	46,63,73	2.04	12 (26%)	53,101,113	2.28	16 (30%)
11	CLA	A	1125	-	43,60,73	2.11	12 (27%)	49,97,113	2.65	16 (32%)
11	CLA	A	1126	-	56,73,73	1.88	11 (19%)	65,113,113	2.09	16 (24%)
11	CLA	A	1127	-	56,73,73	1.85	13 (23%)	65,113,113	2.15	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1128	-	56,73,73	1.86	11 (19%)	65,113,113	2.04	15 (23%)
11	CLA	A	1129	-	37,54,73	2.37	12 (32%)	43,90,113	2.29	12 (27%)
11	CLA	A	1130	-	37,54,73	2.38	13 (35%)	43,90,113	2.29	12 (27%)
11	CLA	A	1131	-	56,73,73	1.88	12 (21%)	65,113,113	2.10	17 (26%)
11	CLA	A	1132	-	56,73,73	1.88	12 (21%)	65,113,113	2.14	13 (20%)
11	CLA	A	1133	-	37,54,73	2.37	12 (32%)	43,90,113	2.50	15 (34%)
11	CLA	A	1134	1	37,54,73	2.36	12 (32%)	43,90,113	2.40	14 (32%)
11	CLA	A	1135	-	42,59,73	2.14	12 (28%)	48,96,113	2.40	15 (31%)
11	CLA	A	1136	-	37,54,73	2.38	12 (32%)	43,90,113	2.35	12 (27%)
11	CLA	A	1137	-	56,73,73	1.91	12 (21%)	65,113,113	2.28	18 (27%)
11	CLA	A	1138	-	37,54,73	2.35	12 (32%)	43,90,113	2.33	16 (37%)
11	CLA	A	1139	-	41,58,73	2.19	12 (29%)	47,95,113	2.32	14 (29%)
11	CLA	A	1140	-	56,73,73	1.87	12 (21%)	65,113,113	2.15	16 (24%)
11	CLA	A	1237	-	46,63,73	2.06	11 (23%)	53,101,113	2.29	14 (26%)
11	CLA	A	1801	15	43,60,73	2.17	12 (27%)	49,97,113	2.51	15 (30%)
12	PQN	A	2001	-	34,34,34	1.44	2 (5%)	43,45,45	1.08	5 (11%)
13	SF4	A	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	A	4001	-	41,41,41	2.79	6 (14%)	56,56,56	6.35	27 (48%)
14	BCR	A	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.28	24 (42%)
14	BCR	A	4003	-	41,41,41	2.86	6 (14%)	56,56,56	6.25	24 (42%)
14	BCR	A	4007	-	41,41,41	2.78	6 (14%)	56,56,56	6.77	23 (41%)
14	BCR	A	4008	-	41,41,41	2.73	7 (17%)	56,56,56	6.65	30 (53%)
15	LHG	A	5001	-	48,48,48	0.91	2 (4%)	49,54,54	1.18	4 (8%)
15	LHG	A	5003	11	48,48,48	0.94	2 (4%)	49,54,54	1.18	4 (8%)
11	CLA	B	1013	-	56,73,73	1.88	12 (21%)	65,113,113	2.10	16 (24%)
11	CLA	B	1021	-	56,73,73	1.83	13 (23%)	65,113,113	2.33	18 (27%)
11	CLA	B	1023	-	56,73,73	1.83	11 (19%)	65,113,113	2.10	16 (24%)
11	CLA	B	1201	-	45,62,73	2.08	12 (26%)	51,99,113	2.35	16 (31%)
11	CLA	B	1202	-	56,73,73	1.92	13 (23%)	65,113,113	2.08	14 (21%)
11	CLA	B	1203	-	56,73,73	1.85	12 (21%)	65,113,113	2.02	13 (20%)
11	CLA	B	1204	-	56,73,73	1.83	11 (19%)	65,113,113	2.06	15 (23%)
11	CLA	B	1205	-	46,63,73	2.02	11 (23%)	53,101,113	2.44	14 (26%)
11	CLA	B	1206	2	56,73,73	1.83	12 (21%)	65,113,113	2.11	16 (24%)
11	CLA	B	1207	-	56,73,73	1.84	11 (19%)	65,113,113	2.15	14 (21%)
11	CLA	B	1208	-	33,53,73	2.29	11 (33%)	37,89,113	2.28	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1209	-	33,53,73	2.26	11 (33%)	37,89,113	2.44	13 (35%)
11	CLA	B	1210	-	56,73,73	1.88	12 (21%)	65,113,113	2.08	17 (26%)
11	CLA	B	1211	-	37,54,73	2.37	11 (29%)	43,90,113	2.31	13 (30%)
11	CLA	B	1212	-	33,53,73	2.28	12 (36%)	37,89,113	2.30	10 (27%)
11	CLA	B	1213	-	56,73,73	1.89	12 (21%)	65,113,113	2.09	15 (23%)
11	CLA	B	1214	-	50,67,73	1.97	13 (26%)	57,105,113	2.34	19 (33%)
11	CLA	B	1215	-	56,73,73	1.85	12 (21%)	65,113,113	2.27	18 (27%)
11	CLA	B	1216	-	56,73,73	1.87	12 (21%)	65,113,113	2.05	15 (23%)
11	CLA	B	1217	-	38,55,73	2.22	12 (31%)	44,91,113	2.45	13 (29%)
11	CLA	B	1218	-	33,53,73	2.27	11 (33%)	37,89,113	2.29	10 (27%)
11	CLA	B	1219	-	46,63,73	2.06	13 (28%)	53,101,113	2.23	16 (30%)
11	CLA	B	1220	-	37,54,73	2.34	12 (32%)	43,90,113	2.26	11 (25%)
11	CLA	B	1221	-	45,62,73	2.07	12 (26%)	51,99,113	2.41	15 (29%)
11	CLA	B	1222	-	47,64,73	2.10	12 (25%)	54,102,113	2.54	19 (35%)
11	CLA	B	1223	-	56,73,73	1.86	13 (23%)	65,113,113	2.16	18 (27%)
11	CLA	B	1224	-	46,63,73	2.07	12 (26%)	53,101,113	2.35	15 (28%)
11	CLA	B	1225	-	56,73,73	1.85	12 (21%)	65,113,113	2.06	15 (23%)
11	CLA	B	1226	-	56,73,73	1.84	11 (19%)	65,113,113	2.20	17 (26%)
11	CLA	B	1227	-	33,53,73	2.25	11 (33%)	37,89,113	2.53	12 (32%)
11	CLA	B	1228	-	41,58,73	2.20	12 (29%)	47,95,113	2.34	14 (29%)
11	CLA	B	1229	-	56,73,73	1.85	12 (21%)	65,113,113	2.10	17 (26%)
11	CLA	B	1230	-	49,66,73	2.02	12 (24%)	56,104,113	2.33	17 (30%)
11	CLA	B	1231	-	33,53,73	2.24	11 (33%)	37,89,113	2.55	14 (37%)
11	CLA	B	1232	-	33,53,73	2.24	11 (33%)	37,89,113	2.43	11 (29%)
11	CLA	B	1234	-	51,68,73	1.93	12 (23%)	59,107,113	2.29	16 (27%)
11	CLA	B	1235	-	51,68,73	1.99	13 (25%)	59,107,113	2.13	13 (22%)
11	CLA	B	1236	-	38,55,73	2.20	12 (31%)	44,91,113	2.47	15 (34%)
11	CLA	B	1238	-	56,73,73	1.86	11 (19%)	65,113,113	1.98	14 (21%)
11	CLA	B	1239	-	37,54,73	2.38	12 (32%)	43,90,113	2.32	12 (27%)
11	CLA	B	1240	15	33,53,73	2.31	11 (33%)	37,89,113	2.32	9 (24%)
12	PQN	B	2002	-	34,34,34	1.44	2 (5%)	43,45,45	1.09	3 (6%)
14	BCR	B	4004	-	41,41,41	2.81	6 (14%)	56,56,56	6.52	27 (48%)
14	BCR	B	4005	-	41,41,41	2.81	7 (17%)	56,56,56	6.50	25 (44%)
14	BCR	B	4006	-	41,41,41	2.76	6 (14%)	56,56,56	6.78	26 (46%)
14	BCR	B	4009	-	41,41,41	2.76	6 (14%)	56,56,56	6.67	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	B	4010	-	41,41,41	2.73	6 (14%)	56,56,56	6.37	26 (46%)
14	BCR	B	4011	-	41,41,41	2.83	7 (17%)	56,56,56	6.67	27 (48%)
14	BCR	B	4014	-	41,41,41	2.79	7 (17%)	56,56,56	6.25	25 (44%)
14	BCR	B	4017	-	41,41,41	2.78	6 (14%)	56,56,56	6.56	31 (55%)
16	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.10	4 (6%)
15	LHG	B	5004	11	48,48,48	0.94	2 (4%)	49,54,54	1.18	4 (8%)
13	SF4	C	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
13	SF4	C	3003	3	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	F	4013	-	41,41,41	2.79	6 (14%)	56,56,56	6.75	21 (37%)
14	BCR	F	4018	-	41,41,41	2.92	7 (17%)	56,56,56	6.53	24 (42%)
14	BCR	F	4020	-	41,41,41	2.80	6 (14%)	56,56,56	6.37	23 (41%)
11	CLA	K	1401	-	56,73,73	1.85	12 (21%)	65,113,113	2.18	16 (24%)
11	CLA	K	1402	-	41,58,73	2.21	12 (29%)	47,95,113	2.28	12 (25%)
11	CLA	L	1501	7	56,73,73	1.86	12 (21%)	65,113,113	2.06	15 (23%)
11	CLA	L	1502	-	37,54,73	2.38	11 (29%)	43,90,113	2.39	12 (27%)
11	CLA	L	1503	-	56,73,73	1.84	11 (19%)	65,113,113	2.14	13 (20%)
14	BCR	L	4019	-	41,41,41	2.71	6 (14%)	56,56,56	6.55	24 (42%)
14	BCR	L	4022	-	41,41,41	2.71	6 (14%)	56,56,56	6.07	25 (44%)
14	BCR	M	4021	-	41,41,41	2.81	6 (14%)	56,56,56	6.54	21 (37%)
11	CLA	a	1011	-	56,73,73	1.88	13 (23%)	65,113,113	2.22	16 (24%)
11	CLA	a	1012	-	56,73,73	1.88	13 (23%)	65,113,113	2.26	16 (24%)
11	CLA	a	1022	-	56,73,73	1.86	13 (23%)	65,113,113	2.17	14 (21%)
11	CLA	a	1101	-	56,73,73	1.88	12 (21%)	65,113,113	2.13	17 (26%)
11	CLA	a	1102	11	56,73,73	1.87	13 (23%)	65,113,113	2.07	13 (20%)
11	CLA	a	1103	-	56,73,73	1.87	13 (23%)	65,113,113	2.11	14 (21%)
11	CLA	a	1104	-	56,73,73	1.84	12 (21%)	65,113,113	2.06	17 (26%)
11	CLA	a	1105	-	39,56,73	2.26	12 (30%)	45,92,113	2.52	15 (33%)
11	CLA	a	1106	1	56,73,73	1.88	13 (23%)	65,113,113	2.13	16 (24%)
11	CLA	a	1107	1	56,73,73	1.84	12 (21%)	65,113,113	2.26	18 (27%)
11	CLA	a	1108	-	33,53,73	2.28	11 (33%)	37,89,113	2.37	11 (29%)
11	CLA	a	1109	11	56,73,73	1.89	13 (23%)	65,113,113	2.10	15 (23%)
11	CLA	a	1110	-	45,62,73	2.10	13 (28%)	51,99,113	2.34	14 (27%)
11	CLA	a	1111	-	51,68,73	1.92	13 (25%)	59,107,113	2.17	17 (28%)
11	CLA	a	1112	-	33,53,73	2.26	11 (33%)	37,89,113	2.24	12 (32%)
11	CLA	a	1113	-	33,53,73	2.28	11 (33%)	37,89,113	2.33	11 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	a	1114	-	37,54,73	2.38	13 (35%)	43,90,113	2.35	12 (27%)
11	CLA	a	1115	-	37,54,73	2.41	12 (32%)	43,90,113	2.20	11 (25%)
11	CLA	a	1116	-	45,62,73	2.11	12 (26%)	51,99,113	2.28	14 (27%)
11	CLA	a	1117	-	56,73,73	1.89	12 (21%)	65,113,113	2.04	16 (24%)
11	CLA	a	1118	-	52,69,73	1.94	11 (21%)	60,108,113	2.12	15 (25%)
11	CLA	a	1119	-	56,73,73	1.86	12 (21%)	65,113,113	2.13	18 (27%)
11	CLA	a	1120	-	37,54,73	2.39	13 (35%)	43,90,113	2.41	13 (30%)
11	CLA	a	1121	-	37,54,73	2.37	13 (35%)	43,90,113	2.37	13 (30%)
11	CLA	a	1122	-	50,67,73	2.01	12 (24%)	57,105,113	2.27	16 (28%)
11	CLA	a	1123	-	56,73,73	1.86	12 (21%)	65,113,113	2.11	16 (24%)
11	CLA	a	1124	-	46,63,73	2.05	13 (28%)	53,101,113	2.36	15 (28%)
11	CLA	a	1125	-	43,60,73	2.09	13 (30%)	49,97,113	2.34	14 (28%)
11	CLA	a	1126	-	56,73,73	1.89	11 (19%)	65,113,113	2.10	15 (23%)
11	CLA	a	1127	-	56,73,73	1.86	12 (21%)	65,113,113	2.23	20 (30%)
11	CLA	a	1128	-	56,73,73	1.88	12 (21%)	65,113,113	2.09	16 (24%)
11	CLA	a	1129	-	37,54,73	2.39	11 (29%)	43,90,113	2.39	13 (30%)
11	CLA	a	1130	-	37,54,73	2.41	12 (32%)	43,90,113	2.31	12 (27%)
11	CLA	a	1131	-	56,73,73	1.88	12 (21%)	65,113,113	2.09	19 (29%)
11	CLA	a	1132	-	56,73,73	1.88	13 (23%)	65,113,113	2.03	14 (21%)
11	CLA	a	1133	-	37,54,73	2.38	12 (32%)	43,90,113	2.44	12 (27%)
11	CLA	a	1134	-	37,54,73	2.38	12 (32%)	43,90,113	2.33	15 (34%)
11	CLA	a	1135	-	42,59,73	2.15	12 (28%)	48,96,113	2.46	15 (31%)
11	CLA	a	1136	-	37,54,73	2.38	12 (32%)	43,90,113	2.36	11 (25%)
11	CLA	a	1137	-	56,73,73	1.89	13 (23%)	65,113,113	2.21	17 (26%)
11	CLA	a	1138	-	37,54,73	2.36	12 (32%)	43,90,113	2.35	16 (37%)
11	CLA	a	1139	-	41,58,73	2.17	13 (31%)	47,95,113	2.46	13 (27%)
11	CLA	a	1140	-	56,73,73	1.87	12 (21%)	65,113,113	2.09	16 (24%)
11	CLA	a	1237	-	46,63,73	2.08	11 (23%)	53,101,113	2.23	13 (24%)
11	CLA	a	1801	15	43,60,73	2.15	13 (30%)	49,97,113	2.43	13 (26%)
12	PQN	a	2001	-	34,34,34	1.43	2 (5%)	43,45,45	0.99	4 (9%)
13	SF4	a	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	a	4001	-	41,41,41	2.75	6 (14%)	56,56,56	6.48	27 (48%)
14	BCR	a	4002	-	41,41,41	2.78	6 (14%)	56,56,56	6.56	25 (44%)
14	BCR	a	4003	-	41,41,41	2.76	6 (14%)	56,56,56	6.16	26 (46%)
14	BCR	a	4007	-	41,41,41	2.74	6 (14%)	56,56,56	6.70	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	a	4008	-	41,41,41	2.75	7 (17%)	56,56,56	6.53	29 (51%)
15	LHG	a	5001	-	48,48,48	0.94	2 (4%)	49,54,54	1.11	3 (6%)
15	LHG	a	5003	11	48,48,48	0.92	2 (4%)	49,54,54	1.08	3 (6%)
11	CLA	b	1013	-	56,73,73	1.88	12 (21%)	65,113,113	2.04	15 (23%)
11	CLA	b	1021	-	56,73,73	1.88	12 (21%)	65,113,113	2.33	22 (33%)
11	CLA	b	1023	-	56,73,73	1.85	12 (21%)	65,113,113	2.10	17 (26%)
11	CLA	b	1201	-	45,62,73	2.13	11 (24%)	51,99,113	2.33	16 (31%)
11	CLA	b	1202	-	56,73,73	1.88	12 (21%)	65,113,113	2.01	14 (21%)
11	CLA	b	1203	-	56,73,73	1.85	13 (23%)	65,113,113	2.10	15 (23%)
11	CLA	b	1204	-	56,73,73	1.85	12 (21%)	65,113,113	2.02	13 (20%)
11	CLA	b	1205	-	46,63,73	2.05	11 (23%)	53,101,113	2.32	14 (26%)
11	CLA	b	1206	2	56,73,73	1.85	12 (21%)	65,113,113	2.09	17 (26%)
11	CLA	b	1207	-	56,73,73	1.86	12 (21%)	65,113,113	2.22	13 (20%)
11	CLA	b	1208	-	33,53,73	2.28	11 (33%)	37,89,113	2.44	10 (27%)
11	CLA	b	1209	-	33,53,73	2.30	11 (33%)	37,89,113	2.37	12 (32%)
11	CLA	b	1210	-	56,73,73	1.88	13 (23%)	65,113,113	2.05	19 (29%)
11	CLA	b	1211	-	37,54,73	2.39	13 (35%)	43,90,113	2.38	13 (30%)
11	CLA	b	1212	-	33,53,73	2.27	12 (36%)	37,89,113	2.39	9 (24%)
11	CLA	b	1213	-	56,73,73	1.90	12 (21%)	65,113,113	2.09	14 (21%)
11	CLA	b	1214	-	50,67,73	1.97	13 (26%)	57,105,113	2.17	17 (29%)
11	CLA	b	1215	-	56,73,73	1.87	12 (21%)	65,113,113	2.23	18 (27%)
11	CLA	b	1216	-	56,73,73	1.88	12 (21%)	65,113,113	2.14	19 (29%)
11	CLA	b	1217	-	38,55,73	2.24	13 (34%)	44,91,113	2.47	13 (29%)
11	CLA	b	1218	-	33,53,73	2.28	12 (36%)	37,89,113	2.31	10 (27%)
11	CLA	b	1219	-	46,63,73	2.10	12 (26%)	53,101,113	2.37	15 (28%)
11	CLA	b	1220	-	37,54,73	2.41	13 (35%)	43,90,113	2.37	13 (30%)
11	CLA	b	1221	-	45,62,73	2.09	12 (26%)	51,99,113	2.45	16 (31%)
11	CLA	b	1222	-	47,64,73	2.04	13 (27%)	54,102,113	2.45	16 (29%)
11	CLA	b	1223	-	56,73,73	1.89	12 (21%)	65,113,113	2.08	16 (24%)
11	CLA	b	1224	-	46,63,73	2.08	13 (28%)	53,101,113	2.35	16 (30%)
11	CLA	b	1225	-	56,73,73	1.87	13 (23%)	65,113,113	2.08	15 (23%)
11	CLA	b	1226	-	56,73,73	1.85	13 (23%)	65,113,113	2.14	16 (24%)
11	CLA	b	1227	-	33,53,73	2.27	12 (36%)	37,89,113	2.47	11 (29%)
11	CLA	b	1228	-	41,58,73	2.19	12 (29%)	47,95,113	2.37	14 (29%)
11	CLA	b	1229	-	56,73,73	1.87	13 (23%)	65,113,113	2.03	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1230	-	49,66,73	2.04	13 (26%)	56,104,113	2.41	16 (28%)
11	CLA	b	1231	-	33,53,73	2.25	12 (36%)	37,89,113	2.26	12 (32%)
11	CLA	b	1232	-	33,53,73	2.28	12 (36%)	37,89,113	2.35	10 (27%)
11	CLA	b	1234	-	51,68,73	1.95	12 (23%)	59,107,113	2.24	15 (25%)
11	CLA	b	1235	-	51,68,73	1.99	13 (25%)	59,107,113	2.23	18 (30%)
11	CLA	b	1236	-	38,55,73	2.23	11 (28%)	44,91,113	2.42	13 (29%)
11	CLA	b	1238	-	56,73,73	1.87	12 (21%)	65,113,113	2.01	13 (20%)
11	CLA	b	1239	-	37,54,73	2.38	12 (32%)	43,90,113	2.42	14 (32%)
11	CLA	b	1240	-	33,53,73	2.30	12 (36%)	37,89,113	2.30	10 (27%)
12	PQN	b	2002	-	34,34,34	1.43	2 (5%)	43,45,45	1.06	4 (9%)
14	BCR	b	4004	-	41,41,41	2.75	6 (14%)	56,56,56	6.53	26 (46%)
14	BCR	b	4005	-	41,41,41	2.77	6 (14%)	56,56,56	6.54	25 (44%)
14	BCR	b	4006	-	41,41,41	2.78	6 (14%)	56,56,56	6.90	27 (48%)
14	BCR	b	4009	-	41,41,41	2.66	6 (14%)	56,56,56	6.89	26 (46%)
14	BCR	b	4010	-	41,41,41	2.80	6 (14%)	56,56,56	6.67	24 (42%)
14	BCR	b	4011	-	41,41,41	2.77	6 (14%)	56,56,56	6.76	25 (44%)
14	BCR	b	4014	-	41,41,41	2.75	7 (17%)	56,56,56	6.45	24 (42%)
14	BCR	b	4017	-	41,41,41	2.83	7 (17%)	56,56,56	6.62	27 (48%)
16	LMG	b	5002	-	55,55,55	0.87	2 (3%)	63,63,63	1.07	5 (7%)
15	LHG	b	5004	-	48,48,48	0.92	2 (4%)	49,54,54	1.09	3 (6%)
13	SF4	c	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
13	SF4	c	3003	3	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	f	4013	-	41,41,41	2.77	6 (14%)	56,56,56	6.58	24 (42%)
14	BCR	f	4018	-	41,41,41	2.87	7 (17%)	56,56,56	6.32	24 (42%)
14	BCR	f	4020	-	41,41,41	2.81	6 (14%)	56,56,56	6.54	22 (39%)
11	CLA	k	1401	-	56,73,73	1.86	12 (21%)	65,113,113	2.19	16 (24%)
11	CLA	k	1402	-	41,58,73	2.23	12 (29%)	47,95,113	2.33	14 (29%)
11	CLA	l	1501	7	56,73,73	1.88	13 (23%)	65,113,113	2.15	16 (24%)
11	CLA	l	1502	-	37,54,73	2.39	12 (32%)	43,90,113	2.43	12 (27%)
11	CLA	l	1503	-	56,73,73	1.86	12 (21%)	65,113,113	2.08	13 (20%)
14	BCR	l	4019	-	41,41,41	2.77	6 (14%)	56,56,56	6.67	23 (41%)
14	BCR	l	4022	-	41,41,41	2.75	6 (14%)	56,56,56	6.38	26 (46%)
14	BCR	m	4021	-	41,41,41	2.86	6 (14%)	56,56,56	6.47	24 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	0	1401	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	0	1402	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	1	1011	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1012	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1022	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1102	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1104	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1105	-	3/3/16/25	0/17/115/135	0/0/9/9
11	CLA	1	1106	1	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1107	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	1	1109	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1110	-	2/2/17/25	0/24/122/135	0/0/9/9
11	CLA	1	1111	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	1	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	1	1113	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	1	1114	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1115	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1116	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	1	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1118	-	3/3/19/25	0/33/131/135	0/0/9/9
11	CLA	1	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1121	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1122	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	1	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	1	1125	-	2/2/17/25	0/22/120/135	0/0/9/9
11	CLA	1	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1128	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1129	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1130	-	1/1/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1131	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1134	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1135	-	2/2/17/25	0/21/119/135	0/0/9/9
11	CLA	1	1136	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1137	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1138	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1139	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	1	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1237	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	1	1801	15	3/3/17/25	0/22/120/135	0/0/9/9
12	PQN	1	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	1	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	1	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4008	-	-	1/29/63/63	0/2/2/2
15	LHG	1	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	1	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	2	1013	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1201	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	2	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1203	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1204	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1205	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	2	1206	2	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1207	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1208	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1209	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1210	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	2	1212	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1213	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1214	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	2	1215	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1217	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	2	1218	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1219	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	2	1220	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	2	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	2	1222	-	3/3/18/25	0/27/125/135	0/0/9/9
11	CLA	2	1223	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1224	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	2	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1227	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	2	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1230	-	2/2/18/25	0/29/127/135	0/0/9/9
11	CLA	2	1231	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1232	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1234	-	2/2/19/25	0/31/129/135	0/0/9/9
11	CLA	2	1235	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	2	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	2	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1239	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	2	1240	15	3/3/16/25	0/11/111/135	0/0/9/9
12	PQN	2	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	2	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4006	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4014	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	2	4017	-	-	2/29/63/63	0/2/2/2
16	LMG	2	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	2	5004	11	-	0/53/53/53	0/0/0/0
13	SF4	3	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	3	3003	-	-	0/0/48/48	0/6/5/5
14	BCR	6	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	6	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	6	4020	-	-	1/29/63/63	0/2/2/2
14	BCR	7	4021	-	-	0/29/63/63	0/2/2/2
11	CLA	8	1501	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	8	1502	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	8	1503	-	3/3/20/25	0/37/135/135	0/0/9/9
14	BCR	8	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	8	4022	-	-	0/29/63/63	0/2/2/2
11	CLA	A	1011	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1012	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1022	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1102	11	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1105	-	3/3/16/25	0/17/115/135	0/0/9/9
11	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	A	1109	11	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1110	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	A	1111	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	A	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	A	1113	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	A	1114	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1115	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1116	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	A	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1118	-	3/3/19/25	0/33/131/135	0/0/9/9
11	CLA	A	1119	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1121	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1122	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	A	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	A	1125	-	2/2/17/25	0/22/120/135	0/0/9/9
11	CLA	A	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1129	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1130	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1131	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1134	1	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1135	-	3/3/17/25	0/21/119/135	0/0/9/9
11	CLA	A	1136	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1137	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1138	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1139	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	A	1140	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1237	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	A	1801	15	3/3/17/25	0/22/120/135	0/0/9/9
12	PQN	A	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	3/29/63/63	0/2/2/2
15	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	A	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	B	1013	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1201	-	3/3/17/25	0/24/122/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1203	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1204	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1205	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	B	1206	2	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1207	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1208	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1209	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	B	1212	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1213	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1214	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	B	1215	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1217	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	B	1218	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1219	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	B	1220	-	1/1/16/25	0/15/113/135	0/0/9/9
11	CLA	B	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	B	1222	-	3/3/18/25	0/27/125/135	0/0/9/9
11	CLA	B	1223	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1224	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	B	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1227	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	B	1229	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1230	-	2/2/18/25	0/29/127/135	0/0/9/9
11	CLA	B	1231	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1232	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	B	1235	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	B	1236	-	3/3/16/25	0/16/114/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1239	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	B	1240	15	3/3/16/25	0/11/111/135	0/0/9/9
12	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	2/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4017	-	-	1/29/63/63	0/2/2/2
16	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	B	5004	11	-	0/53/53/53	0/0/0/0
13	SF4	C	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	C	3003	3	-	0/0/48/48	0/6/5/5
14	BCR	F	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4020	-	-	0/29/63/63	0/2/2/2
11	CLA	K	1401	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	K	1402	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	L	1501	7	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	L	1502	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	L	1503	-	2/2/20/25	0/37/135/135	0/0/9/9
14	BCR	L	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	L	4022	-	-	0/29/63/63	0/2/2/2
14	BCR	M	4021	-	-	0/29/63/63	0/2/2/2
11	CLA	a	1011	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1012	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1022	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1102	11	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1105	-	3/3/16/25	0/17/115/135	0/0/9/9
11	CLA	a	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1108	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1109	11	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1110	-	2/2/17/25	0/24/122/135	0/0/9/9
11	CLA	a	1111	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	a	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	a	1113	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	a	1114	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1115	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1116	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	a	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1118	-	3/3/19/25	0/33/131/135	0/0/9/9
11	CLA	a	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1121	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1122	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	a	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	a	1125	-	2/2/17/25	0/22/120/135	0/0/9/9
11	CLA	a	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1129	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1130	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1131	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1134	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1135	-	2/2/17/25	0/21/119/135	0/0/9/9
11	CLA	a	1136	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1137	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1138	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1139	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	a	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1237	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	a	1801	15	3/3/17/25	0/22/120/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PQN	a	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	a	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	a	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4008	-	-	1/29/63/63	0/2/2/2
15	LHG	a	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	a	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	b	1013	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1201	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	b	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1203	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1204	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1205	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	b	1206	2	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1207	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1208	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1209	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	b	1212	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1213	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1214	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	b	1215	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1217	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	b	1218	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1219	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	b	1220	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	b	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	b	1222	-	3/3/18/25	0/27/125/135	0/0/9/9
11	CLA	b	1223	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1224	-	3/3/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1227	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	b	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1230	-	3/3/18/25	0/29/127/135	0/0/9/9
11	CLA	b	1231	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1232	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	b	1235	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	b	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	b	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1239	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	b	1240	-	3/3/16/25	0/11/111/135	0/0/9/9
12	PQN	b	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	b	4004	-	-	1/29/63/63	0/2/2/2
14	BCR	b	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4006	-	-	2/29/63/63	0/2/2/2
14	BCR	b	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4014	-	-	2/29/63/63	0/2/2/2
14	BCR	b	4017	-	-	1/29/63/63	0/2/2/2
16	LMG	b	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	b	5004	-	-	0/53/53/53	0/0/0/0
13	SF4	c	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	c	3003	3	-	0/0/48/48	0/6/5/5
14	BCR	f	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	f	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	f	4020	-	-	0/29/63/63	0/2/2/2
11	CLA	k	1401	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	k	1402	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	l	1501	7	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	l	1502	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	l	1503	-	2/2/20/25	0/37/135/135	0/0/9/9
14	BCR	l	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	l	4022	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	m	4021	-	-	0/29/63/63	0/2/2/2

All (3697) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4003	BCR	C11-C10	-8.40	1.17	1.43
14	F	4018	BCR	C11-C10	-8.36	1.18	1.43
14	2	4010	BCR	C11-C10	-8.32	1.18	1.43
14	m	4021	BCR	C8-C9	-8.32	1.27	1.45
14	m	4021	BCR	C11-C10	-8.30	1.18	1.43
14	6	4020	BCR	C11-C10	-8.29	1.18	1.43
14	f	4013	BCR	C8-C9	-8.27	1.27	1.45
14	M	4021	BCR	C11-C10	-8.27	1.18	1.43
14	A	4003	BCR	C8-C9	-8.27	1.27	1.45
14	F	4013	BCR	C8-C9	-8.23	1.28	1.45
14	2	4011	BCR	C8-C9	-8.21	1.28	1.45
14	F	4018	BCR	C8-C9	-8.20	1.28	1.45
14	l	4019	BCR	C8-C9	-8.20	1.28	1.45
14	6	4018	BCR	C8-C9	-8.19	1.28	1.45
14	b	4017	BCR	C11-C10	-8.18	1.18	1.43
14	f	4018	BCR	C8-C9	-8.17	1.28	1.45
14	B	4011	BCR	C8-C9	-8.17	1.28	1.45
14	b	4010	BCR	C11-C10	-8.17	1.18	1.43
14	7	4021	BCR	C8-C9	-8.16	1.28	1.45
14	B	4009	BCR	C11-C10	-8.15	1.18	1.43
14	B	4004	BCR	C8-C9	-8.15	1.28	1.45
14	6	4018	BCR	C11-C10	-8.15	1.18	1.43
14	b	4006	BCR	C8-C9	-8.15	1.28	1.45
14	M	4021	BCR	C8-C9	-8.15	1.28	1.45
14	2	4014	BCR	C8-C9	-8.15	1.28	1.45
14	l	4019	BCR	C11-C10	-8.15	1.18	1.43
14	B	4004	BCR	C11-C10	-8.14	1.18	1.43
14	B	4011	BCR	C11-C10	-8.14	1.18	1.43
14	F	4013	BCR	C11-C10	-8.14	1.18	1.43
14	F	4020	BCR	C11-C10	-8.14	1.18	1.43
14	2	4010	BCR	C8-C9	-8.14	1.28	1.45
14	f	4020	BCR	C11-C10	-8.13	1.18	1.43
14	a	4008	BCR	C8-C9	-8.13	1.28	1.45
14	2	4011	BCR	C11-C10	-8.13	1.18	1.43
14	a	4008	BCR	C11-C10	-8.13	1.18	1.43
14	f	4013	BCR	C11-C10	-8.13	1.18	1.43
14	B	4006	BCR	C8-C9	-8.13	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	4003	BCR	C8-C9	-8.13	1.28	1.45
14	b	4010	BCR	C8-C9	-8.12	1.28	1.45
14	6	4013	BCR	C8-C9	-8.11	1.28	1.45
14	7	4021	BCR	C11-C10	-8.11	1.18	1.43
14	6	4020	BCR	C8-C9	-8.11	1.28	1.45
14	B	4010	BCR	C8-C9	-8.11	1.28	1.45
14	8	4019	BCR	C8-C9	-8.11	1.28	1.45
14	1	4003	BCR	C11-C10	-8.10	1.18	1.43
14	8	4022	BCR	C11-C10	-8.10	1.18	1.43
14	2	4005	BCR	C8-C9	-8.09	1.28	1.45
14	a	4002	BCR	C11-C10	-8.09	1.18	1.43
14	b	4014	BCR	C8-C9	-8.09	1.28	1.45
14	1	4003	BCR	C8-C9	-8.09	1.28	1.45
14	B	4005	BCR	C11-C10	-8.08	1.18	1.43
14	2	4017	BCR	C11-C10	-8.08	1.18	1.43
14	2	4014	BCR	C11-C10	-8.07	1.18	1.43
14	f	4020	BCR	C8-C9	-8.07	1.28	1.45
14	b	4005	BCR	C8-C9	-8.07	1.28	1.45
14	b	4004	BCR	C11-C10	-8.06	1.18	1.43
14	B	4005	BCR	C8-C9	-8.06	1.28	1.45
14	f	4018	BCR	C11-C10	-8.06	1.18	1.43
14	A	4007	BCR	C11-C10	-8.05	1.18	1.43
14	A	4001	BCR	C8-C9	-8.05	1.28	1.45
14	1	4008	BCR	C8-C9	-8.05	1.28	1.45
14	1	4008	BCR	C11-C10	-8.05	1.18	1.43
14	b	4006	BCR	C11-C10	-8.05	1.18	1.43
14	b	4011	BCR	C11-C10	-8.04	1.18	1.43
14	b	4005	BCR	C11-C10	-8.04	1.19	1.43
14	F	4020	BCR	C8-C9	-8.03	1.28	1.45
14	L	4022	BCR	C8-C9	-8.02	1.28	1.45
14	B	4017	BCR	C11-C10	-8.02	1.19	1.43
14	2	4005	BCR	C11-C10	-8.01	1.19	1.43
14	l	4022	BCR	C11-C10	-8.01	1.19	1.43
14	a	4002	BCR	C8-C9	-8.01	1.28	1.45
14	a	4007	BCR	C11-C10	-8.01	1.19	1.43
14	a	4003	BCR	C11-C10	-7.99	1.19	1.43
14	1	4001	BCR	C11-C10	-7.97	1.19	1.43
14	2	4009	BCR	C8-C9	-7.97	1.28	1.45
14	1	4007	BCR	C11-C10	-7.97	1.19	1.43
14	b	4014	BCR	C11-C10	-7.97	1.19	1.43
14	8	4019	BCR	C11-C10	-7.96	1.19	1.43
14	a	4001	BCR	C11-C10	-7.96	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4006	BCR	C11-C10	-7.96	1.19	1.43
14	2	4009	BCR	C11-C10	-7.96	1.19	1.43
14	2	4004	BCR	C11-C10	-7.96	1.19	1.43
14	2	4006	BCR	C11-C10	-7.95	1.19	1.43
14	A	4001	BCR	C11-C10	-7.95	1.19	1.43
14	6	4013	BCR	C11-C10	-7.95	1.19	1.43
14	B	4010	BCR	C11-C10	-7.94	1.19	1.43
14	a	4007	BCR	C8-C9	-7.94	1.28	1.45
14	A	4002	BCR	C8-C9	-7.93	1.28	1.45
14	1	4002	BCR	C11-C10	-7.93	1.19	1.43
14	l	4022	BCR	C8-C9	-7.93	1.28	1.45
14	a	4001	BCR	C8-C9	-7.93	1.28	1.45
14	A	4008	BCR	C11-C10	-7.93	1.19	1.43
14	8	4022	BCR	C8-C9	-7.92	1.28	1.45
14	2	4006	BCR	C8-C9	-7.92	1.28	1.45
14	F	4018	BCR	C10-C9	-7.92	1.25	1.35
14	L	4019	BCR	C11-C10	-7.90	1.19	1.43
14	1	4001	BCR	C8-C9	-7.90	1.28	1.45
14	b	4011	BCR	C8-C9	-7.90	1.28	1.45
14	B	4014	BCR	C11-C10	-7.90	1.19	1.43
14	A	4007	BCR	C8-C9	-7.89	1.28	1.45
14	B	4014	BCR	C8-C9	-7.89	1.28	1.45
14	B	4009	BCR	C8-C9	-7.87	1.28	1.45
14	B	4017	BCR	C8-C9	-7.86	1.28	1.45
14	2	4004	BCR	C8-C9	-7.86	1.28	1.45
14	2	4017	BCR	C8-C9	-7.85	1.28	1.45
14	b	4004	BCR	C8-C9	-7.85	1.28	1.45
14	1	4007	BCR	C8-C9	-7.85	1.28	1.45
14	1	4002	BCR	C8-C9	-7.85	1.28	1.45
14	6	4018	BCR	C20-C21	-7.84	1.19	1.43
14	A	4002	BCR	C11-C10	-7.83	1.19	1.43
14	L	4019	BCR	C8-C9	-7.82	1.28	1.45
14	m	4021	BCR	C10-C9	-7.78	1.25	1.35
14	b	4009	BCR	C11-C10	-7.78	1.19	1.43
14	L	4022	BCR	C11-C10	-7.78	1.19	1.43
14	b	4009	BCR	C8-C9	-7.75	1.29	1.45
14	A	4008	BCR	C8-C9	-7.74	1.29	1.45
14	6	4018	BCR	C16-C17	-7.74	1.19	1.43
14	F	4018	BCR	C20-C21	-7.72	1.19	1.43
14	b	4017	BCR	C8-C9	-7.71	1.29	1.45
14	f	4018	BCR	C20-C21	-7.70	1.20	1.43
14	f	4018	BCR	C16-C17	-7.69	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	4013	BCR	C20-C21	-7.67	1.20	1.43
14	2	4017	BCR	C20-C21	-7.66	1.20	1.43
14	B	4017	BCR	C20-C21	-7.66	1.20	1.43
14	6	4020	BCR	C20-C21	-7.65	1.20	1.43
14	2	4014	BCR	C10-C9	-7.63	1.25	1.35
14	b	4017	BCR	C20-C21	-7.62	1.20	1.43
14	2	4010	BCR	C10-C9	-7.61	1.25	1.35
14	F	4018	BCR	C16-C17	-7.61	1.20	1.43
14	a	4003	BCR	C16-C17	-7.57	1.20	1.43
14	A	4003	BCR	C20-C21	-7.57	1.20	1.43
14	b	4017	BCR	C16-C17	-7.57	1.20	1.43
14	M	4021	BCR	C10-C9	-7.56	1.25	1.35
14	6	4020	BCR	C16-C17	-7.56	1.20	1.43
14	A	4003	BCR	C16-C17	-7.55	1.20	1.43
14	8	4022	BCR	C10-C9	-7.55	1.25	1.35
14	a	4003	BCR	C20-C21	-7.54	1.20	1.43
14	f	4013	BCR	C16-C17	-7.53	1.20	1.43
14	L	4022	BCR	C20-C21	-7.53	1.20	1.43
14	B	4014	BCR	C16-C17	-7.52	1.20	1.43
14	8	4022	BCR	C20-C21	-7.52	1.20	1.43
14	B	4014	BCR	C20-C21	-7.51	1.20	1.43
14	F	4020	BCR	C20-C21	-7.50	1.20	1.43
14	b	4006	BCR	C20-C21	-7.50	1.20	1.43
14	B	4005	BCR	C20-C21	-7.50	1.20	1.43
14	B	4011	BCR	C16-C17	-7.50	1.20	1.43
14	8	4019	BCR	C20-C21	-7.49	1.20	1.43
14	6	4020	BCR	C10-C9	-7.49	1.25	1.35
14	2	4010	BCR	C20-C21	-7.49	1.20	1.43
14	B	4004	BCR	C20-C21	-7.48	1.20	1.43
14	B	4011	BCR	C20-C21	-7.48	1.20	1.43
14	f	4020	BCR	C16-C17	-7.48	1.20	1.43
14	m	4021	BCR	C16-C17	-7.47	1.20	1.43
14	f	4020	BCR	C20-C21	-7.47	1.20	1.43
14	2	4005	BCR	C20-C21	-7.46	1.20	1.43
14	B	4009	BCR	C20-C21	-7.45	1.20	1.43
14	l	4019	BCR	C20-C21	-7.45	1.20	1.43
14	B	4004	BCR	C10-C9	-7.45	1.25	1.35
14	6	4013	BCR	C20-C21	-7.45	1.20	1.43
14	2	4011	BCR	C20-C21	-7.44	1.20	1.43
14	B	4005	BCR	C16-C17	-7.44	1.20	1.43
14	b	4004	BCR	C20-C21	-7.43	1.20	1.43
14	1	4003	BCR	C20-C21	-7.43	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	l	4022	BCR	C20-C21	-7.43	1.20	1.43
14	a	4002	BCR	C20-C21	-7.43	1.20	1.43
14	b	4011	BCR	C20-C21	-7.42	1.20	1.43
14	2	4010	BCR	C16-C17	-7.42	1.20	1.43
14	2	4017	BCR	C16-C17	-7.42	1.20	1.43
14	b	4010	BCR	C20-C21	-7.42	1.20	1.43
14	a	4008	BCR	C20-C21	-7.42	1.20	1.43
14	B	4017	BCR	C16-C17	-7.42	1.20	1.43
14	a	4001	BCR	C20-C21	-7.41	1.20	1.43
14	7	4021	BCR	C20-C21	-7.40	1.20	1.43
14	F	4013	BCR	C20-C21	-7.40	1.20	1.43
14	2	4011	BCR	C16-C17	-7.40	1.20	1.43
14	2	4014	BCR	C16-C17	-7.39	1.20	1.43
14	A	4008	BCR	C20-C21	-7.39	1.20	1.43
14	b	4011	BCR	C16-C17	-7.39	1.21	1.43
14	6	4013	BCR	C16-C17	-7.39	1.21	1.43
14	1	4007	BCR	C20-C21	-7.38	1.21	1.43
14	A	4007	BCR	C16-C17	-7.38	1.21	1.43
14	L	4022	BCR	C16-C17	-7.38	1.21	1.43
14	1	4008	BCR	C20-C21	-7.38	1.21	1.43
14	b	4017	BCR	C10-C9	-7.38	1.26	1.35
14	1	4003	BCR	C16-C17	-7.38	1.21	1.43
14	F	4020	BCR	C16-C17	-7.38	1.21	1.43
14	2	4004	BCR	C20-C21	-7.38	1.21	1.43
14	a	4008	BCR	C16-C17	-7.38	1.21	1.43
14	b	4005	BCR	C20-C21	-7.38	1.21	1.43
14	b	4010	BCR	C10-C9	-7.37	1.26	1.35
14	b	4010	BCR	C16-C17	-7.37	1.21	1.43
14	8	4022	BCR	C16-C17	-7.37	1.21	1.43
14	A	4007	BCR	C20-C21	-7.37	1.21	1.43
14	A	4002	BCR	C20-C21	-7.37	1.21	1.43
14	F	4013	BCR	C10-C9	-7.37	1.26	1.35
14	B	4006	BCR	C20-C21	-7.36	1.21	1.43
14	A	4001	BCR	C10-C9	-7.36	1.26	1.35
14	2	4011	BCR	C10-C9	-7.36	1.26	1.35
14	f	4018	BCR	C10-C9	-7.36	1.26	1.35
14	7	4021	BCR	C16-C17	-7.36	1.21	1.43
14	1	4001	BCR	C20-C21	-7.36	1.21	1.43
14	m	4021	BCR	C20-C21	-7.35	1.21	1.43
14	B	4010	BCR	C20-C21	-7.35	1.21	1.43
14	A	4008	BCR	C16-C17	-7.35	1.21	1.43
14	2	4006	BCR	C20-C21	-7.34	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	4004	BCR	C16-C17	-7.34	1.21	1.43
14	a	4007	BCR	C20-C21	-7.33	1.21	1.43
14	b	4006	BCR	C16-C17	-7.33	1.21	1.43
14	F	4020	BCR	C10-C9	-7.32	1.26	1.35
14	1	4008	BCR	C16-C17	-7.32	1.21	1.43
14	A	4001	BCR	C20-C21	-7.32	1.21	1.43
14	b	4005	BCR	C16-C17	-7.32	1.21	1.43
14	A	4007	BCR	C10-C9	-7.32	1.26	1.35
14	B	4005	BCR	C10-C9	-7.32	1.26	1.35
14	A	4001	BCR	C16-C17	-7.31	1.21	1.43
14	b	4014	BCR	C16-C17	-7.31	1.21	1.43
14	6	4018	BCR	C10-C9	-7.31	1.26	1.35
14	1	4002	BCR	C20-C21	-7.31	1.21	1.43
14	1	4003	BCR	C10-C9	-7.30	1.26	1.35
14	A	4003	BCR	C10-C9	-7.30	1.26	1.35
14	2	4005	BCR	C16-C17	-7.30	1.21	1.43
14	2	4009	BCR	C20-C21	-7.30	1.21	1.43
14	a	4002	BCR	C16-C17	-7.30	1.21	1.43
14	f	4020	BCR	C10-C9	-7.30	1.26	1.35
14	2	4004	BCR	C16-C17	-7.30	1.21	1.43
14	a	4007	BCR	C16-C17	-7.29	1.21	1.43
14	1	4007	BCR	C16-C17	-7.29	1.21	1.43
14	l	4019	BCR	C16-C17	-7.29	1.21	1.43
14	A	4002	BCR	C10-C9	-7.29	1.26	1.35
14	1	4001	BCR	C16-C17	-7.29	1.21	1.43
14	B	4011	BCR	C10-C9	-7.29	1.26	1.35
14	F	4013	BCR	C16-C17	-7.28	1.21	1.43
14	l	4022	BCR	C16-C17	-7.28	1.21	1.43
14	B	4010	BCR	C16-C17	-7.27	1.21	1.43
14	M	4021	BCR	C20-C21	-7.27	1.21	1.43
14	8	4019	BCR	C16-C17	-7.27	1.21	1.43
14	1	4002	BCR	C16-C17	-7.27	1.21	1.43
14	L	4019	BCR	C20-C21	-7.26	1.21	1.43
14	A	4002	BCR	C16-C17	-7.26	1.21	1.43
14	M	4021	BCR	C16-C17	-7.26	1.21	1.43
14	8	4019	BCR	C10-C9	-7.26	1.26	1.35
14	B	4009	BCR	C16-C17	-7.25	1.21	1.43
14	2	4009	BCR	C16-C17	-7.25	1.21	1.43
14	B	4006	BCR	C16-C17	-7.24	1.21	1.43
14	b	4004	BCR	C16-C17	-7.24	1.21	1.43
14	b	4009	BCR	C20-C21	-7.24	1.21	1.43
14	2	4006	BCR	C16-C17	-7.23	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	b	4014	BCR	C20-C21	-7.23	1.21	1.43
14	a	4001	BCR	C16-C17	-7.22	1.21	1.43
14	7	4021	BCR	C10-C9	-7.22	1.26	1.35
14	L	4019	BCR	C16-C17	-7.21	1.21	1.43
14	2	4014	BCR	C20-C21	-7.21	1.21	1.43
14	a	4002	BCR	C10-C9	-7.19	1.26	1.35
14	b	4005	BCR	C10-C9	-7.19	1.26	1.35
14	B	4014	BCR	C10-C9	-7.18	1.26	1.35
14	b	4009	BCR	C16-C17	-7.10	1.21	1.43
14	B	4006	BCR	C10-C9	-7.09	1.26	1.35
14	l	4022	BCR	C10-C9	-7.08	1.26	1.35
14	b	4004	BCR	C10-C9	-7.07	1.26	1.35
14	B	4017	BCR	C10-C9	-7.06	1.26	1.35
14	b	4006	BCR	C10-C9	-7.06	1.26	1.35
14	2	4017	BCR	C10-C9	-7.06	1.26	1.35
14	a	4007	BCR	C10-C9	-7.04	1.26	1.35
14	a	4001	BCR	C10-C9	-7.02	1.26	1.35
14	b	4011	BCR	C10-C9	-7.01	1.26	1.35
14	B	4009	BCR	C10-C9	-7.00	1.26	1.35
14	2	4009	BCR	C10-C9	-6.96	1.26	1.35
14	L	4019	BCR	C10-C9	-6.94	1.26	1.35
14	1	4001	BCR	C10-C9	-6.94	1.26	1.35
14	2	4006	BCR	C10-C9	-6.94	1.26	1.35
14	1	4002	BCR	C10-C9	-6.93	1.26	1.35
14	b	4014	BCR	C10-C9	-6.89	1.26	1.35
14	1	4007	BCR	C10-C9	-6.87	1.26	1.35
14	A	4008	BCR	C10-C9	-6.82	1.26	1.35
14	l	4019	BCR	C10-C9	-6.82	1.26	1.35
14	2	4004	BCR	C10-C9	-6.81	1.26	1.35
14	2	4005	BCR	C10-C9	-6.76	1.26	1.35
14	B	4010	BCR	C10-C9	-6.66	1.27	1.35
14	b	4009	BCR	C10-C9	-6.63	1.27	1.35
14	1	4008	BCR	C10-C9	-6.42	1.27	1.35
14	a	4003	BCR	C10-C9	-6.40	1.27	1.35
14	a	4008	BCR	C10-C9	-6.31	1.27	1.35
14	L	4022	BCR	C10-C9	-6.12	1.27	1.35
14	6	4013	BCR	C10-C9	-6.08	1.27	1.35
14	f	4013	BCR	C10-C9	-5.98	1.27	1.35
14	F	4018	BCR	C11-C12	-3.61	1.25	1.34
14	A	4003	BCR	C11-C12	-3.47	1.25	1.34
14	m	4021	BCR	C11-C12	-3.47	1.25	1.34
14	2	4014	BCR	C11-C12	-3.41	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	6	4020	BCR	C11-C12	-3.38	1.25	1.34
14	6	4018	BCR	C11-C12	-3.32	1.25	1.34
14	M	4021	BCR	C11-C12	-3.32	1.25	1.34
14	2	4010	BCR	C11-C12	-3.31	1.26	1.34
14	b	4017	BCR	C11-C12	-3.27	1.26	1.34
14	2	4011	BCR	C11-C12	-3.26	1.26	1.34
14	1	4003	BCR	C11-C12	-3.25	1.26	1.34
14	B	4011	BCR	C11-C12	-3.25	1.26	1.34
14	7	4021	BCR	C11-C12	-3.25	1.26	1.34
14	f	4020	BCR	C11-C12	-3.24	1.26	1.34
14	B	4004	BCR	C11-C12	-3.23	1.26	1.34
14	B	4009	BCR	C11-C12	-3.22	1.26	1.34
14	b	4004	BCR	C11-C12	-3.21	1.26	1.34
14	b	4010	BCR	C11-C12	-3.20	1.26	1.34
14	B	4005	BCR	C11-C12	-3.20	1.26	1.34
14	A	4001	BCR	C11-C12	-3.19	1.26	1.34
14	b	4014	BCR	C11-C12	-3.19	1.26	1.34
14	F	4020	BCR	C11-C12	-3.19	1.26	1.34
14	b	4005	BCR	C11-C12	-3.17	1.26	1.34
14	a	4008	BCR	C11-C12	-3.15	1.26	1.34
14	f	4018	BCR	C11-C12	-3.15	1.26	1.34
14	b	4011	BCR	C11-C12	-3.15	1.26	1.34
14	A	4007	BCR	C11-C12	-3.14	1.26	1.34
14	8	4022	BCR	C11-C12	-3.14	1.26	1.34
14	2	4017	BCR	C11-C12	-3.12	1.26	1.34
14	1	4008	BCR	C11-C12	-3.12	1.26	1.34
14	b	4006	BCR	C11-C12	-3.12	1.26	1.34
14	l	4019	BCR	C11-C12	-3.11	1.26	1.34
14	F	4013	BCR	C11-C12	-3.11	1.26	1.34
14	f	4013	BCR	C11-C12	-3.11	1.26	1.34
14	B	4017	BCR	C11-C12	-3.10	1.26	1.34
14	2	4006	BCR	C11-C12	-3.07	1.26	1.34
14	l	4022	BCR	C11-C12	-3.07	1.26	1.34
14	a	4007	BCR	C11-C12	-3.06	1.26	1.34
14	B	4006	BCR	C11-C12	-3.05	1.26	1.34
14	L	4019	BCR	C11-C12	-3.05	1.26	1.34
14	a	4001	BCR	C11-C12	-3.04	1.26	1.34
14	2	4009	BCR	C11-C12	-3.03	1.26	1.34
14	a	4002	BCR	C11-C12	-3.03	1.26	1.34
14	2	4005	BCR	C11-C12	-3.02	1.26	1.34
14	1	4001	BCR	C11-C12	-3.02	1.26	1.34
14	a	4003	BCR	C11-C12	-3.02	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	4004	BCR	C11-C12	-3.00	1.26	1.34
14	1	4002	BCR	C11-C12	-3.00	1.26	1.34
14	L	4022	BCR	C11-C12	-2.99	1.26	1.34
14	A	4008	BCR	C11-C12	-2.98	1.26	1.34
14	B	4010	BCR	C11-C12	-2.97	1.26	1.34
14	1	4007	BCR	C11-C12	-2.96	1.26	1.34
14	B	4014	BCR	C11-C12	-2.96	1.26	1.34
14	6	4013	BCR	C11-C12	-2.94	1.26	1.34
14	8	4019	BCR	C11-C12	-2.94	1.26	1.34
14	A	4002	BCR	C11-C12	-2.92	1.27	1.34
14	b	4009	BCR	C11-C12	-2.83	1.27	1.34
11	2	1207	CLA	C1C-NC	-2.59	1.33	1.37
11	A	1801	CLA	C1C-NC	-2.55	1.33	1.37
11	A	1140	CLA	C1C-NC	-2.53	1.33	1.37
11	a	1119	CLA	C1C-NC	-2.48	1.33	1.37
11	b	1207	CLA	C1C-NC	-2.45	1.33	1.37
11	B	1230	CLA	C1C-NC	-2.43	1.33	1.37
11	K	1402	CLA	C1C-NC	-2.42	1.33	1.37
11	2	1023	CLA	C1C-NC	-2.40	1.33	1.37
14	f	4018	BCR	C30-C25	-2.38	1.50	1.53
11	a	1125	CLA	C1C-NC	-2.38	1.33	1.37
11	A	1119	CLA	C1C-NC	-2.37	1.33	1.37
11	A	1133	CLA	C1C-NC	-2.36	1.33	1.37
11	2	1230	CLA	C1C-NC	-2.36	1.33	1.37
11	1	1128	CLA	C1C-NC	-2.36	1.33	1.37
11	B	1023	CLA	C1C-NC	-2.35	1.33	1.37
11	a	1128	CLA	C1C-NC	-2.35	1.33	1.37
11	B	1206	CLA	C1C-NC	-2.35	1.33	1.37
11	2	1212	CLA	C1C-NC	-2.34	1.33	1.37
11	A	1135	CLA	C1C-NC	-2.34	1.33	1.37
11	1	1115	CLA	C1C-NC	-2.33	1.34	1.37
11	k	1402	CLA	C1C-NC	-2.32	1.34	1.37
11	B	1234	CLA	C1C-NC	-2.32	1.34	1.37
11	B	1201	CLA	C1C-NC	-2.32	1.34	1.37
11	B	1207	CLA	C1C-NC	-2.31	1.34	1.37
11	A	1123	CLA	C1C-NC	-2.31	1.34	1.37
11	1	1801	CLA	C1C-NC	-2.31	1.34	1.37
11	B	1229	CLA	C1C-NC	-2.31	1.34	1.37
11	b	1234	CLA	C1C-NC	-2.30	1.34	1.37
11	2	1214	CLA	C1C-NC	-2.30	1.34	1.37
14	6	4018	BCR	C30-C25	-2.29	1.50	1.53
11	A	1125	CLA	C1C-NC	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1237	CLA	C1C-NC	-2.29	1.34	1.37
11	B	1218	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1227	CLA	C1C-NC	-2.28	1.34	1.37
11	A	1122	CLA	C1C-NC	-2.28	1.34	1.37
11	B	1228	CLA	C1C-NC	-2.28	1.34	1.37
11	A	1012	CLA	C1C-NC	-2.27	1.34	1.37
11	A	1106	CLA	C1C-NC	-2.27	1.34	1.37
11	b	1239	CLA	C1C-NC	-2.27	1.34	1.37
11	2	1218	CLA	C1C-NC	-2.27	1.34	1.37
11	2	1208	CLA	C1C-NC	-2.27	1.34	1.37
11	A	1110	CLA	C1C-NC	-2.26	1.34	1.37
11	A	1128	CLA	C1C-NC	-2.26	1.34	1.37
11	a	1124	CLA	C1C-NC	-2.26	1.34	1.37
11	B	1203	CLA	C1C-NC	-2.26	1.34	1.37
11	a	1115	CLA	C1C-NC	-2.26	1.34	1.37
11	1	1107	CLA	C1C-NC	-2.26	1.34	1.37
11	a	1118	CLA	C1C-NC	-2.26	1.34	1.37
11	b	1238	CLA	C1C-NC	-2.25	1.34	1.37
11	1	1106	CLA	C1C-NC	-2.25	1.34	1.37
11	B	1205	CLA	C1C-NC	-2.24	1.34	1.37
11	A	1129	CLA	C1C-NC	-2.24	1.34	1.37
11	1	1138	CLA	C1C-NC	-2.24	1.34	1.37
11	a	1110	CLA	C1C-NC	-2.24	1.34	1.37
11	A	1114	CLA	C1C-NC	-2.24	1.34	1.37
11	1	1109	CLA	C1C-NC	-2.24	1.34	1.37
11	B	1210	CLA	C1C-NC	-2.24	1.34	1.37
11	1	1111	CLA	C1C-NC	-2.24	1.34	1.37
11	b	1209	CLA	C1C-NC	-2.24	1.34	1.37
11	1	1133	CLA	C1C-NC	-2.23	1.34	1.37
11	b	1205	CLA	C1C-NC	-2.23	1.34	1.37
11	b	1206	CLA	C1C-NC	-2.23	1.34	1.37
11	B	1013	CLA	C1C-NC	-2.23	1.34	1.37
11	1	1125	CLA	C1C-NC	-2.23	1.34	1.37
11	b	1023	CLA	C1C-NC	-2.23	1.34	1.37
11	A	1136	CLA	C1C-NC	-2.23	1.34	1.37
11	a	1135	CLA	C1C-NC	-2.23	1.34	1.37
11	2	1238	CLA	C1C-NC	-2.22	1.34	1.37
11	2	1240	CLA	C1C-NC	-2.22	1.34	1.37
11	b	1230	CLA	C1C-NC	-2.22	1.34	1.37
11	A	1138	CLA	C1C-NC	-2.22	1.34	1.37
11	2	1224	CLA	C1C-NC	-2.22	1.34	1.37
11	a	1136	CLA	C1C-NC	-2.22	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1021	CLA	C1C-NC	-2.22	1.34	1.37
11	2	1227	CLA	C1C-NC	-2.22	1.34	1.37
11	8	1501	CLA	C1C-NC	-2.22	1.34	1.37
11	2	1226	CLA	C1C-NC	-2.21	1.34	1.37
11	1	1117	CLA	C1C-NC	-2.21	1.34	1.37
11	A	1022	CLA	C1C-NC	-2.21	1.34	1.37
11	a	1237	CLA	C1C-NC	-2.21	1.34	1.37
11	b	1212	CLA	C1C-NC	-2.21	1.34	1.37
11	B	1224	CLA	C1C-NC	-2.21	1.34	1.37
11	a	1106	CLA	C1C-NC	-2.21	1.34	1.37
11	a	1127	CLA	C1C-NC	-2.21	1.34	1.37
11	A	1108	CLA	C1C-NC	-2.21	1.34	1.37
11	a	1133	CLA	C1C-NC	-2.21	1.34	1.37
11	A	1124	CLA	C1C-NC	-2.21	1.34	1.37
11	A	1118	CLA	C1C-NC	-2.21	1.34	1.37
11	2	1206	CLA	C1C-NC	-2.21	1.34	1.37
14	6	4020	BCR	C30-C25	-2.21	1.50	1.53
11	a	1116	CLA	C1C-NC	-2.21	1.34	1.37
11	L	1502	CLA	C1C-NC	-2.20	1.34	1.37
11	a	1138	CLA	C1C-NC	-2.20	1.34	1.37
11	1	1012	CLA	C1C-NC	-2.20	1.34	1.37
11	B	1226	CLA	C1C-NC	-2.20	1.34	1.37
11	B	1232	CLA	C1C-NC	-2.20	1.34	1.37
11	0	1402	CLA	C1C-NC	-2.20	1.34	1.37
11	A	1107	CLA	C1C-NC	-2.20	1.34	1.37
11	2	1205	CLA	C1C-NC	-2.20	1.34	1.37
11	B	1215	CLA	C1C-NC	-2.20	1.34	1.37
11	b	1201	CLA	C1C-NC	-2.20	1.34	1.37
11	A	1134	CLA	C1C-NC	-2.20	1.34	1.37
11	b	1217	CLA	C1C-NC	-2.20	1.34	1.37
11	1	1104	CLA	C1C-NC	-2.19	1.34	1.37
11	1	1131	CLA	C1C-NC	-2.19	1.34	1.37
11	1	1136	CLA	C1C-NC	-2.19	1.34	1.37
11	2	1201	CLA	C1C-NC	-2.19	1.34	1.37
11	2	1203	CLA	C1C-NC	-2.19	1.34	1.37
11	1	1237	CLA	C1C-NC	-2.18	1.34	1.37
11	b	1228	CLA	C1C-NC	-2.18	1.34	1.37
11	a	1134	CLA	C1C-NC	-2.18	1.34	1.37
11	1	1118	CLA	C1C-NC	-2.18	1.34	1.37
11	b	1214	CLA	C1C-NC	-2.18	1.34	1.37
11	1	1105	CLA	C1C-NC	-2.18	1.34	1.37
11	b	1220	CLA	C1C-NC	-2.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1211	CLA	C1C-NC	-2.18	1.34	1.37
11	1	1130	CLA	C1C-NC	-2.18	1.34	1.37
11	2	1239	CLA	C1C-NC	-2.18	1.34	1.37
11	2	1215	CLA	C1C-NC	-2.18	1.34	1.37
11	B	1216	CLA	C1C-NC	-2.17	1.34	1.37
11	1	1140	CLA	C1C-NC	-2.17	1.34	1.37
11	B	1219	CLA	C1C-NC	-2.17	1.34	1.37
11	1	1119	CLA	C1C-NC	-2.17	1.34	1.37
14	2	4017	BCR	C30-C25	-2.17	1.50	1.53
11	A	1109	CLA	C1C-NC	-2.17	1.34	1.37
11	a	1105	CLA	C1C-NC	-2.17	1.34	1.37
14	B	4011	BCR	C1-C6	-2.17	1.50	1.53
11	a	1130	CLA	C1C-NC	-2.17	1.34	1.37
11	B	1238	CLA	C1C-NC	-2.17	1.34	1.37
11	2	1210	CLA	C1C-NC	-2.17	1.34	1.37
11	b	1240	CLA	C1C-NC	-2.17	1.34	1.37
11	8	1502	CLA	C1C-NC	-2.16	1.34	1.37
11	1	1011	CLA	C1C-NC	-2.16	1.34	1.37
11	2	1217	CLA	C1C-NC	-2.16	1.34	1.37
11	k	1401	CLA	C1C-NC	-2.16	1.34	1.37
11	B	1209	CLA	C1C-NC	-2.16	1.34	1.37
11	1	1132	CLA	C1C-NC	-2.16	1.34	1.37
11	2	1220	CLA	C1C-NC	-2.16	1.34	1.37
11	A	1137	CLA	C1C-NC	-2.16	1.34	1.37
11	1	1127	CLA	C1C-NC	-2.16	1.34	1.37
11	A	1132	CLA	C1C-NC	-2.16	1.34	1.37
11	2	1013	CLA	C1C-NC	-2.16	1.34	1.37
11	2	1213	CLA	C1C-NC	-2.15	1.34	1.37
11	a	1120	CLA	C1C-NC	-2.15	1.34	1.37
11	B	1239	CLA	C1C-NC	-2.15	1.34	1.37
11	b	1204	CLA	C1C-NC	-2.15	1.34	1.37
11	b	1222	CLA	C1C-NC	-2.15	1.34	1.37
11	a	1131	CLA	C1C-NC	-2.15	1.34	1.37
11	b	1223	CLA	C1C-NC	-2.15	1.34	1.37
11	a	1022	CLA	C1C-NC	-2.14	1.34	1.37
11	B	1217	CLA	C1C-NC	-2.14	1.34	1.37
11	B	1204	CLA	C1C-NC	-2.14	1.34	1.37
11	a	1101	CLA	C1C-NC	-2.14	1.34	1.37
11	1	1114	CLA	C1C-NC	-2.14	1.34	1.37
11	1	1135	CLA	C1C-NC	-2.14	1.34	1.37
11	1	1101	CLA	C1C-NC	-2.14	1.34	1.37
11	a	1132	CLA	C1C-NC	-2.14	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1401	CLA	C1C-NC	-2.14	1.34	1.37
11	0	1401	CLA	C1C-NC	-2.14	1.34	1.37
11	1	1103	CLA	C1C-NC	-2.14	1.34	1.37
11	A	1117	CLA	C1C-NC	-2.14	1.34	1.37
11	b	1208	CLA	C1C-NC	-2.14	1.34	1.37
11	L	1501	CLA	C1C-NC	-2.14	1.34	1.37
11	a	1111	CLA	C1C-NC	-2.13	1.34	1.37
11	A	1120	CLA	C1C-NC	-2.13	1.34	1.37
11	B	1231	CLA	C1C-NC	-2.13	1.34	1.37
11	1	1022	CLA	C1C-NC	-2.13	1.34	1.37
11	B	1221	CLA	C1C-NC	-2.13	1.34	1.37
14	F	4018	BCR	C30-C25	-2.13	1.50	1.53
11	1	1124	CLA	C1C-NC	-2.13	1.34	1.37
11	a	1140	CLA	C1C-NC	-2.13	1.34	1.37
11	b	1219	CLA	C1C-NC	-2.13	1.34	1.37
11	a	1117	CLA	C1C-NC	-2.13	1.34	1.37
11	2	1234	CLA	C1C-NC	-2.12	1.34	1.37
11	a	1122	CLA	C1C-NC	-2.12	1.34	1.37
11	a	1103	CLA	C1C-NC	-2.12	1.34	1.37
11	A	1127	CLA	C1C-NC	-2.12	1.34	1.37
11	B	1220	CLA	C1C-NC	-2.12	1.34	1.37
11	A	1105	CLA	C1C-NC	-2.12	1.34	1.37
11	a	1129	CLA	C1C-NC	-2.12	1.34	1.37
11	a	1114	CLA	C1C-NC	-2.12	1.34	1.37
11	A	1104	CLA	C1C-NC	-2.12	1.34	1.37
11	A	1101	CLA	C1C-NC	-2.12	1.34	1.37
11	a	1137	CLA	C1C-NC	-2.12	1.34	1.37
14	b	4017	BCR	C30-C25	-2.12	1.50	1.53
11	b	1229	CLA	C1C-NC	-2.11	1.34	1.37
11	2	1228	CLA	C1C-NC	-2.11	1.34	1.37
11	a	1801	CLA	C1C-NC	-2.11	1.34	1.37
11	A	1115	CLA	C1C-NC	-2.11	1.34	1.37
11	B	1222	CLA	C1C-NC	-2.11	1.34	1.37
11	l	1501	CLA	C1C-NC	-2.11	1.34	1.37
11	b	1210	CLA	C1C-NC	-2.11	1.34	1.37
11	2	1204	CLA	C1C-NC	-2.11	1.34	1.37
11	b	1013	CLA	C1C-NC	-2.11	1.34	1.37
11	2	1202	CLA	C1C-NC	-2.11	1.34	1.37
11	b	1218	CLA	C1C-NC	-2.11	1.34	1.37
11	L	1503	CLA	C1C-NC	-2.11	1.34	1.37
11	B	1236	CLA	C1C-NC	-2.11	1.34	1.37
11	B	1214	CLA	C1C-NC	-2.11	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	1503	CLA	C1C-NC	-2.11	1.34	1.37
14	a	4008	BCR	C30-C25	-2.11	1.50	1.53
11	a	1012	CLA	C1C-NC	-2.10	1.34	1.37
11	1	1137	CLA	C1C-NC	-2.10	1.34	1.37
11	a	1107	CLA	C1C-NC	-2.10	1.34	1.37
11	b	1224	CLA	C1C-NC	-2.10	1.34	1.37
11	b	1203	CLA	C1C-NC	-2.10	1.34	1.37
11	1	1134	CLA	C1C-NC	-2.10	1.34	1.37
11	1	1110	CLA	C1C-NC	-2.10	1.34	1.37
11	A	1130	CLA	C1C-NC	-2.10	1.34	1.37
11	l	1502	CLA	C1C-NC	-2.10	1.34	1.37
11	A	1103	CLA	C1C-NC	-2.09	1.34	1.37
11	2	1209	CLA	C1C-NC	-2.09	1.34	1.37
11	1	1120	CLA	C1C-NC	-2.09	1.34	1.37
11	A	1121	CLA	C1C-NC	-2.09	1.34	1.37
11	A	1011	CLA	C1C-NC	-2.09	1.34	1.37
11	2	1223	CLA	C1C-NC	-2.09	1.34	1.37
11	A	1111	CLA	C1C-NC	-2.08	1.34	1.37
11	1	1108	CLA	C1C-NC	-2.08	1.34	1.37
11	a	1108	CLA	C1C-NC	-2.08	1.34	1.37
11	a	1104	CLA	C1C-NC	-2.08	1.34	1.37
11	1	1122	CLA	C1C-NC	-2.08	1.34	1.37
11	B	1021	CLA	C4C-NC	-2.08	1.34	1.37
11	b	1215	CLA	C1C-NC	-2.08	1.34	1.37
11	2	1211	CLA	C1C-NC	-2.08	1.34	1.37
11	B	1202	CLA	C1C-NC	-2.08	1.34	1.37
11	1	1121	CLA	C1C-NC	-2.08	1.34	1.37
11	2	1231	CLA	C1C-NC	-2.07	1.34	1.37
14	A	4008	BCR	C30-C25	-2.07	1.50	1.53
11	a	1102	CLA	C1C-NC	-2.07	1.34	1.37
11	b	1211	CLA	C1C-NC	-2.07	1.34	1.37
14	B	4014	BCR	C30-C25	-2.07	1.51	1.53
11	1	1129	CLA	C1C-NC	-2.07	1.34	1.37
11	8	1503	CLA	C1C-NC	-2.07	1.34	1.37
11	a	1011	CLA	C1C-NC	-2.06	1.34	1.37
11	b	1226	CLA	C1C-NC	-2.06	1.34	1.37
11	A	1131	CLA	C1C-NC	-2.06	1.34	1.37
14	B	4005	BCR	C30-C25	-2.06	1.51	1.53
11	a	1121	CLA	C1C-NC	-2.06	1.34	1.37
11	2	1235	CLA	C1C-NC	-2.06	1.34	1.37
11	2	1222	CLA	C1C-NC	-2.06	1.34	1.37
11	2	1229	CLA	C1C-NC	-2.06	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1219	CLA	C1C-NC	-2.05	1.34	1.37
11	B	1223	CLA	C1C-NC	-2.05	1.34	1.37
11	1	1126	CLA	C1C-NC	-2.05	1.34	1.37
11	A	1011	CLA	C4C-NC	-2.05	1.34	1.37
11	B	1208	CLA	C1C-NC	-2.05	1.34	1.37
11	b	1021	CLA	C1C-NC	-2.05	1.34	1.37
11	A	1102	CLA	C1C-NC	-2.05	1.34	1.37
11	B	1212	CLA	C1C-NC	-2.05	1.34	1.37
11	b	1231	CLA	C1C-NC	-2.05	1.34	1.37
11	B	1225	CLA	C1C-NC	-2.04	1.34	1.37
11	1	1123	CLA	C1C-NC	-2.04	1.34	1.37
11	1	1139	CLA	C1C-NC	-2.04	1.34	1.37
11	B	1213	CLA	C1C-NC	-2.04	1.34	1.37
11	b	1227	CLA	C1C-NC	-2.04	1.34	1.37
11	a	1109	CLA	C1C-NC	-2.04	1.34	1.37
11	b	1202	CLA	C1C-NC	-2.04	1.34	1.37
11	2	1021	CLA	C1C-NC	-2.04	1.34	1.37
11	A	1113	CLA	C1C-NC	-2.04	1.34	1.37
11	A	1104	CLA	C4C-NC	-2.03	1.34	1.37
11	A	1118	CLA	C4C-NC	-2.03	1.34	1.37
11	2	1221	CLA	C1C-NC	-2.03	1.34	1.37
11	2	1232	CLA	C1C-NC	-2.02	1.34	1.37
11	2	1236	CLA	C1C-NC	-2.01	1.34	1.37
11	b	1235	CLA	C1C-NC	-2.01	1.34	1.37
11	a	1139	CLA	C1C-NC	-2.01	1.34	1.37
14	b	4014	BCR	C30-C25	-2.01	1.51	1.53
11	B	1235	CLA	C1C-NC	-2.01	1.34	1.37
11	1	1113	CLA	C1C-NC	-2.01	1.34	1.37
11	b	1225	CLA	C1C-NC	-2.00	1.34	1.37
11	2	1205	CLA	C4C-NC	-2.00	1.34	1.37
11	b	1232	CLA	C1C-NC	-2.00	1.34	1.37
11	a	1137	CLA	C1C-C2C	2.00	1.48	1.44
11	1	1137	CLA	C1C-C2C	2.00	1.48	1.44
11	2	1221	CLA	C4C-C3C	2.00	1.48	1.45
11	a	1114	CLA	C1C-C2C	2.00	1.48	1.44
11	1	1113	CLA	C1C-C2C	2.00	1.48	1.44
11	B	1021	CLA	C4C-C3C	2.00	1.48	1.45
11	1	1114	CLA	C1C-C2C	2.00	1.48	1.44
11	2	1212	CLA	C1C-C2C	2.00	1.48	1.44
11	a	1801	CLA	C1C-C2C	2.00	1.48	1.44
11	a	1125	CLA	C4C-C3C	2.01	1.48	1.45
11	B	1203	CLA	C1C-C2C	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1125	CLA	C1C-C2C	2.01	1.48	1.44
11	1	1011	CLA	C4C-C3C	2.01	1.48	1.45
11	2	1239	CLA	C1C-C2C	2.01	1.48	1.44
11	1	1011	CLA	C1A-CHA	2.01	1.51	1.43
11	1	1112	CLA	C1C-C2C	2.01	1.48	1.44
11	l	1501	CLA	C4C-C3C	2.01	1.48	1.45
11	1	1801	CLA	C1C-C2C	2.01	1.48	1.44
11	1	1131	CLA	C1C-C2C	2.01	1.48	1.44
11	2	1231	CLA	C1C-C2C	2.01	1.48	1.44
11	1	1115	CLA	C1C-C2C	2.02	1.48	1.44
11	2	1208	CLA	C4C-C3C	2.02	1.48	1.45
11	b	1211	CLA	C1C-C2C	2.02	1.48	1.44
11	1	1104	CLA	C1C-C2C	2.02	1.48	1.44
11	B	1239	CLA	C1C-C2C	2.02	1.48	1.44
11	a	1124	CLA	C1C-C2C	2.03	1.48	1.44
11	a	1125	CLA	C1C-C2C	2.03	1.48	1.44
11	b	1218	CLA	C1C-C2C	2.03	1.48	1.44
11	b	1225	CLA	C1C-C2C	2.03	1.48	1.44
11	A	1121	CLA	C1C-C2C	2.03	1.48	1.44
11	1	1122	CLA	C4C-C3C	2.03	1.48	1.45
11	a	1122	CLA	C4C-C3C	2.03	1.48	1.45
11	2	1219	CLA	C4C-C3C	2.03	1.48	1.45
11	b	1230	CLA	C1C-C2C	2.03	1.48	1.44
11	a	1132	CLA	C1C-C2C	2.03	1.48	1.44
11	B	1219	CLA	C1C-C2C	2.03	1.48	1.44
11	A	1113	CLA	C4C-C3C	2.03	1.48	1.45
11	1	1124	CLA	C1C-C2C	2.04	1.48	1.44
11	A	1105	CLA	C1C-C2C	2.04	1.48	1.44
11	l	1503	CLA	C1C-C2C	2.04	1.48	1.44
11	A	1139	CLA	C4C-C3C	2.04	1.48	1.45
11	b	1231	CLA	C1C-C2C	2.04	1.48	1.44
11	a	1139	CLA	C1C-C2C	2.04	1.48	1.44
11	B	1212	CLA	C4C-C3C	2.04	1.48	1.45
11	1	1118	CLA	C1C-C2C	2.04	1.48	1.44
11	2	1203	CLA	C4C-C3C	2.04	1.48	1.45
11	2	1224	CLA	C1C-C2C	2.04	1.48	1.44
11	A	1120	CLA	C1C-C2C	2.04	1.48	1.44
11	8	1503	CLA	C1C-C2C	2.05	1.48	1.44
11	2	1202	CLA	C4C-C3C	2.05	1.48	1.45
11	A	1102	CLA	C1C-C2C	2.05	1.48	1.44
11	a	1022	CLA	C1C-C2C	2.05	1.48	1.44
11	1	1138	CLA	C4C-C3C	2.05	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1221	CLA	C4C-C3C	2.05	1.48	1.45
11	A	1113	CLA	C1C-C2C	2.05	1.48	1.44
11	1	1116	CLA	C1C-C2C	2.05	1.48	1.44
11	A	1105	CLA	C4C-C3C	2.05	1.48	1.45
11	2	1204	CLA	C1C-C2C	2.05	1.48	1.44
11	a	1110	CLA	C1C-C2C	2.05	1.48	1.44
11	2	1238	CLA	C1C-C2C	2.05	1.48	1.44
11	2	1235	CLA	C4C-C3C	2.05	1.48	1.45
11	a	1111	CLA	C4C-C3C	2.05	1.48	1.45
11	b	1216	CLA	C1C-C2C	2.05	1.48	1.44
11	A	1130	CLA	C1C-C2C	2.05	1.48	1.44
11	2	1205	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1137	CLA	C4C-C3C	2.06	1.48	1.45
11	2	1207	CLA	C4C-C3C	2.06	1.48	1.45
11	2	1222	CLA	C4C-C3C	2.06	1.48	1.45
11	A	1127	CLA	C1C-C2C	2.06	1.48	1.44
11	2	1224	CLA	C4C-C3C	2.06	1.48	1.45
11	A	1108	CLA	C4C-C3C	2.06	1.48	1.45
11	B	1214	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1119	CLA	C1C-C2C	2.06	1.48	1.44
11	B	1202	CLA	C1C-C2C	2.06	1.48	1.44
11	b	1227	CLA	C1C-C2C	2.06	1.48	1.44
11	b	1222	CLA	C1C-C2C	2.06	1.48	1.44
11	a	1103	CLA	C1C-C2C	2.06	1.48	1.44
11	2	1218	CLA	C4C-C3C	2.06	1.48	1.45
11	a	1109	CLA	C1C-C2C	2.06	1.48	1.44
11	1	1135	CLA	C4C-C3C	2.06	1.48	1.45
11	A	1130	CLA	C4C-C3C	2.06	1.48	1.45
11	b	1204	CLA	C4C-C3C	2.07	1.48	1.45
11	K	1402	CLA	C4C-C3C	2.07	1.48	1.45
11	a	1123	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1107	CLA	C1A-CHA	2.07	1.51	1.43
11	1	1130	CLA	C1C-C2C	2.07	1.48	1.44
11	A	1012	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1226	CLA	C1C-C2C	2.07	1.48	1.44
11	B	1013	CLA	C4C-C3C	2.07	1.48	1.45
11	0	1402	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1203	CLA	C4C-C3C	2.07	1.48	1.45
11	L	1501	CLA	C1C-C2C	2.07	1.48	1.44
11	1	1123	CLA	C1C-C2C	2.07	1.48	1.44
11	a	1112	CLA	C1C-C2C	2.07	1.48	1.44
11	2	1228	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1124	CLA	C4C-C3C	2.07	1.48	1.45
11	a	1106	CLA	C1C-C2C	2.07	1.48	1.44
11	1	1022	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1214	CLA	C1C-C2C	2.07	1.48	1.44
11	b	1210	CLA	C1C-C2C	2.08	1.48	1.44
11	a	1011	CLA	C1A-CHA	2.08	1.51	1.43
11	B	1221	CLA	C1C-C2C	2.08	1.48	1.44
11	a	1012	CLA	C4C-C3C	2.08	1.48	1.45
11	2	1228	CLA	C4C-C3C	2.08	1.48	1.45
11	b	1220	CLA	C1C-C2C	2.08	1.48	1.44
11	1	1126	CLA	C4C-C3C	2.08	1.48	1.45
11	2	1222	CLA	C1C-C2C	2.08	1.48	1.44
11	1	1108	CLA	C1C-C2C	2.08	1.48	1.44
11	1	1122	CLA	C1C-C2C	2.08	1.48	1.44
11	a	1121	CLA	C1C-C2C	2.08	1.48	1.44
11	A	1022	CLA	C1C-C2C	2.08	1.48	1.44
11	b	1229	CLA	C4C-C3C	2.08	1.48	1.45
11	a	1120	CLA	C1C-C2C	2.09	1.48	1.44
11	b	1229	CLA	C1C-C2C	2.09	1.48	1.44
11	1	1107	CLA	C4C-C3C	2.09	1.48	1.45
11	2	1013	CLA	C4C-C3C	2.09	1.48	1.45
11	1	1129	CLA	C1C-C2C	2.09	1.48	1.44
11	b	1232	CLA	C1C-C2C	2.09	1.48	1.44
11	a	1113	CLA	C1C-C2C	2.09	1.48	1.44
11	2	1210	CLA	C4C-C3C	2.09	1.48	1.45
11	a	1102	CLA	C1C-C2C	2.09	1.48	1.44
11	a	1117	CLA	C4C-C3C	2.09	1.48	1.45
11	l	1502	CLA	C1C-C2C	2.09	1.48	1.44
11	A	1127	CLA	C4C-C3C	2.09	1.48	1.45
11	A	1012	CLA	C4C-C3C	2.09	1.48	1.45
11	a	1111	CLA	C1C-C2C	2.09	1.48	1.44
11	A	1109	CLA	C4C-C3C	2.09	1.48	1.45
11	b	1023	CLA	C4C-C3C	2.10	1.48	1.45
11	B	1217	CLA	C1C-C2C	2.10	1.48	1.44
11	a	1132	CLA	C4C-C3C	2.10	1.48	1.45
11	2	1216	CLA	C1C-C2C	2.10	1.48	1.44
11	b	1217	CLA	C1C-C2C	2.10	1.48	1.44
11	b	1226	CLA	C4C-C3C	2.10	1.48	1.45
11	B	1221	CLA	CHD-C4C	2.10	1.47	1.41
11	a	1120	CLA	C4C-C3C	2.10	1.48	1.45
11	2	1205	CLA	CHD-C4C	2.10	1.47	1.41
11	b	1224	CLA	C1C-C2C	2.10	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1225	CLA	C4C-C3C	2.10	1.48	1.45
11	b	1240	CLA	C1C-C2C	2.10	1.48	1.44
11	1	1120	CLA	C1C-C2C	2.10	1.48	1.44
11	B	1202	CLA	C4C-C3C	2.10	1.48	1.45
11	a	1136	CLA	C4C-C3C	2.11	1.48	1.45
11	2	1221	CLA	C1C-C2C	2.11	1.48	1.44
11	2	1232	CLA	C1C-C2C	2.11	1.48	1.44
11	B	1224	CLA	C1C-C2C	2.11	1.48	1.44
11	b	1212	CLA	C4C-C3C	2.11	1.48	1.45
11	B	1235	CLA	C1C-C2C	2.11	1.48	1.44
11	B	1235	CLA	C4C-C3C	2.11	1.48	1.45
11	2	1235	CLA	C1C-C2C	2.11	1.48	1.44
11	b	1235	CLA	C1C-C2C	2.11	1.48	1.44
11	1	1139	CLA	C1C-C2C	2.11	1.48	1.44
11	A	1115	CLA	C4C-C3C	2.11	1.48	1.45
11	B	1214	CLA	C4C-C3C	2.11	1.48	1.45
11	B	1213	CLA	C4C-C3C	2.11	1.48	1.45
11	2	1234	CLA	C4C-C3C	2.11	1.48	1.45
11	2	1236	CLA	C1C-C2C	2.11	1.48	1.44
11	a	1101	CLA	C4C-C3C	2.11	1.48	1.45
11	b	1207	CLA	C4C-C3C	2.11	1.48	1.45
11	8	1502	CLA	C1C-C2C	2.11	1.48	1.44
11	b	1213	CLA	C1C-C2C	2.12	1.48	1.44
11	b	1212	CLA	C1C-C2C	2.12	1.48	1.44
11	B	1230	CLA	C4C-C3C	2.12	1.48	1.45
11	A	1116	CLA	C4C-C3C	2.12	1.48	1.45
11	A	1121	CLA	C4C-C3C	2.12	1.48	1.45
11	b	1222	CLA	C4C-C3C	2.12	1.48	1.45
11	1	1131	CLA	C4C-C3C	2.12	1.48	1.45
11	B	1208	CLA	C1C-C2C	2.12	1.48	1.44
11	b	1214	CLA	C4C-C3C	2.12	1.48	1.45
11	1	1140	CLA	C4C-C3C	2.13	1.48	1.45
11	1	1140	CLA	C1C-C2C	2.13	1.48	1.44
11	2	1229	CLA	C1C-C2C	2.13	1.48	1.44
11	b	1236	CLA	C1C-C2C	2.13	1.48	1.44
11	1	1237	CLA	C4C-C3C	2.13	1.48	1.45
11	B	1224	CLA	CHD-C4C	2.13	1.47	1.41
11	A	1122	CLA	CHD-C4C	2.13	1.47	1.41
11	1	1012	CLA	CHD-C4C	2.13	1.47	1.41
11	A	1107	CLA	CHD-C4C	2.13	1.47	1.41
11	A	1137	CLA	C1C-C2C	2.13	1.48	1.44
11	1	1102	CLA	C4C-C3C	2.13	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1130	CLA	C4C-C3C	2.14	1.48	1.45
11	b	1213	CLA	C4C-C3C	2.14	1.48	1.45
11	a	1140	CLA	C4C-C3C	2.14	1.48	1.45
11	1	1135	CLA	C1C-C2C	2.14	1.48	1.44
11	A	1112	CLA	C4C-C3C	2.14	1.48	1.45
11	A	1116	CLA	C1C-C2C	2.14	1.48	1.44
11	b	1221	CLA	CHD-C4C	2.14	1.47	1.41
11	8	1503	CLA	C4C-C3C	2.14	1.48	1.45
11	b	1217	CLA	C4C-C3C	2.14	1.48	1.45
11	B	1023	CLA	CHD-C4C	2.14	1.47	1.41
11	1	1108	CLA	C4C-C3C	2.14	1.48	1.45
11	A	1138	CLA	C4C-C3C	2.15	1.48	1.45
11	1	1117	CLA	C4C-C3C	2.15	1.48	1.45
11	B	1236	CLA	CHD-C4C	2.15	1.47	1.41
11	1	1022	CLA	C4C-C3C	2.15	1.48	1.45
11	a	1011	CLA	C4C-C3C	2.15	1.48	1.45
11	a	1137	CLA	C4C-C3C	2.15	1.48	1.45
11	B	1215	CLA	C4C-C3C	2.15	1.48	1.45
11	2	1213	CLA	C1C-C2C	2.15	1.48	1.44
11	B	1223	CLA	C4C-C3C	2.15	1.48	1.45
11	b	1235	CLA	C4C-C3C	2.15	1.48	1.45
11	8	1502	CLA	CHD-C4C	2.15	1.47	1.41
11	a	1237	CLA	CHD-C4C	2.15	1.47	1.41
11	1	1111	CLA	CHD-C4C	2.15	1.47	1.41
11	2	1213	CLA	C4C-C3C	2.15	1.48	1.45
11	a	1022	CLA	C4C-C3C	2.16	1.48	1.45
11	A	1112	CLA	C1C-C2C	2.16	1.48	1.44
11	B	1223	CLA	C1C-C2C	2.16	1.48	1.44
11	1	1129	CLA	C4C-C3C	2.16	1.48	1.45
11	A	1117	CLA	C4C-C3C	2.16	1.48	1.45
11	B	1212	CLA	C1C-C2C	2.16	1.48	1.44
11	B	1230	CLA	CHD-C4C	2.16	1.47	1.41
11	a	1106	CLA	C4C-C3C	2.16	1.48	1.45
11	b	1202	CLA	C1C-C2C	2.16	1.48	1.44
11	B	1219	CLA	C4C-C3C	2.16	1.48	1.45
11	B	1205	CLA	CHD-C4C	2.16	1.47	1.41
11	2	1238	CLA	C4C-C3C	2.16	1.48	1.45
11	l	1501	CLA	C1C-C2C	2.17	1.48	1.44
11	a	1104	CLA	C1C-C2C	2.17	1.48	1.44
11	l	1502	CLA	CHD-C4C	2.17	1.47	1.41
11	8	1501	CLA	C4C-C3C	2.17	1.48	1.45
11	b	1218	CLA	C4C-C3C	2.17	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1215	CLA	C4C-C3C	2.17	1.48	1.45
11	B	1236	CLA	C1C-C2C	2.18	1.48	1.44
11	b	1238	CLA	C4C-C3C	2.18	1.48	1.45
11	b	1203	CLA	C1C-C2C	2.18	1.48	1.44
11	a	1102	CLA	C4C-C3C	2.18	1.48	1.45
11	1	1105	CLA	C4C-C3C	2.18	1.48	1.45
11	b	1013	CLA	C4C-C3C	2.18	1.48	1.45
11	B	1218	CLA	C4C-C3C	2.18	1.48	1.45
11	1	1109	CLA	C4C-C3C	2.19	1.48	1.45
11	k	1401	CLA	C4C-C3C	2.19	1.48	1.45
11	b	1240	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1112	CLA	C4C-C3C	2.19	1.48	1.45
11	a	1115	CLA	C1C-C2C	2.19	1.48	1.44
11	1	1113	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1115	CLA	C4C-C3C	2.19	1.48	1.45
11	b	1219	CLA	C4C-C3C	2.19	1.48	1.45
11	a	1107	CLA	CHD-C4C	2.19	1.47	1.41
11	a	1115	CLA	CHD-C4C	2.19	1.47	1.41
11	0	1402	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1101	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1121	CLA	C4C-C3C	2.19	1.48	1.45
11	1	1132	CLA	C4C-C3C	2.19	1.48	1.45
11	b	1207	CLA	CHD-C4C	2.20	1.47	1.41
11	1	1106	CLA	C4C-C3C	2.20	1.48	1.45
11	2	1226	CLA	CHD-C4C	2.20	1.47	1.41
11	1	1136	CLA	C4C-C3C	2.20	1.48	1.45
11	b	1224	CLA	C4C-C3C	2.20	1.48	1.45
11	2	1212	CLA	C4C-C3C	2.20	1.48	1.45
11	1	1127	CLA	C4C-C3C	2.20	1.48	1.45
11	2	1230	CLA	CHD-C4C	2.20	1.47	1.41
11	A	1120	CLA	C4C-C3C	2.20	1.48	1.45
11	2	1221	CLA	CHD-C4C	2.20	1.47	1.41
11	1	1107	CLA	CHD-C4C	2.20	1.47	1.41
11	A	1012	CLA	CHD-C4C	2.20	1.47	1.41
11	K	1401	CLA	C4C-C3C	2.21	1.48	1.45
11	B	1240	CLA	C4C-C3C	2.21	1.48	1.45
11	A	1101	CLA	C1C-C2C	2.21	1.48	1.44
11	2	1214	CLA	C4C-C3C	2.21	1.48	1.45
11	A	1111	CLA	C4C-C3C	2.21	1.48	1.45
11	A	1135	CLA	C4C-C3C	2.21	1.48	1.45
11	B	1222	CLA	CHD-C4C	2.21	1.47	1.41
11	B	1234	CLA	C4C-C3C	2.21	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1801	CLA	C4C-C3C	2.21	1.48	1.45
11	1	1012	CLA	C1C-C2C	2.21	1.48	1.44
11	a	1012	CLA	C1C-C2C	2.21	1.48	1.44
11	A	1113	CLA	CHD-C4C	2.22	1.47	1.41
11	2	1224	CLA	CHD-C4C	2.22	1.47	1.41
11	2	1229	CLA	C4C-C3C	2.22	1.48	1.45
11	a	1112	CLA	C4C-C3C	2.22	1.49	1.45
11	A	1132	CLA	C4C-C3C	2.22	1.49	1.45
11	0	1401	CLA	C4C-C3C	2.22	1.49	1.45
11	A	1129	CLA	C4C-C3C	2.22	1.49	1.45
11	b	1215	CLA	C4C-C3C	2.22	1.49	1.45
11	A	1136	CLA	C4C-C3C	2.22	1.49	1.45
11	b	1231	CLA	C4C-C3C	2.22	1.49	1.45
11	B	1226	CLA	CHD-C4C	2.22	1.47	1.41
11	2	1206	CLA	C4C-C3C	2.22	1.49	1.45
11	B	1214	CLA	CHD-C4C	2.23	1.47	1.41
11	2	1223	CLA	C1C-C2C	2.23	1.48	1.44
11	A	1129	CLA	CHD-C4C	2.23	1.47	1.41
11	A	1116	CLA	CHD-C4C	2.23	1.47	1.41
11	1	1126	CLA	C1C-C2C	2.23	1.48	1.44
11	2	1211	CLA	CHD-C4C	2.23	1.47	1.41
11	2	1235	CLA	CHD-C4C	2.23	1.47	1.41
11	A	1102	CLA	C4C-C3C	2.23	1.49	1.45
11	b	1202	CLA	CHD-C4C	2.23	1.47	1.41
11	b	1205	CLA	CHD-C4C	2.24	1.47	1.41
11	a	1128	CLA	C4C-C3C	2.24	1.49	1.45
11	a	1108	CLA	C4C-C3C	2.24	1.49	1.45
11	2	1230	CLA	C4C-C3C	2.24	1.49	1.45
11	2	1210	CLA	CHD-C4C	2.24	1.47	1.41
11	a	1131	CLA	C4C-C3C	2.24	1.49	1.45
11	a	1111	CLA	CHD-C4C	2.24	1.47	1.41
11	k	1402	CLA	C4C-C3C	2.24	1.49	1.45
11	a	1110	CLA	C4C-C3C	2.24	1.49	1.45
11	1	1128	CLA	C4C-C3C	2.24	1.49	1.45
11	a	1126	CLA	CHD-C4C	2.24	1.47	1.41
11	A	1104	CLA	CHD-C4C	2.24	1.47	1.41
11	A	1128	CLA	CHD-C4C	2.25	1.47	1.41
11	2	1236	CLA	CHD-C4C	2.25	1.47	1.41
11	1	1137	CLA	CHD-C4C	2.25	1.47	1.41
11	B	1021	CLA	CHD-C4C	2.25	1.47	1.41
11	b	1210	CLA	CHD-C4C	2.25	1.47	1.41
11	B	1222	CLA	C1C-C2C	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1216	CLA	CHD-C4C	2.25	1.47	1.41
11	A	1101	CLA	CHD-C4C	2.25	1.47	1.41
11	a	1122	CLA	CHD-C4C	2.25	1.47	1.41
11	a	1012	CLA	CHD-C4C	2.25	1.47	1.41
11	B	1210	CLA	CHD-C4C	2.25	1.47	1.41
11	A	1140	CLA	C4C-C3C	2.25	1.49	1.45
11	B	1201	CLA	C4C-C3C	2.25	1.49	1.45
11	2	1021	CLA	C4C-C3C	2.25	1.49	1.45
11	1	1011	CLA	CHD-C4C	2.25	1.47	1.41
11	K	1402	CLA	CHD-C4C	2.25	1.47	1.41
11	B	1206	CLA	C4C-C3C	2.25	1.49	1.45
11	1	1135	CLA	CHD-C4C	2.26	1.47	1.41
11	b	1211	CLA	C4C-C3C	2.26	1.49	1.45
11	2	1207	CLA	CHD-C4C	2.26	1.47	1.41
11	a	1124	CLA	C4C-C3C	2.26	1.49	1.45
11	a	1109	CLA	C4C-C3C	2.26	1.49	1.45
11	1	1122	CLA	CHD-C4C	2.26	1.47	1.41
11	b	1023	CLA	CHD-C4C	2.26	1.47	1.41
11	A	1137	CLA	CHD-C4C	2.26	1.47	1.41
11	A	1106	CLA	C4C-C3C	2.26	1.49	1.45
11	b	1021	CLA	C4C-C3C	2.26	1.49	1.45
11	a	1125	CLA	CHD-C4C	2.26	1.47	1.41
11	L	1501	CLA	CHD-C4C	2.26	1.47	1.41
11	B	1207	CLA	CHD-C4C	2.26	1.47	1.41
11	1	1116	CLA	C4C-C3C	2.27	1.49	1.45
11	b	1214	CLA	CHD-C4C	2.27	1.48	1.41
11	b	1221	CLA	C1C-C2C	2.27	1.48	1.44
11	b	1230	CLA	CHD-C4C	2.27	1.48	1.41
11	a	1114	CLA	C4C-C3C	2.27	1.49	1.45
11	2	1231	CLA	C4C-C3C	2.27	1.49	1.45
11	1	1120	CLA	C4C-C3C	2.27	1.49	1.45
11	b	1224	CLA	CHD-C4C	2.27	1.48	1.41
11	a	1116	CLA	C4C-C3C	2.27	1.49	1.45
11	a	1130	CLA	C4C-C3C	2.27	1.49	1.45
11	A	1127	CLA	CHD-C4C	2.27	1.48	1.41
11	L	1502	CLA	CHD-C4C	2.27	1.48	1.41
11	1	1103	CLA	C4C-C3C	2.27	1.49	1.45
11	2	1225	CLA	C4C-C3C	2.27	1.49	1.45
11	a	1118	CLA	CHD-C4C	2.28	1.48	1.41
11	1	1118	CLA	CHD-C4C	2.28	1.48	1.41
11	l	1501	CLA	CHD-C4C	2.28	1.48	1.41
11	A	1126	CLA	C1C-C2C	2.28	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1129	CLA	CHD-C4C	2.28	1.48	1.41
11	a	1103	CLA	C4C-C3C	2.28	1.49	1.45
11	a	1105	CLA	C4C-C3C	2.28	1.49	1.45
11	0	1401	CLA	CHD-C4C	2.28	1.48	1.41
11	2	1212	CLA	CHD-C4C	2.28	1.48	1.41
11	2	1023	CLA	C4C-C3C	2.28	1.49	1.45
11	1	1136	CLA	CHD-C4C	2.28	1.48	1.41
11	A	1103	CLA	CHD-C4C	2.28	1.48	1.41
11	k	1401	CLA	CHD-C4C	2.28	1.48	1.41
11	A	1131	CLA	C4C-C3C	2.29	1.49	1.45
11	1	1134	CLA	C4C-C3C	2.29	1.49	1.45
11	a	1113	CLA	C4C-C3C	2.29	1.49	1.45
11	b	1228	CLA	C4C-C3C	2.29	1.49	1.45
11	1	1102	CLA	C1C-C2C	2.29	1.49	1.44
11	a	1120	CLA	CHD-C4C	2.29	1.48	1.41
11	a	1121	CLA	C4C-C3C	2.29	1.49	1.45
11	K	1401	CLA	CHD-C4C	2.29	1.48	1.41
11	A	1115	CLA	C1C-C2C	2.29	1.49	1.44
11	2	1023	CLA	CHD-C4C	2.29	1.48	1.41
11	B	1213	CLA	CHD-C4C	2.29	1.48	1.41
11	A	1136	CLA	CHD-C4C	2.30	1.48	1.41
11	a	1113	CLA	CHD-C4C	2.30	1.48	1.41
11	1	1104	CLA	CHD-C4C	2.30	1.48	1.41
11	B	1217	CLA	CHD-C4C	2.30	1.48	1.41
11	B	1240	CLA	C1C-C2C	2.30	1.49	1.44
11	1	1108	CLA	CHD-C4C	2.30	1.48	1.41
11	a	1104	CLA	CHD-C4C	2.30	1.48	1.41
11	A	1112	CLA	CHD-C4C	2.30	1.48	1.41
11	b	1227	CLA	C4C-C3C	2.30	1.49	1.45
11	1	1140	CLA	CHD-C4C	2.30	1.48	1.41
11	B	1238	CLA	CHD-C4C	2.30	1.48	1.41
11	1	1113	CLA	CHD-C4C	2.30	1.48	1.41
11	2	1219	CLA	C1C-C2C	2.30	1.49	1.44
11	2	1021	CLA	CHD-C4C	2.30	1.48	1.41
11	A	1110	CLA	C4C-C3C	2.30	1.49	1.45
11	A	1237	CLA	CHD-C4C	2.30	1.48	1.41
11	b	1223	CLA	CHD-C4C	2.30	1.48	1.41
11	b	1212	CLA	CHD-C4C	2.30	1.48	1.41
11	b	1232	CLA	C4C-C3C	2.31	1.49	1.45
11	a	1123	CLA	C4C-C3C	2.31	1.49	1.45
11	b	1021	CLA	CHD-C4C	2.31	1.48	1.41
11	A	1133	CLA	CHD-C4C	2.31	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1225	CLA	CHD-C4C	2.31	1.48	1.41
11	B	1013	CLA	CHD-C4C	2.31	1.48	1.41
11	b	1226	CLA	CHD-C4C	2.31	1.48	1.41
11	A	1111	CLA	CHD-C4C	2.31	1.48	1.41
11	2	1219	CLA	CHD-C4C	2.31	1.48	1.41
11	a	1022	CLA	CHD-C4C	2.31	1.48	1.41
11	1	1129	CLA	CHD-C4C	2.31	1.48	1.41
11	B	1223	CLA	CHD-C4C	2.31	1.48	1.41
11	A	1011	CLA	CHD-C4C	2.31	1.48	1.41
11	1	1237	CLA	CHD-C4C	2.32	1.48	1.41
11	B	1229	CLA	C4C-C3C	2.32	1.49	1.45
11	a	1119	CLA	C4C-C3C	2.32	1.49	1.45
11	B	1234	CLA	CHD-C4C	2.32	1.48	1.41
11	b	1223	CLA	C4C-C3C	2.32	1.49	1.45
11	a	1134	CLA	C4C-C3C	2.32	1.49	1.45
11	2	1223	CLA	CHD-C4C	2.32	1.48	1.41
11	a	1106	CLA	CHD-C4C	2.32	1.48	1.41
11	a	1011	CLA	CHD-C4C	2.32	1.48	1.41
11	a	1127	CLA	CHD-C4C	2.32	1.48	1.41
11	B	1211	CLA	CHD-C4C	2.32	1.48	1.41
11	a	1136	CLA	CHD-C4C	2.33	1.48	1.41
11	B	1219	CLA	CHD-C4C	2.33	1.48	1.41
11	b	1203	CLA	CHD-C4C	2.33	1.48	1.41
11	L	1503	CLA	CHD-C4C	2.33	1.48	1.41
11	B	1206	CLA	CHD-C4C	2.33	1.48	1.41
11	A	1105	CLA	CHD-C4C	2.33	1.48	1.41
11	A	1139	CLA	C1C-C2C	2.33	1.49	1.44
11	B	1212	CLA	CHD-C4C	2.33	1.48	1.41
11	2	1203	CLA	CHD-C4C	2.33	1.48	1.41
11	k	1402	CLA	CHD-C4C	2.33	1.48	1.41
11	b	1219	CLA	CHD-C4C	2.33	1.48	1.41
11	b	1220	CLA	CHD-C4C	2.33	1.48	1.41
11	B	1235	CLA	CHD-C4C	2.33	1.48	1.41
11	a	1108	CLA	CHD-C4C	2.33	1.48	1.41
11	a	1116	CLA	CHD-C4C	2.34	1.48	1.41
11	b	1234	CLA	CHD-C4C	2.34	1.48	1.41
11	8	1501	CLA	CHD-C4C	2.34	1.48	1.41
11	B	1240	CLA	CHD-C4C	2.34	1.48	1.41
11	2	1227	CLA	C4C-C3C	2.34	1.49	1.45
11	b	1213	CLA	CHD-C4C	2.34	1.48	1.41
11	A	1140	CLA	CHD-C4C	2.34	1.48	1.41
11	2	1206	CLA	CHD-C4C	2.34	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1138	CLA	CHD-C4C	2.34	1.48	1.41
11	A	1110	CLA	CHD-C4C	2.34	1.48	1.41
11	a	1124	CLA	CHD-C4C	2.34	1.48	1.41
11	2	1216	CLA	C4C-C3C	2.34	1.49	1.45
11	2	1220	CLA	CHD-C4C	2.34	1.48	1.41
11	b	1206	CLA	C4C-C3C	2.34	1.49	1.45
11	a	1137	CLA	CHD-C4C	2.34	1.48	1.41
11	A	1108	CLA	CHD-C4C	2.35	1.48	1.41
11	1	1139	CLA	C4C-C3C	2.35	1.49	1.45
11	2	1201	CLA	C4C-C3C	2.35	1.49	1.45
11	a	1133	CLA	CHD-C4C	2.35	1.48	1.41
11	b	1211	CLA	CHD-C4C	2.35	1.48	1.41
11	A	1124	CLA	C4C-C3C	2.35	1.49	1.45
11	2	1218	CLA	CHD-C4C	2.35	1.48	1.41
11	1	1125	CLA	CHD-C4C	2.35	1.48	1.41
11	1	1103	CLA	CHD-C4C	2.35	1.48	1.41
11	B	1201	CLA	CHD-C4C	2.35	1.48	1.41
11	B	1220	CLA	C4C-C3C	2.35	1.49	1.45
11	0	1402	CLA	CHD-C4C	2.35	1.48	1.41
11	2	1238	CLA	CHD-C4C	2.35	1.48	1.41
11	1	1022	CLA	CHD-C4C	2.35	1.48	1.41
11	b	1201	CLA	CHD-C4C	2.35	1.48	1.41
11	b	1222	CLA	CHD-C4C	2.35	1.48	1.41
11	a	1117	CLA	CHD-C4C	2.35	1.48	1.41
11	A	1114	CLA	CHD-C4C	2.36	1.48	1.41
11	B	1209	CLA	CHD-C4C	2.36	1.48	1.41
11	B	1202	CLA	CHD-C4C	2.36	1.48	1.41
11	b	1235	CLA	CHD-C4C	2.36	1.48	1.41
11	1	1119	CLA	CHD-C4C	2.36	1.48	1.41
11	2	1232	CLA	C4C-C3C	2.36	1.49	1.45
11	B	1203	CLA	CHD-C4C	2.36	1.48	1.41
11	b	1236	CLA	CHD-C4C	2.36	1.48	1.41
11	b	1225	CLA	CHD-C4C	2.36	1.48	1.41
11	A	1022	CLA	CHD-C4C	2.36	1.48	1.41
11	a	1801	CLA	C4C-C3C	2.36	1.49	1.45
11	l	1503	CLA	CHD-C4C	2.36	1.48	1.41
11	1	1112	CLA	CHD-C4C	2.36	1.48	1.41
11	b	1225	CLA	C4C-C3C	2.37	1.49	1.45
11	b	1216	CLA	CHD-C4C	2.37	1.48	1.41
11	2	1234	CLA	CHD-C4C	2.37	1.48	1.41
11	2	1228	CLA	CHD-C4C	2.37	1.48	1.41
11	A	1135	CLA	CHD-C4C	2.37	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1102	CLA	CHD-C4C	2.37	1.48	1.41
11	b	1216	CLA	C4C-C3C	2.37	1.49	1.45
11	b	1204	CLA	CHD-C4C	2.37	1.48	1.41
11	B	1204	CLA	CHD-C4C	2.37	1.48	1.41
11	1	1124	CLA	CHD-C4C	2.37	1.48	1.41
11	A	1130	CLA	CHD-C4C	2.37	1.48	1.41
11	1	1134	CLA	CHD-C4C	2.37	1.48	1.41
11	2	1239	CLA	C4C-C3C	2.37	1.49	1.45
11	a	1126	CLA	C1C-C2C	2.37	1.49	1.44
11	a	1102	CLA	CHD-C4C	2.37	1.48	1.41
11	2	1240	CLA	CHD-C4C	2.37	1.48	1.41
11	A	1123	CLA	CHD-C4C	2.37	1.48	1.41
11	1	1116	CLA	CHD-C4C	2.38	1.48	1.41
11	A	1119	CLA	CHD-C4C	2.38	1.48	1.41
11	B	1239	CLA	CHD-C4C	2.38	1.48	1.41
11	1	1801	CLA	CHD-C4C	2.38	1.48	1.41
11	2	1229	CLA	CHD-C4C	2.38	1.48	1.41
11	2	1222	CLA	CHD-C4C	2.38	1.48	1.41
11	1	1133	CLA	CHD-C4C	2.38	1.48	1.41
11	b	1239	CLA	C4C-C3C	2.38	1.49	1.45
11	A	1134	CLA	CHD-C4C	2.38	1.48	1.41
11	2	1214	CLA	CHD-C4C	2.38	1.48	1.41
11	2	1208	CLA	CHD-C4C	2.38	1.48	1.41
11	A	1118	CLA	CHD-C4C	2.38	1.48	1.41
11	1	1128	CLA	CHD-C4C	2.38	1.48	1.41
11	2	1240	CLA	C4C-C3C	2.38	1.49	1.45
11	a	1128	CLA	CHD-C4C	2.38	1.48	1.41
11	b	1238	CLA	CHD-C4C	2.38	1.48	1.41
11	1	1115	CLA	CHD-C4C	2.38	1.48	1.41
11	2	1213	CLA	CHD-C4C	2.38	1.48	1.41
11	A	1126	CLA	CHD-C4C	2.38	1.48	1.41
11	B	1215	CLA	CHD-C4C	2.38	1.48	1.41
11	1	1120	CLA	CHD-C4C	2.38	1.48	1.41
11	A	1132	CLA	CHD-C4C	2.38	1.48	1.41
11	B	1208	CLA	CHD-C4C	2.38	1.48	1.41
11	b	1240	CLA	CHD-C4C	2.39	1.48	1.41
11	2	1204	CLA	CHD-C4C	2.39	1.48	1.41
11	A	1133	CLA	C4C-C3C	2.39	1.49	1.45
11	a	1121	CLA	CHD-C4C	2.39	1.48	1.41
11	B	1216	CLA	C4C-C3C	2.39	1.49	1.45
11	a	1132	CLA	CHD-C4C	2.39	1.48	1.41
11	1	1106	CLA	CHD-C4C	2.39	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1140	CLA	CHD-C4C	2.39	1.48	1.41
11	a	1119	CLA	CHD-C4C	2.39	1.48	1.41
11	B	1228	CLA	C4C-C3C	2.39	1.49	1.45
11	A	1119	CLA	C4C-C3C	2.39	1.49	1.45
11	B	1218	CLA	CHD-C4C	2.39	1.48	1.41
11	a	1131	CLA	CHD-C4C	2.39	1.48	1.41
11	A	1115	CLA	CHD-C4C	2.39	1.48	1.41
11	2	1227	CLA	CHD-C4C	2.39	1.48	1.41
11	8	1503	CLA	CHD-C4C	2.39	1.48	1.41
11	2	1239	CLA	CHD-C4C	2.39	1.48	1.41
11	a	1112	CLA	CHD-C4C	2.40	1.48	1.41
11	1	1126	CLA	CHD-C4C	2.40	1.48	1.41
11	1	1123	CLA	C4C-C3C	2.40	1.49	1.45
11	A	1139	CLA	CHD-C4C	2.40	1.48	1.41
11	a	1114	CLA	CHD-C4C	2.40	1.48	1.41
11	A	1114	CLA	C4C-C3C	2.40	1.49	1.45
11	1	1131	CLA	CHD-C4C	2.40	1.48	1.41
11	2	1201	CLA	CHD-C4C	2.40	1.48	1.41
11	1	1125	CLA	C4C-C3C	2.40	1.49	1.45
11	b	1217	CLA	CHD-C4C	2.40	1.48	1.41
11	a	1101	CLA	CHD-C4C	2.40	1.48	1.41
11	b	1210	CLA	C4C-C3C	2.40	1.49	1.45
11	a	1103	CLA	CHD-C4C	2.40	1.48	1.41
11	b	1230	CLA	C4C-C3C	2.40	1.49	1.45
11	A	1106	CLA	CHD-C4C	2.40	1.48	1.41
11	b	1229	CLA	CHD-C4C	2.40	1.48	1.41
11	1	1117	CLA	CHD-C4C	2.40	1.48	1.41
11	a	1134	CLA	CHD-C4C	2.40	1.48	1.41
11	A	1125	CLA	CHD-C4C	2.41	1.48	1.41
11	2	1209	CLA	CHD-C4C	2.41	1.48	1.41
11	2	1202	CLA	CHD-C4C	2.41	1.48	1.41
11	B	1229	CLA	CHD-C4C	2.41	1.48	1.41
11	1	1110	CLA	C4C-C3C	2.41	1.49	1.45
11	b	1228	CLA	CHD-C4C	2.41	1.48	1.41
11	b	1209	CLA	CHD-C4C	2.41	1.48	1.41
11	1	1123	CLA	CHD-C4C	2.41	1.48	1.41
11	b	1218	CLA	CHD-C4C	2.41	1.48	1.41
11	1	1132	CLA	CHD-C4C	2.41	1.48	1.41
11	b	1227	CLA	CHD-C4C	2.41	1.48	1.41
11	a	1135	CLA	CHD-C4C	2.42	1.48	1.41
11	b	1208	CLA	C4C-C3C	2.42	1.49	1.45
11	1	1114	CLA	C4C-C3C	2.42	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1131	CLA	CHD-C4C	2.42	1.48	1.41
11	a	1110	CLA	CHD-C4C	2.42	1.48	1.41
11	a	1133	CLA	C4C-C3C	2.42	1.49	1.45
11	A	1138	CLA	CHD-C4C	2.42	1.48	1.41
11	2	1220	CLA	C4C-C3C	2.42	1.49	1.45
11	a	1105	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1110	CLA	CHD-C4C	2.42	1.48	1.41
11	2	1215	CLA	CHD-C4C	2.42	1.48	1.41
11	a	1123	CLA	CHD-C4C	2.42	1.48	1.41
11	2	1217	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1105	CLA	CHD-C4C	2.42	1.48	1.41
11	b	1215	CLA	CHD-C4C	2.42	1.48	1.41
11	1	1121	CLA	CHD-C4C	2.43	1.48	1.41
11	1	1130	CLA	CHD-C4C	2.43	1.48	1.41
11	2	1013	CLA	CHD-C4C	2.43	1.48	1.41
11	a	1135	CLA	C4C-C3C	2.43	1.49	1.45
11	A	1124	CLA	CHD-C4C	2.43	1.48	1.41
11	b	1206	CLA	CHD-C4C	2.43	1.48	1.41
11	1	1109	CLA	CHD-C4C	2.44	1.48	1.41
11	B	1209	CLA	C4C-C3C	2.44	1.49	1.45
11	b	1239	CLA	CHD-C4C	2.44	1.48	1.41
11	1	1101	CLA	CHD-C4C	2.44	1.48	1.41
11	1	1139	CLA	CHD-C4C	2.44	1.48	1.41
11	b	1232	CLA	CHD-C4C	2.44	1.48	1.41
11	a	1138	CLA	C4C-C3C	2.44	1.49	1.45
11	A	1102	CLA	CHD-C4C	2.44	1.48	1.41
11	B	1220	CLA	CHD-C4C	2.44	1.48	1.41
11	1	1114	CLA	CHD-C4C	2.44	1.48	1.41
11	b	1013	CLA	CHD-C4C	2.44	1.48	1.41
11	A	1134	CLA	C4C-C3C	2.44	1.49	1.45
11	b	1234	CLA	C4C-C3C	2.45	1.49	1.45
11	2	1232	CLA	CHD-C4C	2.45	1.48	1.41
11	a	1801	CLA	CHD-C4C	2.45	1.48	1.41
11	a	1130	CLA	CHD-C4C	2.45	1.48	1.41
11	b	1231	CLA	CHD-C4C	2.45	1.48	1.41
11	B	1228	CLA	CHD-C4C	2.46	1.48	1.41
11	B	1227	CLA	CHD-C4C	2.46	1.48	1.41
11	A	1801	CLA	CHD-C4C	2.46	1.48	1.41
11	B	1231	CLA	CHD-C4C	2.47	1.48	1.41
11	A	1117	CLA	CHD-C4C	2.47	1.48	1.41
11	2	1209	CLA	C4C-C3C	2.47	1.49	1.45
11	1	1127	CLA	CHD-C4C	2.47	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1120	CLA	CHD-C4C	2.47	1.48	1.41
11	B	1232	CLA	C4C-C3C	2.47	1.49	1.45
11	a	1138	CLA	CHD-C4C	2.47	1.48	1.41
11	b	1208	CLA	CHD-C4C	2.48	1.48	1.41
11	A	1109	CLA	CHD-C4C	2.48	1.48	1.41
11	2	1217	CLA	C4C-C3C	2.48	1.49	1.45
11	B	1232	CLA	CHD-C4C	2.48	1.48	1.41
11	a	1109	CLA	CHD-C4C	2.48	1.48	1.41
11	B	1216	CLA	CHD-C4C	2.48	1.48	1.41
11	a	1139	CLA	CHD-C4C	2.51	1.48	1.41
11	A	1123	CLA	C4C-C3C	2.51	1.49	1.45
11	a	1127	CLA	C4C-C3C	2.51	1.49	1.45
11	2	1225	CLA	CHD-C4C	2.52	1.48	1.41
11	B	1227	CLA	C4C-C3C	2.52	1.49	1.45
11	A	1121	CLA	CHD-C4C	2.52	1.48	1.41
11	1	1133	CLA	C4C-C3C	2.53	1.49	1.45
11	a	1139	CLA	C4C-C3C	2.54	1.49	1.45
11	2	1231	CLA	CHD-C4C	2.54	1.48	1.41
11	b	1209	CLA	C4C-C3C	2.55	1.49	1.45
11	b	1220	CLA	C4C-C3C	2.55	1.49	1.45
11	B	1231	CLA	C4C-C3C	2.57	1.49	1.45
11	B	1210	CLA	C4C-C3C	2.61	1.49	1.45
11	2	1023	CLA	C1B-CHB	2.69	1.47	1.40
11	A	1801	CLA	C4C-C3C	2.71	1.49	1.45
11	2	1021	CLA	C1B-CHB	2.77	1.47	1.40
11	A	1135	CLA	C1B-CHB	2.77	1.47	1.40
11	A	1011	CLA	C1B-CHB	2.78	1.47	1.40
11	2	1013	CLA	C1B-CHB	2.79	1.47	1.40
11	B	1231	CLA	C1B-CHB	2.80	1.47	1.40
11	A	1124	CLA	C1B-CHB	2.81	1.47	1.40
11	b	1231	CLA	C1B-CHB	2.81	1.47	1.40
11	A	1801	CLA	C1B-CHB	2.82	1.47	1.40
11	A	1126	CLA	C1B-CHB	2.82	1.47	1.40
11	2	1231	CLA	C1B-CHB	2.83	1.47	1.40
11	A	1022	CLA	C1B-CHB	2.84	1.47	1.40
11	A	1125	CLA	C4C-C3C	2.85	1.50	1.45
11	b	1234	CLA	C4B-CHC	2.85	1.47	1.40
11	a	1104	CLA	C1B-CHB	2.86	1.47	1.40
11	B	1206	CLA	C4B-CHC	2.87	1.47	1.40
11	b	1013	CLA	C1B-CHB	2.87	1.47	1.40
11	B	1234	CLA	C4B-CHC	2.88	1.47	1.40
11	1	1111	CLA	C1B-CHB	2.88	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1011	CLA	C4B-CHC	2.88	1.47	1.40
11	B	1211	CLA	C3D-C2D	2.89	1.46	1.39
11	A	1119	CLA	C1B-CHB	2.89	1.47	1.40
11	8	1501	CLA	C1B-CHB	2.89	1.47	1.40
11	A	1133	CLA	C4B-CHC	2.90	1.47	1.40
11	2	1206	CLA	C4B-CHC	2.90	1.47	1.40
11	B	1021	CLA	C1B-CHB	2.90	1.47	1.40
11	B	1227	CLA	C4B-CHC	2.90	1.47	1.40
11	A	1117	CLA	C1B-CHB	2.90	1.47	1.40
11	b	1206	CLA	C4B-CHC	2.90	1.47	1.40
11	b	1207	CLA	C4B-CHC	2.90	1.47	1.40
11	A	1125	CLA	C4B-CHC	2.90	1.47	1.40
11	B	1023	CLA	C1B-CHB	2.91	1.47	1.40
11	2	1207	CLA	C1B-CHB	2.91	1.47	1.40
11	B	1013	CLA	C1B-CHB	2.91	1.47	1.40
11	A	1116	CLA	C1B-CHB	2.91	1.47	1.40
11	a	1112	CLA	C1B-CHB	2.91	1.47	1.40
11	B	1021	CLA	C4B-CHC	2.92	1.47	1.40
11	A	1102	CLA	C1B-CHB	2.92	1.47	1.40
11	a	1011	CLA	C1B-CHB	2.92	1.47	1.40
11	a	1124	CLA	C1B-CHB	2.93	1.47	1.40
11	a	1132	CLA	C1B-CHB	2.93	1.47	1.40
11	A	1012	CLA	C1B-CHB	2.93	1.47	1.40
11	a	1135	CLA	C4B-CHC	2.93	1.47	1.40
11	B	1222	CLA	C1B-CHB	2.93	1.47	1.40
11	a	1801	CLA	C1B-CHB	2.93	1.47	1.40
11	B	1232	CLA	C4B-CHC	2.94	1.47	1.40
11	A	1106	CLA	C1B-CHB	2.94	1.47	1.40
11	1	1110	CLA	C1B-CHB	2.94	1.47	1.40
11	L	1501	CLA	C1B-CHB	2.94	1.47	1.40
11	1	1102	CLA	C1B-CHB	2.94	1.47	1.40
11	a	1102	CLA	C1B-CHB	2.94	1.47	1.40
11	A	1134	CLA	C4B-CHC	2.94	1.48	1.40
11	a	1127	CLA	C4B-CHC	2.95	1.48	1.40
11	a	1119	CLA	C4B-CHC	2.95	1.48	1.40
11	b	1023	CLA	C1B-CHB	2.95	1.48	1.40
11	2	1201	CLA	C4B-CHC	2.95	1.48	1.40
11	a	1138	CLA	C1B-CHB	2.96	1.48	1.40
11	a	1106	CLA	C1B-CHB	2.96	1.48	1.40
11	B	1230	CLA	C4B-CHC	2.96	1.48	1.40
11	B	1204	CLA	C4B-CHC	2.96	1.48	1.40
11	B	1225	CLA	C1B-CHB	2.96	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1132	CLA	C1B-CHB	2.96	1.48	1.40
11	B	1207	CLA	C1B-CHB	2.96	1.48	1.40
11	a	1011	CLA	C4B-CHC	2.96	1.48	1.40
11	B	1231	CLA	C4B-CHC	2.96	1.48	1.40
11	1	1125	CLA	C1B-CHB	2.97	1.48	1.40
11	L	1503	CLA	C4B-CHC	2.97	1.48	1.40
11	a	1116	CLA	C1B-CHB	2.97	1.48	1.40
11	2	1234	CLA	C4B-CHC	2.97	1.48	1.40
11	A	1138	CLA	C4B-CHC	2.97	1.48	1.40
11	B	1220	CLA	C1B-CHB	2.97	1.48	1.40
11	A	1123	CLA	C4B-CHC	2.97	1.48	1.40
11	b	1225	CLA	C1B-CHB	2.97	1.48	1.40
11	B	1216	CLA	C1B-CHB	2.97	1.48	1.40
11	B	1214	CLA	C1B-CHB	2.97	1.48	1.40
11	b	1239	CLA	C4B-CHC	2.97	1.48	1.40
11	a	1139	CLA	C4B-CHC	2.98	1.48	1.40
11	b	1203	CLA	C1B-CHB	2.98	1.48	1.40
11	b	1215	CLA	C1B-CHB	2.98	1.48	1.40
11	A	1112	CLA	C1B-CHB	2.98	1.48	1.40
11	B	1224	CLA	C3D-C2D	2.98	1.46	1.39
11	2	1229	CLA	C1B-CHB	2.98	1.48	1.40
11	2	1225	CLA	C1B-CHB	2.98	1.48	1.40
11	l	1503	CLA	C1B-CHB	2.98	1.48	1.40
11	1	1104	CLA	C1B-CHB	2.98	1.48	1.40
11	B	1204	CLA	C1B-CHB	2.98	1.48	1.40
11	a	1134	CLA	C1B-CHB	2.98	1.48	1.40
11	1	1801	CLA	C1B-CHB	2.99	1.48	1.40
11	2	1203	CLA	C1B-CHB	2.99	1.48	1.40
11	A	1120	CLA	C1B-CHB	2.99	1.48	1.40
11	B	1215	CLA	C1B-CHB	2.99	1.48	1.40
11	b	1228	CLA	C1B-CHB	2.99	1.48	1.40
11	A	1127	CLA	C1B-CHB	2.99	1.48	1.40
11	2	1227	CLA	C4B-CHC	2.99	1.48	1.40
11	2	1203	CLA	C4B-CHC	2.99	1.48	1.40
11	A	1106	CLA	C4B-CHC	2.99	1.48	1.40
11	2	1209	CLA	C1B-CHB	3.00	1.48	1.40
11	a	1133	CLA	C4B-CHC	3.00	1.48	1.40
11	B	1220	CLA	C4B-CHC	3.00	1.48	1.40
11	1	1022	CLA	C1B-CHB	3.00	1.48	1.40
11	2	1207	CLA	C4B-CHC	3.00	1.48	1.40
11	B	1201	CLA	C1B-CHB	3.00	1.48	1.40
11	8	1501	CLA	C4B-CHC	3.00	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1111	CLA	C1B-CHB	3.00	1.48	1.40
11	1	1124	CLA	C1B-CHB	3.00	1.48	1.40
11	1	1138	CLA	C4B-CHC	3.01	1.48	1.40
11	A	1107	CLA	C1B-CHB	3.01	1.48	1.40
11	b	1223	CLA	C4B-CHC	3.01	1.48	1.40
11	1	1103	CLA	C1B-CHB	3.01	1.48	1.40
11	A	1118	CLA	C4B-CHC	3.01	1.48	1.40
11	B	1201	CLA	C4B-CHC	3.01	1.48	1.40
11	2	1228	CLA	C1B-CHB	3.01	1.48	1.40
11	1	1109	CLA	C4B-CHC	3.01	1.48	1.40
11	B	1221	CLA	C1B-CHB	3.01	1.48	1.40
11	a	1022	CLA	C1B-CHB	3.01	1.48	1.40
11	a	1107	CLA	C1B-CHB	3.01	1.48	1.40
11	2	1222	CLA	C1B-CHB	3.01	1.48	1.40
11	B	1202	CLA	C1B-CHB	3.01	1.48	1.40
11	b	1214	CLA	C1B-CHB	3.01	1.48	1.40
11	1	1011	CLA	C1B-CHB	3.01	1.48	1.40
11	1	1128	CLA	C4B-CHC	3.01	1.48	1.40
11	B	1205	CLA	C4B-CHC	3.02	1.48	1.40
11	a	1138	CLA	C4B-CHC	3.02	1.48	1.40
11	B	1212	CLA	C1B-CHB	3.02	1.48	1.40
11	A	1011	CLA	C4B-CHC	3.02	1.48	1.40
11	A	1139	CLA	C1B-CHB	3.02	1.48	1.40
11	l	1501	CLA	C1B-CHB	3.02	1.48	1.40
11	B	1226	CLA	C1B-CHB	3.02	1.48	1.40
11	2	1238	CLA	C1B-CHB	3.02	1.48	1.40
11	2	1221	CLA	C1B-CHB	3.02	1.48	1.40
11	1	1130	CLA	C1B-CHB	3.02	1.48	1.40
11	B	1209	CLA	C4B-CHC	3.02	1.48	1.40
11	2	1021	CLA	C4B-CHC	3.02	1.48	1.40
11	b	1205	CLA	C4B-CHC	3.02	1.48	1.40
11	1	1120	CLA	C1B-CHB	3.02	1.48	1.40
11	A	1237	CLA	C4B-CHC	3.02	1.48	1.40
11	A	1123	CLA	C1B-CHB	3.02	1.48	1.40
11	2	1235	CLA	C1B-CHB	3.02	1.48	1.40
11	1	1126	CLA	C1B-CHB	3.03	1.48	1.40
11	2	1230	CLA	C1B-CHB	3.03	1.48	1.40
11	a	1101	CLA	C4B-CHC	3.03	1.48	1.40
11	a	1103	CLA	C1B-CHB	3.03	1.48	1.40
11	b	1021	CLA	C1B-CHB	3.03	1.48	1.40
11	A	1109	CLA	C1B-CHB	3.03	1.48	1.40
11	1	1133	CLA	C4B-CHC	3.03	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	1401	CLA	C1B-CHB	3.03	1.48	1.40
11	1	1115	CLA	C1B-CHB	3.03	1.48	1.40
11	1	1117	CLA	C4B-CHC	3.03	1.48	1.40
11	8	1502	CLA	C1B-CHB	3.03	1.48	1.40
11	b	1205	CLA	C1B-CHB	3.03	1.48	1.40
11	b	1238	CLA	C1B-CHB	3.03	1.48	1.40
11	B	1215	CLA	C4B-CHC	3.04	1.48	1.40
11	0	1401	CLA	C1B-CHB	3.04	1.48	1.40
11	a	1109	CLA	C1B-CHB	3.04	1.48	1.40
11	a	1121	CLA	C1B-CHB	3.04	1.48	1.40
11	a	1130	CLA	C1B-CHB	3.04	1.48	1.40
11	B	1218	CLA	C4B-CHC	3.04	1.48	1.40
11	2	1209	CLA	C4B-CHC	3.04	1.48	1.40
11	2	1215	CLA	C4B-CHC	3.04	1.48	1.40
11	0	1401	CLA	C4B-CHC	3.04	1.48	1.40
11	1	1237	CLA	C4B-CHC	3.04	1.48	1.40
11	b	1202	CLA	C1B-CHB	3.04	1.48	1.40
11	L	1502	CLA	C1B-CHB	3.04	1.48	1.40
11	1	1135	CLA	C1B-CHB	3.04	1.48	1.40
11	1	1114	CLA	C4B-CHC	3.04	1.48	1.40
11	b	1210	CLA	C1B-CHB	3.04	1.48	1.40
11	b	1222	CLA	C1B-CHB	3.04	1.48	1.40
11	a	1012	CLA	C1B-CHB	3.04	1.48	1.40
11	b	1217	CLA	C1B-CHB	3.04	1.48	1.40
11	K	1401	CLA	C4B-CHC	3.04	1.48	1.40
11	a	1118	CLA	C4B-CHC	3.04	1.48	1.40
11	K	1402	CLA	C4B-CHC	3.05	1.48	1.40
11	1	1123	CLA	C1B-CHB	3.05	1.48	1.40
11	2	1232	CLA	C1B-CHB	3.05	1.48	1.40
11	B	1240	CLA	C1B-CHB	3.05	1.48	1.40
11	2	1224	CLA	C3D-C2D	3.05	1.46	1.39
11	B	1238	CLA	C4B-CHC	3.05	1.48	1.40
11	a	1101	CLA	C1B-CHB	3.05	1.48	1.40
11	1	1117	CLA	C1B-CHB	3.05	1.48	1.40
11	1	1119	CLA	C1B-CHB	3.05	1.48	1.40
11	2	1219	CLA	C1B-CHB	3.05	1.48	1.40
11	1	1103	CLA	C4B-CHC	3.05	1.48	1.40
11	A	1119	CLA	C4B-CHC	3.05	1.48	1.40
11	1	1139	CLA	C1B-CHB	3.05	1.48	1.40
11	2	1220	CLA	C4B-CHC	3.05	1.48	1.40
11	a	1128	CLA	C4B-CHC	3.06	1.48	1.40
11	b	1215	CLA	C4B-CHC	3.06	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1101	CLA	C1B-CHB	3.06	1.48	1.40
11	a	1114	CLA	C4B-CHC	3.06	1.48	1.40
11	2	1215	CLA	C1B-CHB	3.06	1.48	1.40
11	k	1401	CLA	C4B-CHC	3.06	1.48	1.40
11	2	1225	CLA	C4B-CHC	3.06	1.48	1.40
11	2	1210	CLA	C1B-CHB	3.06	1.48	1.40
11	2	1214	CLA	C4B-CHC	3.06	1.48	1.40
11	B	1209	CLA	C1B-CHB	3.06	1.48	1.40
11	A	1140	CLA	C4B-CHC	3.06	1.48	1.40
11	a	1136	CLA	C4B-CHC	3.06	1.48	1.40
11	b	1219	CLA	C4B-CHC	3.06	1.48	1.40
11	1	1132	CLA	C4B-CHC	3.06	1.48	1.40
11	B	1203	CLA	C1B-CHB	3.06	1.48	1.40
11	B	1228	CLA	C1B-CHB	3.06	1.48	1.40
11	a	1022	CLA	C4B-CHC	3.06	1.48	1.40
11	k	1401	CLA	C1B-CHB	3.06	1.48	1.40
11	b	1230	CLA	C4B-CHC	3.06	1.48	1.40
11	b	1229	CLA	C1B-CHB	3.06	1.48	1.40
11	a	1105	CLA	C4B-CHC	3.06	1.48	1.40
11	2	1212	CLA	C4B-CHC	3.06	1.48	1.40
11	8	1503	CLA	C1B-CHB	3.06	1.48	1.40
11	2	1204	CLA	C1B-CHB	3.07	1.48	1.40
11	a	1120	CLA	C4B-CHC	3.07	1.48	1.40
11	B	1229	CLA	C4B-CHC	3.07	1.48	1.40
11	a	1122	CLA	C1B-CHB	3.07	1.48	1.40
11	2	1217	CLA	C1B-CHB	3.07	1.48	1.40
11	A	1136	CLA	C4B-CHC	3.07	1.48	1.40
11	K	1402	CLA	C1B-CHB	3.07	1.48	1.40
11	b	1023	CLA	C4B-CHC	3.07	1.48	1.40
11	a	1123	CLA	C4B-CHC	3.07	1.48	1.40
11	k	1402	CLA	C1B-CHB	3.07	1.48	1.40
11	b	1207	CLA	C1B-CHB	3.07	1.48	1.40
11	b	1204	CLA	C1B-CHB	3.07	1.48	1.40
11	A	1138	CLA	C1B-CHB	3.07	1.48	1.40
11	1	1123	CLA	C4B-CHC	3.07	1.48	1.40
11	a	1107	CLA	C4B-CHC	3.07	1.48	1.40
11	a	1127	CLA	C1B-CHB	3.07	1.48	1.40
11	a	1110	CLA	C1B-CHB	3.07	1.48	1.40
11	2	1214	CLA	C1B-CHB	3.07	1.48	1.40
11	b	1235	CLA	C1B-CHB	3.07	1.48	1.40
11	A	1101	CLA	C1B-CHB	3.07	1.48	1.40
11	A	1114	CLA	C4B-CHC	3.07	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1137	CLA	C1B-CHB	3.07	1.48	1.40
11	2	1218	CLA	C1B-CHB	3.08	1.48	1.40
11	a	1123	CLA	C1B-CHB	3.08	1.48	1.40
11	a	1125	CLA	C1B-CHB	3.08	1.48	1.40
11	B	1219	CLA	C1B-CHB	3.08	1.48	1.40
11	B	1225	CLA	C4B-CHC	3.08	1.48	1.40
11	A	1128	CLA	C4B-CHC	3.08	1.48	1.40
11	a	1128	CLA	C1B-CHB	3.08	1.48	1.40
11	A	1115	CLA	C1B-CHB	3.08	1.48	1.40
11	b	1204	CLA	C4B-CHC	3.08	1.48	1.40
11	B	1235	CLA	C1B-CHB	3.08	1.48	1.40
11	b	1240	CLA	C1B-CHB	3.08	1.48	1.40
11	A	1107	CLA	C3D-C2D	3.08	1.46	1.39
11	1	1109	CLA	C1B-CHB	3.08	1.48	1.40
11	A	1137	CLA	C1B-CHB	3.08	1.48	1.40
11	a	1120	CLA	C1B-CHB	3.08	1.48	1.40
11	L	1503	CLA	C1B-CHB	3.08	1.48	1.40
11	2	1217	CLA	C4B-CHC	3.08	1.48	1.40
11	2	1223	CLA	C1B-CHB	3.08	1.48	1.40
11	A	1133	CLA	C1B-CHB	3.09	1.48	1.40
11	A	1104	CLA	C1B-CHB	3.09	1.48	1.40
11	b	1201	CLA	C1B-CHB	3.09	1.48	1.40
11	A	1801	CLA	C4B-CHC	3.09	1.48	1.40
11	A	1132	CLA	C4B-CHC	3.09	1.48	1.40
11	B	1221	CLA	C4B-CHC	3.09	1.48	1.40
11	b	1208	CLA	C4B-CHC	3.09	1.48	1.40
11	2	1208	CLA	C4B-CHC	3.09	1.48	1.40
11	1	1140	CLA	C1B-CHB	3.09	1.48	1.40
11	A	1113	CLA	C1B-CHB	3.09	1.48	1.40
11	b	1228	CLA	C4B-CHC	3.09	1.48	1.40
11	2	1224	CLA	C4B-CHC	3.09	1.48	1.40
11	a	1126	CLA	C1B-CHB	3.09	1.48	1.40
11	B	1207	CLA	C4B-CHC	3.09	1.48	1.40
11	2	1218	CLA	C4B-CHC	3.09	1.48	1.40
11	B	1228	CLA	C4B-CHC	3.09	1.48	1.40
11	1	1128	CLA	C1B-CHB	3.09	1.48	1.40
11	1	1801	CLA	C4B-CHC	3.09	1.48	1.40
11	a	1237	CLA	C4B-CHC	3.09	1.48	1.40
11	b	1230	CLA	C1B-CHB	3.09	1.48	1.40
11	a	1103	CLA	C4B-CHC	3.09	1.48	1.40
11	a	1140	CLA	C4B-CHC	3.09	1.48	1.40
11	A	1130	CLA	C1B-CHB	3.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1112	CLA	C1B-CHB	3.10	1.48	1.40
11	B	1217	CLA	C1B-CHB	3.10	1.48	1.40
11	2	1211	CLA	C4B-CHC	3.10	1.48	1.40
11	2	1234	CLA	C1B-CHB	3.10	1.48	1.40
11	A	1108	CLA	C1B-CHB	3.10	1.48	1.40
11	a	1140	CLA	C1B-CHB	3.10	1.48	1.40
11	a	1102	CLA	C4B-CHC	3.10	1.48	1.40
11	1	1121	CLA	C1B-CHB	3.10	1.48	1.40
11	A	1135	CLA	C4B-CHC	3.10	1.48	1.40
11	a	1131	CLA	C1B-CHB	3.10	1.48	1.40
11	b	1209	CLA	C4B-CHC	3.10	1.48	1.40
11	1	1118	CLA	C1B-CHB	3.10	1.48	1.40
11	1	1121	CLA	C4B-CHC	3.10	1.48	1.40
11	l	1503	CLA	C4B-CHC	3.10	1.48	1.40
11	B	1223	CLA	C1B-CHB	3.10	1.48	1.40
11	1	1116	CLA	C1B-CHB	3.10	1.48	1.40
11	B	1238	CLA	C1B-CHB	3.10	1.48	1.40
11	1	1101	CLA	C4B-CHC	3.10	1.48	1.40
11	1	1131	CLA	C4B-CHC	3.10	1.48	1.40
11	2	1226	CLA	C3D-C2D	3.11	1.46	1.39
11	b	1218	CLA	C1B-CHB	3.11	1.48	1.40
11	a	1135	CLA	C1B-CHB	3.11	1.48	1.40
11	1	1106	CLA	C4B-CHC	3.11	1.48	1.40
11	b	1227	CLA	C4B-CHC	3.11	1.48	1.40
11	2	1206	CLA	C1B-CHB	3.11	1.48	1.40
11	1	1105	CLA	C1B-CHB	3.11	1.48	1.40
11	A	1237	CLA	C1B-CHB	3.11	1.48	1.40
11	1	1134	CLA	C1B-CHB	3.11	1.48	1.40
11	a	1117	CLA	C1B-CHB	3.11	1.48	1.40
11	1	1140	CLA	C4B-CHC	3.11	1.48	1.40
11	b	1225	CLA	C4B-CHC	3.11	1.48	1.40
11	b	1232	CLA	C1B-CHB	3.11	1.48	1.40
11	2	1240	CLA	C4B-CHC	3.11	1.48	1.40
11	1	1127	CLA	C4B-CHC	3.11	1.48	1.40
11	A	1122	CLA	C4B-CHC	3.11	1.48	1.40
11	2	1221	CLA	C4B-CHC	3.11	1.48	1.40
11	B	1206	CLA	C1B-CHB	3.11	1.48	1.40
11	2	1239	CLA	C4B-CHC	3.11	1.48	1.40
11	b	1206	CLA	C1B-CHB	3.11	1.48	1.40
11	1	1118	CLA	C4B-CHC	3.11	1.48	1.40
11	1	1115	CLA	C4B-CHC	3.11	1.48	1.40
11	a	1131	CLA	C4B-CHC	3.11	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1239	CLA	C4B-CHC	3.11	1.48	1.40
11	b	1212	CLA	C4B-CHC	3.11	1.48	1.40
11	A	1121	CLA	C1B-CHB	3.11	1.48	1.40
11	A	1124	CLA	C4B-CHC	3.12	1.48	1.40
11	A	1110	CLA	C4B-CHC	3.12	1.48	1.40
11	A	1104	CLA	C4B-CHC	3.12	1.48	1.40
11	b	1222	CLA	C4B-CHC	3.12	1.48	1.40
11	2	1228	CLA	C4B-CHC	3.12	1.48	1.40
11	B	1229	CLA	C1B-CHB	3.12	1.48	1.40
11	A	1104	CLA	C3D-C2D	3.12	1.46	1.39
11	b	1226	CLA	C1B-CHB	3.12	1.48	1.40
11	b	1239	CLA	C1B-CHB	3.12	1.48	1.40
11	A	1122	CLA	C1B-CHB	3.12	1.48	1.40
11	1	1110	CLA	C4B-CHC	3.12	1.48	1.40
11	B	1203	CLA	C4B-CHC	3.12	1.48	1.40
11	b	1227	CLA	C1B-CHB	3.12	1.48	1.40
11	1	1104	CLA	C4B-CHC	3.12	1.48	1.40
11	A	1101	CLA	C3D-C2D	3.12	1.46	1.39
11	A	1129	CLA	C1B-CHB	3.12	1.48	1.40
11	B	1219	CLA	C4B-CHC	3.12	1.48	1.40
11	a	1119	CLA	C1B-CHB	3.12	1.48	1.40
11	1	1012	CLA	C4B-CHC	3.12	1.48	1.40
11	2	1240	CLA	C1B-CHB	3.12	1.48	1.40
11	A	1134	CLA	C1B-CHB	3.12	1.48	1.40
11	B	1239	CLA	C1B-CHB	3.12	1.48	1.40
11	B	1217	CLA	C4B-CHC	3.12	1.48	1.40
11	a	1137	CLA	C4B-CHC	3.12	1.48	1.40
11	B	1211	CLA	C4B-CHC	3.12	1.48	1.40
11	2	1220	CLA	C1B-CHB	3.12	1.48	1.40
11	2	1222	CLA	C4B-CHC	3.12	1.48	1.40
11	b	1220	CLA	C1B-CHB	3.12	1.48	1.40
11	2	1212	CLA	C1B-CHB	3.13	1.48	1.40
11	B	1205	CLA	C1B-CHB	3.13	1.48	1.40
11	a	1109	CLA	C4B-CHC	3.13	1.48	1.40
11	A	1131	CLA	C4B-CHC	3.13	1.48	1.40
11	B	1211	CLA	C1B-CHB	3.13	1.48	1.40
11	B	1210	CLA	C1B-CHB	3.13	1.48	1.40
11	1	1127	CLA	C1B-CHB	3.13	1.48	1.40
11	1	1022	CLA	C4B-CHC	3.13	1.48	1.40
11	1	1237	CLA	C1B-CHB	3.13	1.48	1.40
11	a	1108	CLA	C4B-CHC	3.13	1.48	1.40
11	1	1106	CLA	C1B-CHB	3.13	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1023	CLA	C4B-CHC	3.13	1.48	1.40
11	a	1129	CLA	C4B-CHC	3.13	1.48	1.40
11	A	1012	CLA	C4B-CHC	3.13	1.48	1.40
11	1	1138	CLA	C1B-CHB	3.13	1.48	1.40
11	A	1105	CLA	C4B-CHC	3.13	1.48	1.40
11	A	1102	CLA	C4B-CHC	3.13	1.48	1.40
11	A	1128	CLA	C1B-CHB	3.13	1.48	1.40
11	2	1211	CLA	C1B-CHB	3.13	1.48	1.40
11	B	1216	CLA	C4B-CHC	3.13	1.48	1.40
11	2	1227	CLA	C1B-CHB	3.13	1.48	1.40
11	A	1131	CLA	C1B-CHB	3.13	1.48	1.40
11	A	1103	CLA	C1B-CHB	3.13	1.48	1.40
11	1	1108	CLA	C1B-CHB	3.14	1.48	1.40
11	1	1113	CLA	C4B-CHC	3.14	1.48	1.40
11	a	1110	CLA	C4B-CHC	3.14	1.48	1.40
11	b	1209	CLA	C1B-CHB	3.14	1.48	1.40
11	b	1224	CLA	C1B-CHB	3.14	1.48	1.40
11	1	1105	CLA	C4B-CHC	3.14	1.48	1.40
11	1	1136	CLA	C4B-CHC	3.14	1.48	1.40
11	2	1239	CLA	C1B-CHB	3.14	1.48	1.40
11	B	1236	CLA	C1B-CHB	3.14	1.48	1.40
11	a	1137	CLA	C1B-CHB	3.14	1.48	1.40
11	b	1236	CLA	C1B-CHB	3.14	1.48	1.40
11	a	1129	CLA	C1B-CHB	3.14	1.48	1.40
11	1	1137	CLA	C4B-CHC	3.14	1.48	1.40
11	0	1402	CLA	C1B-CHB	3.14	1.48	1.40
11	1	1012	CLA	C1B-CHB	3.14	1.48	1.40
11	L	1502	CLA	C4B-CHC	3.14	1.48	1.40
11	2	1226	CLA	C4B-CHC	3.14	1.48	1.40
11	1	1131	CLA	C1B-CHB	3.14	1.48	1.40
11	a	1124	CLA	C4B-CHC	3.14	1.48	1.40
11	B	1210	CLA	C4B-CHC	3.14	1.48	1.40
11	B	1023	CLA	C4B-CHC	3.14	1.48	1.40
11	A	1109	CLA	C4B-CHC	3.14	1.48	1.40
11	b	1211	CLA	C4B-CHC	3.15	1.48	1.40
11	2	1230	CLA	C4B-CHC	3.15	1.48	1.40
11	2	1238	CLA	C4B-CHC	3.15	1.48	1.40
11	l	1502	CLA	C1B-CHB	3.15	1.48	1.40
11	1	1135	CLA	C4B-CHC	3.15	1.48	1.40
11	b	1217	CLA	C4B-CHC	3.15	1.48	1.40
11	2	1216	CLA	C1B-CHB	3.15	1.48	1.40
11	b	1220	CLA	C4B-CHC	3.15	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1129	CLA	C4B-CHC	3.15	1.48	1.40
11	b	1232	CLA	C4B-CHC	3.15	1.48	1.40
11	b	1021	CLA	C4B-CHC	3.15	1.48	1.40
11	a	1134	CLA	C4B-CHC	3.15	1.48	1.40
11	B	1230	CLA	C1B-CHB	3.15	1.48	1.40
11	A	1127	CLA	C4B-CHC	3.15	1.48	1.40
11	a	1139	CLA	C1B-CHB	3.15	1.48	1.40
11	2	1201	CLA	C1B-CHB	3.15	1.48	1.40
11	1	1107	CLA	C4B-CHC	3.15	1.48	1.40
11	a	1801	CLA	C4B-CHC	3.15	1.48	1.40
11	B	1218	CLA	C1B-CHB	3.15	1.48	1.40
11	2	1224	CLA	C1B-CHB	3.15	1.48	1.40
11	A	1108	CLA	C4B-CHC	3.15	1.48	1.40
11	2	1013	CLA	C4B-CHC	3.15	1.48	1.40
11	b	1216	CLA	C1B-CHB	3.16	1.48	1.40
11	a	1130	CLA	C4B-CHC	3.16	1.48	1.40
11	1	1124	CLA	C4B-CHC	3.16	1.48	1.40
11	A	1107	CLA	C4B-CHC	3.16	1.48	1.40
11	B	1224	CLA	C1B-CHB	3.16	1.48	1.40
11	b	1213	CLA	C1B-CHB	3.16	1.48	1.40
11	a	1113	CLA	C4B-CHC	3.16	1.48	1.40
11	b	1238	CLA	C4B-CHC	3.16	1.48	1.40
11	A	1103	CLA	C3D-C2D	3.16	1.46	1.39
11	a	1117	CLA	C4B-CHC	3.16	1.48	1.40
11	2	1205	CLA	C3D-C2D	3.16	1.46	1.39
11	1	1133	CLA	C1B-CHB	3.16	1.48	1.40
11	a	1106	CLA	C4B-CHC	3.16	1.48	1.40
11	k	1402	CLA	C4B-CHC	3.16	1.48	1.40
11	a	1012	CLA	C4B-CHC	3.16	1.48	1.40
11	A	1114	CLA	C1B-CHB	3.16	1.48	1.40
11	a	1108	CLA	C1B-CHB	3.16	1.48	1.40
11	b	1219	CLA	C1B-CHB	3.16	1.48	1.40
11	a	1121	CLA	C4B-CHC	3.16	1.48	1.40
11	1	1139	CLA	C4B-CHC	3.16	1.48	1.40
11	a	1113	CLA	C1B-CHB	3.16	1.48	1.40
11	b	1231	CLA	C4B-CHC	3.16	1.48	1.40
11	B	1208	CLA	C1B-CHB	3.16	1.48	1.40
11	2	1205	CLA	C4B-CHC	3.16	1.48	1.40
11	B	1226	CLA	C4B-CHC	3.16	1.48	1.40
11	2	1202	CLA	C3D-C2D	3.16	1.46	1.39
11	A	1140	CLA	C1B-CHB	3.17	1.48	1.40
11	b	1224	CLA	C4B-CHC	3.17	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1113	CLA	C1B-CHB	3.17	1.48	1.40
11	2	1213	CLA	C1B-CHB	3.17	1.48	1.40
11	b	1203	CLA	C4B-CHC	3.17	1.48	1.40
11	B	1213	CLA	C4B-CHC	3.17	1.48	1.40
11	1	1114	CLA	C1B-CHB	3.17	1.48	1.40
11	1	1120	CLA	C4B-CHC	3.17	1.48	1.40
11	b	1236	CLA	C3D-C2D	3.17	1.46	1.39
11	2	1204	CLA	C4B-CHC	3.17	1.48	1.40
11	2	1225	CLA	C3D-C2D	3.17	1.46	1.39
11	1	1119	CLA	C4B-CHC	3.17	1.48	1.40
11	B	1013	CLA	C4B-CHC	3.17	1.48	1.40
11	a	1107	CLA	C3D-C2D	3.17	1.46	1.39
11	2	1219	CLA	C3D-C2D	3.17	1.46	1.39
11	a	1114	CLA	C1B-CHB	3.17	1.48	1.40
11	a	1118	CLA	C1B-CHB	3.17	1.48	1.40
11	1	1122	CLA	C1B-CHB	3.17	1.48	1.40
11	1	1116	CLA	C4B-CHC	3.17	1.48	1.40
11	1	1102	CLA	C4B-CHC	3.17	1.48	1.40
11	A	1022	CLA	C4B-CHC	3.18	1.48	1.40
11	B	1232	CLA	C1B-CHB	3.18	1.48	1.40
11	1	1134	CLA	C4B-CHC	3.18	1.48	1.40
11	L	1501	CLA	C4B-CHC	3.18	1.48	1.40
11	2	1216	CLA	C4B-CHC	3.18	1.48	1.40
11	b	1229	CLA	C4B-CHC	3.18	1.48	1.40
11	1	1107	CLA	C1B-CHB	3.18	1.48	1.40
11	a	1115	CLA	C1B-CHB	3.18	1.48	1.40
11	a	1105	CLA	C1B-CHB	3.18	1.48	1.40
11	1	1129	CLA	C1B-CHB	3.18	1.48	1.40
11	a	1136	CLA	C1B-CHB	3.18	1.48	1.40
11	A	1125	CLA	C1B-CHB	3.18	1.48	1.40
11	1	1130	CLA	C4B-CHC	3.18	1.48	1.40
11	1	1108	CLA	C4B-CHC	3.19	1.48	1.40
11	1	1129	CLA	C4B-CHC	3.19	1.48	1.40
11	2	1232	CLA	C4B-CHC	3.19	1.48	1.40
11	B	1213	CLA	C1B-CHB	3.19	1.48	1.40
11	b	1211	CLA	C1B-CHB	3.19	1.48	1.40
11	A	1130	CLA	C4B-CHC	3.19	1.48	1.40
11	b	1225	CLA	C3D-C2D	3.19	1.46	1.39
11	A	1112	CLA	C3D-C2D	3.19	1.46	1.39
11	a	1125	CLA	C4B-CHC	3.19	1.48	1.40
11	A	1113	CLA	C4B-CHC	3.19	1.48	1.40
11	B	1201	CLA	C3D-C2D	3.19	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1111	CLA	C1B-CHB	3.19	1.48	1.40
11	A	1121	CLA	C4B-CHC	3.19	1.48	1.40
11	b	1216	CLA	C4B-CHC	3.19	1.48	1.40
11	b	1201	CLA	C4B-CHC	3.19	1.48	1.40
11	l	1501	CLA	C4B-CHC	3.19	1.48	1.40
11	b	1221	CLA	C1B-CHB	3.19	1.48	1.40
11	B	1223	CLA	C4B-CHC	3.20	1.48	1.40
11	A	1118	CLA	C3D-C2D	3.20	1.46	1.39
11	b	1240	CLA	C4B-CHC	3.20	1.48	1.40
11	l	1502	CLA	C4B-CHC	3.20	1.48	1.40
11	2	1208	CLA	C1B-CHB	3.20	1.48	1.40
11	1	1112	CLA	C4B-CHC	3.20	1.48	1.40
11	b	1218	CLA	C4B-CHC	3.20	1.48	1.40
11	8	1502	CLA	C4B-CHC	3.20	1.48	1.40
11	B	1227	CLA	C1B-CHB	3.20	1.48	1.40
11	2	1231	CLA	C4B-CHC	3.20	1.48	1.40
11	a	1132	CLA	C4B-CHC	3.20	1.48	1.40
11	A	1120	CLA	C4B-CHC	3.20	1.48	1.40
11	1	1111	CLA	C3D-C2D	3.20	1.46	1.39
11	B	1226	CLA	C3D-C2D	3.21	1.46	1.39
11	A	1126	CLA	C3D-C2D	3.21	1.46	1.39
11	A	1123	CLA	C3D-C2D	3.21	1.46	1.39
11	b	1226	CLA	C4B-CHC	3.21	1.48	1.40
11	b	1234	CLA	C1B-CHB	3.21	1.48	1.40
11	A	1105	CLA	C1B-CHB	3.21	1.48	1.40
11	b	1212	CLA	C1B-CHB	3.21	1.48	1.40
11	B	1212	CLA	C4B-CHC	3.22	1.48	1.40
11	A	1132	CLA	C1B-CHB	3.22	1.48	1.40
11	B	1234	CLA	C1B-CHB	3.22	1.48	1.40
11	B	1207	CLA	C3D-C2D	3.22	1.46	1.39
11	2	1226	CLA	C1B-CHB	3.22	1.48	1.40
11	1	1107	CLA	C3D-C2D	3.22	1.46	1.39
11	b	1013	CLA	C4B-CHC	3.22	1.48	1.40
11	2	1210	CLA	C4B-CHC	3.22	1.48	1.40
11	a	1133	CLA	C1B-CHB	3.22	1.48	1.40
11	1	1136	CLA	C1B-CHB	3.22	1.48	1.40
11	b	1236	CLA	C4B-CHC	3.22	1.48	1.40
11	2	1229	CLA	C4B-CHC	3.22	1.48	1.40
11	A	1110	CLA	C1B-CHB	3.22	1.48	1.40
11	1	1103	CLA	C3D-C2D	3.22	1.46	1.39
11	8	1503	CLA	C4B-CHC	3.22	1.48	1.40
11	a	1115	CLA	C3D-C2D	3.23	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1236	CLA	C3D-C2D	3.23	1.46	1.39
11	a	1125	CLA	C3D-C2D	3.23	1.46	1.39
11	2	1231	CLA	C3D-C2D	3.23	1.46	1.39
11	B	1225	CLA	C3D-C2D	3.23	1.46	1.39
11	A	1136	CLA	C1B-CHB	3.23	1.48	1.40
11	1	1129	CLA	C3D-C2D	3.23	1.46	1.39
11	A	1139	CLA	C4B-CHC	3.23	1.48	1.40
11	2	1205	CLA	C1B-CHB	3.23	1.48	1.40
11	1	1125	CLA	C4B-CHC	3.23	1.48	1.40
11	1	1011	CLA	C3D-C2D	3.23	1.46	1.39
11	B	1205	CLA	C3D-C2D	3.24	1.46	1.39
11	B	1203	CLA	C3D-C2D	3.24	1.46	1.39
11	b	1235	CLA	C4B-CHC	3.24	1.48	1.40
11	2	1236	CLA	C1B-CHB	3.24	1.48	1.40
11	A	1137	CLA	C3D-C2D	3.24	1.46	1.39
11	B	1236	CLA	C4B-CHC	3.24	1.48	1.40
11	b	1208	CLA	C1B-CHB	3.24	1.48	1.40
11	B	1217	CLA	C3D-C2D	3.24	1.46	1.39
11	2	1202	CLA	C1B-CHB	3.25	1.48	1.40
11	A	1122	CLA	C3D-C2D	3.25	1.46	1.39
11	a	1122	CLA	C4B-CHC	3.25	1.48	1.40
11	2	1216	CLA	C3D-C2D	3.25	1.46	1.39
11	b	1224	CLA	C3D-C2D	3.25	1.46	1.39
11	a	1111	CLA	C4B-CHC	3.25	1.48	1.40
11	A	1105	CLA	C3D-C2D	3.25	1.46	1.39
11	b	1202	CLA	C3D-C2D	3.25	1.46	1.39
11	B	1208	CLA	C4B-CHC	3.25	1.48	1.40
11	1	1237	CLA	C3D-C2D	3.25	1.46	1.39
11	A	1111	CLA	C4B-CHC	3.25	1.48	1.40
11	2	1201	CLA	C3D-C2D	3.25	1.46	1.39
11	1	1122	CLA	C4B-CHC	3.26	1.48	1.40
11	B	1235	CLA	C4B-CHC	3.26	1.48	1.40
11	B	1240	CLA	C4B-CHC	3.26	1.48	1.40
11	A	1136	CLA	C3D-C2D	3.26	1.46	1.39
11	b	1213	CLA	C4B-CHC	3.26	1.48	1.40
11	b	1207	CLA	C3D-C2D	3.26	1.46	1.39
11	b	1223	CLA	C1B-CHB	3.26	1.48	1.40
11	A	1101	CLA	C4B-CHC	3.26	1.48	1.40
11	B	1224	CLA	C4B-CHC	3.26	1.48	1.40
11	A	1118	CLA	C1B-CHB	3.26	1.48	1.40
11	b	1223	CLA	C3D-C2D	3.26	1.46	1.39
11	a	1104	CLA	C4B-CHC	3.26	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1202	CLA	C4B-CHC	3.26	1.48	1.40
11	B	1223	CLA	C3D-C2D	3.26	1.46	1.39
11	B	1222	CLA	C4B-CHC	3.26	1.48	1.40
11	B	1214	CLA	C4B-CHC	3.26	1.48	1.40
11	A	1120	CLA	C3D-C2D	3.27	1.47	1.39
11	B	1221	CLA	C3D-C2D	3.27	1.47	1.39
11	a	1116	CLA	C3D-C2D	3.27	1.47	1.39
11	b	1221	CLA	C3D-C2D	3.27	1.47	1.39
11	1	1111	CLA	C4B-CHC	3.27	1.48	1.40
11	a	1111	CLA	C3D-C2D	3.27	1.47	1.39
11	2	1203	CLA	C3D-C2D	3.27	1.47	1.39
11	a	1139	CLA	C3D-C2D	3.27	1.47	1.39
11	A	1129	CLA	C3D-C2D	3.27	1.47	1.39
11	2	1222	CLA	C3D-C2D	3.28	1.47	1.39
11	1	1136	CLA	C3D-C2D	3.28	1.47	1.39
11	2	1235	CLA	C4B-CHC	3.28	1.48	1.40
11	B	1218	CLA	C3D-C2D	3.28	1.47	1.39
11	a	1116	CLA	C4B-CHC	3.28	1.48	1.40
11	b	1231	CLA	C3D-C2D	3.28	1.47	1.39
11	1	1106	CLA	C3D-C2D	3.28	1.47	1.39
11	a	1118	CLA	C3D-C2D	3.28	1.47	1.39
11	a	1135	CLA	C3D-C2D	3.28	1.47	1.39
11	a	1237	CLA	C3D-C2D	3.28	1.47	1.39
11	b	1235	CLA	C3D-C2D	3.28	1.47	1.39
11	2	1219	CLA	C4B-CHC	3.28	1.48	1.40
11	B	1238	CLA	C3D-C2D	3.29	1.47	1.39
11	a	1121	CLA	C3D-C2D	3.29	1.47	1.39
11	2	1214	CLA	C3D-C2D	3.29	1.47	1.39
11	1	1125	CLA	C3D-C2D	3.29	1.47	1.39
11	A	1138	CLA	C3D-C2D	3.29	1.47	1.39
11	2	1236	CLA	C4B-CHC	3.29	1.48	1.40
11	k	1401	CLA	C3D-C2D	3.29	1.47	1.39
11	b	1221	CLA	C4B-CHC	3.29	1.48	1.40
11	A	1115	CLA	C3D-C2D	3.30	1.47	1.39
11	B	1023	CLA	C3D-C2D	3.30	1.47	1.39
11	A	1137	CLA	C4B-CHC	3.30	1.48	1.40
11	A	1134	CLA	C3D-C2D	3.30	1.47	1.39
11	K	1401	CLA	C3D-C2D	3.30	1.47	1.39
11	1	1124	CLA	C3D-C2D	3.30	1.47	1.39
11	1	1116	CLA	C3D-C2D	3.30	1.47	1.39
11	0	1402	CLA	C4B-CHC	3.30	1.48	1.40
11	A	1103	CLA	C4B-CHC	3.30	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1116	CLA	C4B-CHC	3.30	1.48	1.40
11	2	1221	CLA	C3D-C2D	3.31	1.47	1.39
11	a	1138	CLA	C3D-C2D	3.31	1.47	1.39
11	2	1213	CLA	C4B-CHC	3.31	1.48	1.40
11	2	1223	CLA	C4B-CHC	3.31	1.48	1.40
11	B	1214	CLA	C3D-C2D	3.31	1.47	1.39
11	A	1132	CLA	C3D-C2D	3.31	1.47	1.39
11	b	1213	CLA	C3D-C2D	3.31	1.47	1.39
11	A	1121	CLA	C3D-C2D	3.31	1.47	1.39
11	2	1223	CLA	C3D-C2D	3.31	1.47	1.39
11	A	1119	CLA	C3D-C2D	3.31	1.47	1.39
11	b	1214	CLA	C4B-CHC	3.31	1.48	1.40
11	b	1202	CLA	C4B-CHC	3.32	1.48	1.40
11	B	1202	CLA	C3D-C2D	3.32	1.47	1.39
11	a	1120	CLA	C3D-C2D	3.32	1.47	1.39
11	B	1021	CLA	C3D-C2D	3.32	1.47	1.39
11	b	1222	CLA	C3D-C2D	3.32	1.47	1.39
11	b	1210	CLA	C4B-CHC	3.32	1.49	1.40
11	b	1226	CLA	C3D-C2D	3.32	1.47	1.39
11	2	1220	CLA	C3D-C2D	3.32	1.47	1.39
11	a	1113	CLA	C3D-C2D	3.32	1.47	1.39
11	0	1401	CLA	C3D-C2D	3.32	1.47	1.39
11	b	1205	CLA	C3D-C2D	3.33	1.47	1.39
11	A	1117	CLA	C4B-CHC	3.33	1.49	1.40
11	2	1235	CLA	C3D-C2D	3.33	1.47	1.39
11	a	1104	CLA	C3D-C2D	3.33	1.47	1.39
11	a	1112	CLA	C4B-CHC	3.33	1.49	1.40
11	L	1502	CLA	C3D-C2D	3.34	1.47	1.39
11	b	1201	CLA	C3D-C2D	3.34	1.47	1.39
11	B	1202	CLA	C4B-CHC	3.34	1.49	1.40
11	a	1136	CLA	C3D-C2D	3.34	1.47	1.39
11	A	1140	CLA	C3D-C2D	3.34	1.47	1.39
11	A	1125	CLA	C3D-C2D	3.34	1.47	1.39
11	B	1222	CLA	C3D-C2D	3.34	1.47	1.39
11	1	1108	CLA	C3D-C2D	3.34	1.47	1.39
11	a	1140	CLA	C3D-C2D	3.34	1.47	1.39
11	a	1112	CLA	C3D-C2D	3.34	1.47	1.39
11	A	1113	CLA	C3D-C2D	3.34	1.47	1.39
11	L	1501	CLA	C3D-C2D	3.34	1.47	1.39
11	B	1216	CLA	C3D-C2D	3.34	1.47	1.39
11	A	1139	CLA	C3D-C2D	3.34	1.47	1.39
11	b	1220	CLA	C3D-C2D	3.35	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1801	CLA	C3D-C2D	3.35	1.47	1.39
11	1	1115	CLA	C3D-C2D	3.35	1.47	1.39
11	a	1237	CLA	C1B-CHB	3.35	1.49	1.40
11	b	1021	CLA	C3D-C2D	3.35	1.47	1.39
11	2	1211	CLA	C3D-C2D	3.35	1.47	1.39
11	1	1113	CLA	C3D-C2D	3.35	1.47	1.39
11	A	1115	CLA	C4B-CHC	3.35	1.49	1.40
11	b	1210	CLA	C3D-C2D	3.35	1.47	1.39
11	1	1140	CLA	C3D-C2D	3.35	1.47	1.39
11	b	1216	CLA	C3D-C2D	3.35	1.47	1.39
11	1	1104	CLA	C3D-C2D	3.35	1.47	1.39
11	1	1134	CLA	C3D-C2D	3.35	1.47	1.39
11	B	1219	CLA	C3D-C2D	3.35	1.47	1.39
11	1	1126	CLA	C4B-CHC	3.35	1.49	1.40
11	2	1232	CLA	C3D-C2D	3.35	1.47	1.39
11	2	1210	CLA	C3D-C2D	3.36	1.47	1.39
11	2	1218	CLA	C3D-C2D	3.36	1.47	1.39
11	a	1103	CLA	C3D-C2D	3.36	1.47	1.39
11	1	1131	CLA	C3D-C2D	3.36	1.47	1.39
11	a	1115	CLA	C4B-CHC	3.36	1.49	1.40
11	a	1108	CLA	C3D-C2D	3.36	1.47	1.39
11	L	1503	CLA	C3D-C2D	3.36	1.47	1.39
11	2	1207	CLA	C3D-C2D	3.36	1.47	1.39
11	B	1240	CLA	C3D-C2D	3.36	1.47	1.39
11	1	1112	CLA	C3D-C2D	3.36	1.47	1.39
11	1	1127	CLA	C3D-C2D	3.36	1.47	1.39
11	a	1124	CLA	C3D-C2D	3.36	1.47	1.39
11	A	1110	CLA	C3D-C2D	3.36	1.47	1.39
11	1	1139	CLA	C3D-C2D	3.37	1.47	1.39
11	8	1501	CLA	C3D-C2D	3.37	1.47	1.39
11	b	1227	CLA	C3D-C2D	3.37	1.47	1.39
11	1	1118	CLA	C3D-C2D	3.37	1.47	1.39
11	b	1209	CLA	C3D-C2D	3.37	1.47	1.39
11	8	1502	CLA	C3D-C2D	3.37	1.47	1.39
11	b	1212	CLA	C3D-C2D	3.37	1.47	1.39
11	B	1220	CLA	C3D-C2D	3.37	1.47	1.39
11	a	1129	CLA	C3D-C2D	3.37	1.47	1.39
11	a	1134	CLA	C3D-C2D	3.37	1.47	1.39
11	0	1402	CLA	C3D-C2D	3.37	1.47	1.39
11	a	1127	CLA	C3D-C2D	3.37	1.47	1.39
11	B	1239	CLA	C3D-C2D	3.37	1.47	1.39
11	1	1121	CLA	C3D-C2D	3.37	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1208	CLA	C3D-C2D	3.37	1.47	1.39
11	2	1209	CLA	C3D-C2D	3.37	1.47	1.39
11	b	1023	CLA	C3D-C2D	3.37	1.47	1.39
11	a	1106	CLA	C3D-C2D	3.38	1.47	1.39
11	a	1126	CLA	C4B-CHC	3.38	1.49	1.40
11	B	1234	CLA	C3D-C2D	3.38	1.47	1.39
11	A	1112	CLA	C4B-CHC	3.38	1.49	1.40
11	B	1204	CLA	C3D-C2D	3.38	1.47	1.39
11	B	1227	CLA	C3D-C2D	3.38	1.47	1.39
11	a	1137	CLA	C3D-C2D	3.38	1.47	1.39
11	2	1229	CLA	C3D-C2D	3.38	1.47	1.39
11	b	1214	CLA	C3D-C2D	3.38	1.47	1.39
11	b	1240	CLA	C3D-C2D	3.38	1.47	1.39
11	2	1238	CLA	C3D-C2D	3.38	1.47	1.39
11	1	1102	CLA	C3D-C2D	3.38	1.47	1.39
11	b	1217	CLA	C3D-C2D	3.38	1.47	1.39
11	2	1234	CLA	C3D-C2D	3.38	1.47	1.39
11	A	1237	CLA	C3D-C2D	3.38	1.47	1.39
11	a	1801	CLA	C3D-C2D	3.39	1.47	1.39
11	1	1138	CLA	C3D-C2D	3.39	1.47	1.39
11	A	1108	CLA	C3D-C2D	3.39	1.47	1.39
11	A	1116	CLA	C3D-C2D	3.39	1.47	1.39
11	2	1240	CLA	C3D-C2D	3.39	1.47	1.39
11	8	1503	CLA	C3D-C2D	3.39	1.47	1.39
11	a	1101	CLA	C3D-C2D	3.39	1.47	1.39
11	B	1215	CLA	C3D-C2D	3.39	1.47	1.39
11	a	1105	CLA	C3D-C2D	3.39	1.47	1.39
11	1	1135	CLA	C3D-C2D	3.39	1.47	1.39
11	1	1122	CLA	C3D-C2D	3.39	1.47	1.39
11	A	1011	CLA	C3D-C2D	3.39	1.47	1.39
11	b	1234	CLA	C3D-C2D	3.39	1.47	1.39
11	1	1123	CLA	C3D-C2D	3.39	1.47	1.39
11	b	1239	CLA	C3D-C2D	3.39	1.47	1.39
11	a	1011	CLA	C3D-C2D	3.40	1.47	1.39
11	b	1204	CLA	C3D-C2D	3.40	1.47	1.39
11	A	1124	CLA	C3D-C2D	3.40	1.47	1.39
11	B	1210	CLA	C3D-C2D	3.40	1.47	1.39
11	1	1119	CLA	C3D-C2D	3.40	1.47	1.39
11	a	1122	CLA	C3D-C2D	3.40	1.47	1.39
11	B	1235	CLA	C3D-C2D	3.40	1.47	1.39
11	2	1206	CLA	C3D-C2D	3.40	1.47	1.39
11	l	1502	CLA	C3D-C2D	3.40	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1111	CLA	C3D-C2D	3.40	1.47	1.39
11	a	1123	CLA	C3D-C2D	3.41	1.47	1.39
11	b	1206	CLA	C3D-C2D	3.41	1.47	1.39
11	K	1402	CLA	C3D-C2D	3.41	1.47	1.39
11	B	1213	CLA	C3D-C2D	3.41	1.47	1.39
11	1	1109	CLA	C3D-C2D	3.41	1.47	1.39
11	b	1218	CLA	C3D-C2D	3.41	1.47	1.39
11	a	1102	CLA	C3D-C2D	3.41	1.47	1.39
11	2	1213	CLA	C3D-C2D	3.41	1.47	1.39
11	2	1021	CLA	C3D-C2D	3.41	1.47	1.39
11	2	1228	CLA	C3D-C2D	3.41	1.47	1.39
11	1	1130	CLA	C3D-C2D	3.42	1.47	1.39
11	1	1801	CLA	C3D-C2D	3.42	1.47	1.39
11	a	1126	CLA	C3D-C2D	3.42	1.47	1.39
11	1	1101	CLA	C3D-C2D	3.42	1.47	1.39
11	1	1126	CLA	C3D-C2D	3.42	1.47	1.39
11	2	1239	CLA	C3D-C2D	3.42	1.47	1.39
11	l	1501	CLA	C3D-C2D	3.43	1.47	1.39
11	A	1135	CLA	C3D-C2D	3.43	1.47	1.39
11	a	1133	CLA	C3D-C2D	3.43	1.47	1.39
11	b	1203	CLA	C3D-C2D	3.43	1.47	1.39
11	A	1114	CLA	C3D-C2D	3.43	1.47	1.39
11	B	1206	CLA	C3D-C2D	3.43	1.47	1.39
11	A	1106	CLA	C3D-C2D	3.43	1.47	1.39
11	A	1130	CLA	C3D-C2D	3.43	1.47	1.39
11	2	1204	CLA	C3D-C2D	3.43	1.47	1.39
11	2	1227	CLA	C3D-C2D	3.44	1.47	1.39
11	B	1229	CLA	C3D-C2D	3.44	1.47	1.39
11	1	1132	CLA	C3D-C2D	3.44	1.47	1.39
11	1	1105	CLA	C3D-C2D	3.44	1.47	1.39
11	b	1238	CLA	C3D-C2D	3.44	1.47	1.39
11	a	1131	CLA	C3D-C2D	3.44	1.47	1.39
11	B	1212	CLA	C3D-C2D	3.44	1.47	1.39
11	b	1230	CLA	C3D-C2D	3.45	1.47	1.39
11	2	1236	CLA	C3D-C2D	3.45	1.47	1.39
11	1	1133	CLA	C3D-C2D	3.45	1.47	1.39
11	1	1128	CLA	C3D-C2D	3.45	1.47	1.39
11	a	1132	CLA	C3D-C2D	3.45	1.47	1.39
11	B	1232	CLA	C3D-C2D	3.45	1.47	1.39
11	B	1228	CLA	C3D-C2D	3.45	1.47	1.39
11	1	1137	CLA	C3D-C2D	3.45	1.47	1.39
11	2	1215	CLA	C3D-C2D	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1209	CLA	C3D-C2D	3.45	1.47	1.39
11	a	1117	CLA	C3D-C2D	3.45	1.47	1.39
11	b	1211	CLA	C3D-C2D	3.46	1.47	1.39
11	b	1229	CLA	C3D-C2D	3.46	1.47	1.39
11	b	1228	CLA	C3D-C2D	3.46	1.47	1.39
11	A	1126	CLA	C4B-CHC	3.46	1.49	1.40
11	a	1110	CLA	C3D-C2D	3.46	1.47	1.39
11	2	1217	CLA	C3D-C2D	3.46	1.47	1.39
11	k	1402	CLA	C3D-C2D	3.46	1.47	1.39
11	A	1133	CLA	C3D-C2D	3.47	1.47	1.39
11	a	1114	CLA	C3D-C2D	3.47	1.47	1.39
11	1	1120	CLA	C3D-C2D	3.47	1.47	1.39
11	2	1023	CLA	C3D-C2D	3.47	1.47	1.39
11	l	1503	CLA	C3D-C2D	3.47	1.47	1.39
11	1	1117	CLA	C3D-C2D	3.48	1.47	1.39
11	A	1109	CLA	C3D-C2D	3.48	1.47	1.39
11	A	1131	CLA	C3D-C2D	3.48	1.47	1.39
11	a	1109	CLA	C3D-C2D	3.48	1.47	1.39
11	1	1110	CLA	C3D-C2D	3.48	1.47	1.39
11	a	1128	CLA	C3D-C2D	3.48	1.47	1.39
11	2	1013	CLA	C3D-C2D	3.49	1.47	1.39
11	A	1102	CLA	C3D-C2D	3.49	1.47	1.39
11	a	1119	CLA	C3D-C2D	3.49	1.47	1.39
11	B	1230	CLA	C3D-C2D	3.49	1.47	1.39
11	b	1208	CLA	C3D-C2D	3.49	1.47	1.39
11	a	1130	CLA	C3D-C2D	3.49	1.47	1.39
11	b	1013	CLA	C3D-C2D	3.49	1.47	1.39
11	b	1219	CLA	C3D-C2D	3.49	1.47	1.39
11	B	1231	CLA	C3D-C2D	3.50	1.47	1.39
11	1	1114	CLA	C3D-C2D	3.50	1.47	1.39
11	2	1230	CLA	C3D-C2D	3.50	1.47	1.39
11	A	1117	CLA	C3D-C2D	3.51	1.47	1.39
11	2	1212	CLA	C3D-C2D	3.51	1.47	1.39
11	A	1128	CLA	C3D-C2D	3.53	1.47	1.39
11	A	1127	CLA	C3D-C2D	3.53	1.47	1.39
11	2	1208	CLA	C3D-C2D	3.53	1.47	1.39
11	b	1215	CLA	C3D-C2D	3.54	1.47	1.39
11	b	1232	CLA	C3D-C2D	3.54	1.47	1.39
11	1	1022	CLA	C3D-C2D	3.56	1.47	1.39
11	A	1022	CLA	C3D-C2D	3.59	1.47	1.39
11	B	1013	CLA	C3D-C2D	3.59	1.47	1.39
11	a	1022	CLA	C3D-C2D	3.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1012	CLA	C3D-C2D	3.75	1.48	1.39
11	a	1012	CLA	C3D-C2D	3.80	1.48	1.39
16	b	5002	LMG	O7-C10	3.87	1.45	1.34
11	A	1012	CLA	C3D-C2D	3.87	1.48	1.39
15	A	5003	LHG	O7-C7	3.88	1.45	1.34
11	A	1125	CLA	OBD-CAD	3.91	1.28	1.22
15	a	5003	LHG	O7-C7	3.93	1.45	1.34
11	B	1236	CLA	OBD-CAD	3.95	1.28	1.22
15	b	5004	LHG	O7-C7	3.95	1.45	1.34
16	2	5002	LMG	O7-C10	3.97	1.45	1.34
11	A	1119	CLA	OBD-CAD	3.98	1.28	1.22
16	B	5002	LMG	O7-C10	4.00	1.45	1.34
15	A	5001	LHG	O7-C7	4.01	1.45	1.34
15	1	5003	LHG	O7-C7	4.02	1.46	1.34
15	1	5001	LHG	O7-C7	4.05	1.46	1.34
15	a	5001	LHG	O7-C7	4.05	1.46	1.34
11	A	1123	CLA	C3B-C2B	4.06	1.45	1.40
15	B	5004	LHG	O7-C7	4.07	1.46	1.34
11	a	1125	CLA	OBD-CAD	4.12	1.28	1.22
15	2	5004	LHG	O7-C7	4.13	1.46	1.34
15	A	5001	LHG	O8-C23	4.13	1.45	1.33
11	b	1217	CLA	O2A-C1	4.14	1.60	1.46
16	B	5002	LMG	O8-C28	4.15	1.45	1.33
11	A	1138	CLA	C3C-C2C	4.16	1.45	1.36
11	2	1210	CLA	C3C-C2C	4.16	1.45	1.36
11	1	1111	CLA	C3C-C2C	4.16	1.45	1.36
11	1	1115	CLA	OBD-CAD	4.17	1.28	1.22
11	B	1223	CLA	OBD-CAD	4.18	1.28	1.22
11	A	1125	CLA	CHC-C1C	4.19	1.47	1.35
11	A	1112	CLA	C3B-C2B	4.20	1.45	1.40
11	a	1111	CLA	C3C-C2C	4.21	1.45	1.36
11	a	1119	CLA	OBD-CAD	4.22	1.28	1.22
16	b	5002	LMG	O8-C28	4.22	1.45	1.33
15	b	5004	LHG	O8-C23	4.22	1.45	1.33
11	A	1123	CLA	CHC-C1C	4.23	1.47	1.35
11	1	1237	CLA	OBD-CAD	4.23	1.28	1.22
15	2	5004	LHG	O8-C23	4.23	1.45	1.33
11	B	1206	CLA	CHC-C1C	4.23	1.47	1.35
11	A	1133	CLA	CHC-C1C	4.24	1.47	1.35
11	A	1127	CLA	OBD-CAD	4.24	1.28	1.22
11	b	1207	CLA	CHC-C1C	4.24	1.47	1.35
11	B	1234	CLA	CHC-C1C	4.24	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	5002	LMG	O8-C28	4.25	1.45	1.33
11	2	1236	CLA	O2A-C1	4.26	1.60	1.46
15	a	5003	LHG	O8-C23	4.26	1.45	1.33
11	2	1236	CLA	OBD-CAD	4.26	1.28	1.22
15	1	5001	LHG	O8-C23	4.26	1.45	1.33
11	B	1227	CLA	CHC-C1C	4.27	1.47	1.35
11	2	1207	CLA	C3C-C2C	4.27	1.45	1.36
11	1	1011	CLA	CHC-C1C	4.28	1.47	1.35
15	B	5004	LHG	O8-C23	4.28	1.45	1.33
11	a	1119	CLA	CHC-C1C	4.29	1.47	1.35
11	B	1230	CLA	CHC-C1C	4.29	1.47	1.35
11	A	1111	CLA	C3C-C2C	4.29	1.45	1.36
11	A	1134	CLA	CHC-C1C	4.29	1.47	1.35
11	B	1230	CLA	C3C-C2C	4.30	1.45	1.36
11	b	1206	CLA	CHC-C1C	4.30	1.47	1.35
11	b	1234	CLA	CHC-C1C	4.31	1.47	1.35
11	A	1138	CLA	CHC-C1C	4.31	1.47	1.35
11	b	1236	CLA	O2A-C1	4.31	1.61	1.46
11	B	1217	CLA	OBD-CAD	4.31	1.28	1.22
11	A	1106	CLA	C3B-C2B	4.31	1.46	1.40
11	1	1133	CLA	CHC-C1C	4.31	1.47	1.35
11	b	1226	CLA	OBD-CAD	4.31	1.28	1.22
11	2	1206	CLA	CHC-C1C	4.31	1.47	1.35
11	2	1206	CLA	C3B-C2B	4.32	1.46	1.40
11	1	1115	CLA	CHC-C1C	4.32	1.47	1.35
11	2	1223	CLA	OBD-CAD	4.32	1.28	1.22
11	2	1229	CLA	C3B-C2B	4.32	1.46	1.40
11	A	1121	CLA	OBD-CAD	4.32	1.28	1.22
11	A	1140	CLA	CHC-C1C	4.32	1.47	1.35
11	2	1234	CLA	CHC-C1C	4.33	1.47	1.35
15	1	5003	LHG	O8-C23	4.33	1.46	1.33
11	B	1236	CLA	O2A-C1	4.33	1.61	1.46
11	B	1232	CLA	CHC-C1C	4.33	1.48	1.35
11	a	1237	CLA	C3C-C2C	4.33	1.46	1.36
11	2	1207	CLA	CHC-C1C	4.33	1.48	1.35
11	A	1123	CLA	C3C-C2C	4.33	1.46	1.36
15	a	5001	LHG	O8-C23	4.33	1.46	1.33
11	2	1217	CLA	O2A-C1	4.33	1.61	1.46
11	A	1118	CLA	C3C-C2C	4.34	1.46	1.36
11	A	1119	CLA	C3B-C2B	4.34	1.46	1.40
11	1	1125	CLA	OBD-CAD	4.34	1.28	1.22
11	B	1205	CLA	CHC-C1C	4.34	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1123	CLA	C3C-C2C	4.34	1.46	1.36
11	a	1133	CLA	CHC-C1C	4.34	1.48	1.35
11	2	1212	CLA	CHC-C1C	4.34	1.48	1.35
11	2	1217	CLA	OBD-CAD	4.34	1.28	1.22
11	a	1011	CLA	CHC-C1C	4.34	1.48	1.35
11	L	1503	CLA	CHC-C1C	4.35	1.48	1.35
11	A	1022	CLA	C3B-C2B	4.35	1.46	1.40
11	B	1023	CLA	C3C-C2C	4.35	1.46	1.36
11	a	1135	CLA	CHC-C1C	4.35	1.48	1.35
11	B	1021	CLA	CHC-C1C	4.35	1.48	1.35
11	2	1227	CLA	CHC-C1C	4.35	1.48	1.35
11	a	1139	CLA	CHC-C1C	4.35	1.48	1.35
11	B	1231	CLA	CHC-C1C	4.35	1.48	1.35
11	1	1109	CLA	CHC-C1C	4.35	1.48	1.35
15	A	5003	LHG	O8-C23	4.36	1.46	1.33
11	a	1127	CLA	CHC-C1C	4.36	1.48	1.35
11	2	1232	CLA	C3B-C2B	4.36	1.46	1.40
11	b	1239	CLA	CHC-C1C	4.36	1.48	1.35
11	2	1235	CLA	C3C-C2C	4.36	1.46	1.36
11	B	1210	CLA	C3C-C2C	4.36	1.46	1.36
11	A	1114	CLA	CHC-C1C	4.36	1.48	1.35
11	1	1012	CLA	OBD-CAD	4.36	1.28	1.22
11	1	1123	CLA	C3C-C2C	4.37	1.46	1.36
11	B	1226	CLA	C3B-C2B	4.37	1.46	1.40
11	A	1118	CLA	CHC-C1C	4.37	1.48	1.35
11	a	1118	CLA	CHC-C1C	4.37	1.48	1.35
11	b	1236	CLA	OBD-CAD	4.37	1.28	1.22
11	1	1103	CLA	C3C-C2C	4.38	1.46	1.36
11	B	1229	CLA	CHC-C1C	4.38	1.48	1.35
11	A	1128	CLA	C3B-C2B	4.38	1.46	1.40
11	a	1105	CLA	CHC-C1C	4.38	1.48	1.35
11	2	1215	CLA	CHC-C1C	4.38	1.48	1.35
11	b	1223	CLA	CHC-C1C	4.38	1.48	1.35
11	b	1205	CLA	CHC-C1C	4.38	1.48	1.35
11	B	1214	CLA	C3C-C2C	4.39	1.46	1.36
11	1	1128	CLA	CHC-C1C	4.39	1.48	1.35
11	B	1201	CLA	CHC-C1C	4.39	1.48	1.35
11	B	1205	CLA	C3C-C2C	4.39	1.46	1.36
11	b	1210	CLA	C3C-C2C	4.39	1.46	1.36
11	2	1201	CLA	CHC-C1C	4.39	1.48	1.35
11	b	1212	CLA	CHC-C1C	4.39	1.48	1.35
11	B	1204	CLA	CHC-C1C	4.39	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1136	CLA	CHC-C1C	4.39	1.48	1.35
11	b	1207	CLA	C3C-C2C	4.39	1.46	1.36
11	A	1140	CLA	C3C-C2C	4.39	1.46	1.36
11	2	1203	CLA	CHC-C1C	4.40	1.48	1.35
11	A	1103	CLA	C3C-C2C	4.40	1.46	1.36
11	8	1501	CLA	CHC-C1C	4.40	1.48	1.35
11	B	1217	CLA	O2A-C1	4.40	1.61	1.46
11	A	1116	CLA	C3C-C2C	4.40	1.46	1.36
11	1	1128	CLA	C3B-C2B	4.40	1.46	1.40
11	2	1205	CLA	C3C-C2C	4.40	1.46	1.36
11	1	1011	CLA	C3B-C2B	4.40	1.46	1.40
11	B	1221	CLA	OBD-CAD	4.40	1.28	1.22
11	b	1208	CLA	CHC-C1C	4.41	1.48	1.35
11	2	1238	CLA	CHC-C1C	4.41	1.48	1.35
11	b	1238	CLA	OBD-CAD	4.41	1.28	1.22
11	a	1103	CLA	OBD-CAD	4.41	1.28	1.22
11	1	1237	CLA	C3C-C2C	4.41	1.46	1.36
11	2	1239	CLA	CHC-C1C	4.41	1.48	1.35
11	2	1234	CLA	C3C-C2C	4.41	1.46	1.36
11	2	1206	CLA	C3C-C2C	4.41	1.46	1.36
11	B	1215	CLA	CHC-C1C	4.41	1.48	1.35
11	B	1220	CLA	CHC-C1C	4.42	1.48	1.35
11	1	1135	CLA	OBD-CAD	4.42	1.28	1.22
11	2	1234	CLA	OBD-CAD	4.42	1.28	1.22
11	B	1206	CLA	C3C-C2C	4.42	1.46	1.36
11	A	1801	CLA	C3B-C2B	4.42	1.46	1.40
11	b	1214	CLA	C3C-C2C	4.42	1.46	1.36
11	A	1801	CLA	CHC-C1C	4.42	1.48	1.35
11	1	1022	CLA	C3B-C2B	4.42	1.46	1.40
11	A	1115	CLA	OBD-CAD	4.42	1.28	1.22
11	A	1106	CLA	CHC-C1C	4.42	1.48	1.35
11	a	1127	CLA	OBD-CAD	4.42	1.28	1.22
11	a	1110	CLA	CHC-C1C	4.42	1.48	1.35
11	a	1136	CLA	CHC-C1C	4.42	1.48	1.35
11	2	1023	CLA	C3C-C2C	4.43	1.46	1.36
11	K	1402	CLA	CHC-C1C	4.43	1.48	1.35
11	1	1117	CLA	CHC-C1C	4.43	1.48	1.35
11	1	1114	CLA	CHC-C1C	4.43	1.48	1.35
11	A	1011	CLA	CHC-C1C	4.43	1.48	1.35
11	B	1234	CLA	C3C-C2C	4.43	1.46	1.36
11	2	1220	CLA	CHC-C1C	4.43	1.48	1.35
11	b	1214	CLA	OBD-CAD	4.43	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1104	CLA	CHC-C1C	4.43	1.48	1.35
11	B	1203	CLA	CHC-C1C	4.43	1.48	1.35
11	2	1214	CLA	CHC-C1C	4.43	1.48	1.35
11	1	1237	CLA	CHC-C1C	4.43	1.48	1.35
11	2	1203	CLA	OBD-CAD	4.43	1.28	1.22
11	b	1222	CLA	CHC-C1C	4.43	1.48	1.35
11	A	1237	CLA	CHC-C1C	4.43	1.48	1.35
11	b	1219	CLA	CHC-C1C	4.44	1.48	1.35
11	a	1131	CLA	CHC-C1C	4.44	1.48	1.35
11	1	1121	CLA	OBD-CAD	4.44	1.28	1.22
11	a	1114	CLA	CHC-C1C	4.44	1.48	1.35
11	a	1022	CLA	CHC-C1C	4.44	1.48	1.35
11	B	1219	CLA	OBD-CAD	4.44	1.28	1.22
11	b	1228	CLA	CHC-C1C	4.44	1.48	1.35
11	A	1110	CLA	CHC-C1C	4.44	1.48	1.35
11	a	1120	CLA	CHC-C1C	4.44	1.48	1.35
11	a	1128	CLA	CHC-C1C	4.44	1.48	1.35
11	A	1132	CLA	CHC-C1C	4.44	1.48	1.35
11	a	1138	CLA	CHC-C1C	4.44	1.48	1.35
11	1	1137	CLA	OBD-CAD	4.44	1.28	1.22
11	a	1237	CLA	CHC-C1C	4.44	1.48	1.35
11	b	1205	CLA	C3C-C2C	4.45	1.46	1.36
11	b	1021	CLA	CHC-C1C	4.45	1.48	1.35
11	L	1503	CLA	C3C-C2C	4.45	1.46	1.36
11	b	1211	CLA	OBD-CAD	4.45	1.28	1.22
11	a	1125	CLA	CHC-C1C	4.45	1.48	1.35
11	A	1106	CLA	OBD-CAD	4.45	1.28	1.22
11	B	1218	CLA	CHC-C1C	4.45	1.48	1.35
11	A	1137	CLA	OBD-CAD	4.45	1.28	1.22
11	b	1219	CLA	OBD-CAD	4.45	1.28	1.22
11	2	1208	CLA	CHC-C1C	4.45	1.48	1.35
11	1	1103	CLA	CHC-C1C	4.45	1.48	1.35
11	1	1123	CLA	CHC-C1C	4.45	1.48	1.35
11	B	1232	CLA	C3C-C2C	4.45	1.46	1.36
11	1	1118	CLA	C3C-C2C	4.45	1.46	1.36
11	2	1240	CLA	CHC-C1C	4.45	1.48	1.35
11	2	1205	CLA	CHC-C1C	4.45	1.48	1.35
11	A	1129	CLA	OBD-CAD	4.45	1.28	1.22
11	a	1102	CLA	CHC-C1C	4.45	1.48	1.35
11	1	1101	CLA	CHC-C1C	4.45	1.48	1.35
11	2	1217	CLA	CHC-C1C	4.45	1.48	1.35
11	1	1131	CLA	CHC-C1C	4.46	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1021	CLA	CHC-C1C	4.46	1.48	1.35
11	1	1107	CLA	CHC-C1C	4.46	1.48	1.35
11	b	1230	CLA	CHC-C1C	4.46	1.48	1.35
11	b	1023	CLA	CHC-C1C	4.46	1.48	1.35
11	a	1107	CLA	OBD-CAD	4.46	1.28	1.22
11	2	1224	CLA	CHC-C1C	4.46	1.48	1.35
11	1	1140	CLA	CHC-C1C	4.46	1.48	1.35
11	B	1209	CLA	CHC-C1C	4.46	1.48	1.35
11	B	1232	CLA	C3B-C2B	4.46	1.46	1.40
11	B	1207	CLA	CHC-C1C	4.46	1.48	1.35
11	B	1023	CLA	CHC-C1C	4.46	1.48	1.35
11	B	1238	CLA	CHC-C1C	4.46	1.48	1.35
11	a	1121	CLA	CHC-C1C	4.46	1.48	1.35
11	B	1204	CLA	C3C-C2C	4.46	1.46	1.36
11	2	1216	CLA	OBD-CAD	4.46	1.28	1.22
11	2	1202	CLA	C3C-C2C	4.46	1.46	1.36
11	1	1105	CLA	CHC-C1C	4.46	1.48	1.35
11	b	1221	CLA	C3C-C2C	4.46	1.46	1.36
11	A	1237	CLA	OBD-CAD	4.46	1.28	1.22
11	2	1227	CLA	C3B-C2B	4.46	1.46	1.40
11	2	1203	CLA	C3C-C2C	4.46	1.46	1.36
11	1	1132	CLA	CHC-C1C	4.46	1.48	1.35
11	2	1023	CLA	CHC-C1C	4.46	1.48	1.35
11	B	1023	CLA	OBD-CAD	4.46	1.28	1.22
11	1	1138	CLA	CHC-C1C	4.46	1.48	1.35
11	b	1227	CLA	CHC-C1C	4.46	1.48	1.35
11	A	1134	CLA	C3C-C2C	4.46	1.46	1.36
11	A	1119	CLA	CHC-C1C	4.47	1.48	1.35
11	a	1124	CLA	OBD-CAD	4.47	1.28	1.22
11	A	1135	CLA	CHC-C1C	4.47	1.48	1.35
11	b	1023	CLA	C3C-C2C	4.47	1.46	1.36
11	B	1214	CLA	OBD-CAD	4.47	1.28	1.22
11	a	1140	CLA	CHC-C1C	4.47	1.48	1.35
11	a	1103	CLA	CHC-C1C	4.47	1.48	1.35
11	a	1123	CLA	CHC-C1C	4.47	1.48	1.35
11	b	1217	CLA	CHC-C1C	4.47	1.48	1.35
11	A	1113	CLA	OBD-CAD	4.47	1.28	1.22
11	a	1107	CLA	CHC-C1C	4.47	1.48	1.35
11	1	1110	CLA	CHC-C1C	4.47	1.48	1.35
11	B	1226	CLA	CHC-C1C	4.47	1.48	1.35
11	b	1228	CLA	OBD-CAD	4.47	1.28	1.22
11	2	1231	CLA	CHC-C1C	4.47	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1124	CLA	CHC-C1C	4.47	1.48	1.35
11	1	1012	CLA	CHC-C1C	4.47	1.48	1.35
11	b	1238	CLA	CHC-C1C	4.47	1.48	1.35
11	B	1211	CLA	CHC-C1C	4.47	1.48	1.35
11	b	1232	CLA	CHC-C1C	4.47	1.48	1.35
11	a	1126	CLA	C3C-C2C	4.48	1.46	1.36
11	2	1220	CLA	C3C-C2C	4.48	1.46	1.36
11	B	1216	CLA	OBD-CAD	4.48	1.28	1.22
11	1	1139	CLA	CHC-C1C	4.48	1.48	1.35
11	A	1104	CLA	CHC-C1C	4.48	1.48	1.35
11	A	1133	CLA	C3B-C2B	4.48	1.46	1.40
11	a	1101	CLA	CHC-C1C	4.48	1.48	1.35
11	2	1224	CLA	OBD-CAD	4.48	1.28	1.22
11	a	1108	CLA	CHC-C1C	4.48	1.48	1.35
11	B	1228	CLA	CHC-C1C	4.48	1.48	1.35
11	A	1131	CLA	CHC-C1C	4.48	1.48	1.35
11	b	1206	CLA	C3B-C2B	4.48	1.46	1.40
11	A	1129	CLA	CHC-C1C	4.48	1.48	1.35
11	2	1220	CLA	OBD-CAD	4.48	1.28	1.22
11	b	1209	CLA	CHC-C1C	4.48	1.48	1.35
11	A	1136	CLA	OBD-CAD	4.48	1.28	1.22
11	B	1211	CLA	OBD-CAD	4.48	1.28	1.22
11	b	1224	CLA	OBD-CAD	4.48	1.28	1.22
11	b	1204	CLA	OBD-CAD	4.48	1.28	1.22
11	b	1204	CLA	CHC-C1C	4.48	1.48	1.35
11	l	1503	CLA	CHC-C1C	4.48	1.48	1.35
11	2	1228	CLA	CHC-C1C	4.48	1.48	1.35
11	1	1135	CLA	CHC-C1C	4.48	1.48	1.35
11	1	1127	CLA	CHC-C1C	4.48	1.48	1.35
11	A	1107	CLA	C3C-C2C	4.48	1.46	1.36
11	1	1118	CLA	CHC-C1C	4.48	1.48	1.35
11	1	1119	CLA	OBD-CAD	4.48	1.28	1.22
11	2	1230	CLA	CHC-C1C	4.49	1.48	1.35
11	B	1207	CLA	C3C-C2C	4.49	1.46	1.36
11	b	1229	CLA	CHC-C1C	4.49	1.48	1.35
11	L	1501	CLA	OBD-CAD	4.49	1.28	1.22
11	b	1217	CLA	OBD-CAD	4.49	1.28	1.22
11	a	1137	CLA	CHC-C1C	4.49	1.48	1.35
11	A	1237	CLA	C3C-C2C	4.49	1.46	1.36
11	L	1502	CLA	CHC-C1C	4.49	1.48	1.35
11	b	1235	CLA	OBD-CAD	4.49	1.28	1.22
11	A	1104	CLA	OBD-CAD	4.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1108	CLA	C3C-C2C	4.49	1.46	1.36
11	a	1022	CLA	OBD-CAD	4.49	1.28	1.22
11	1	1124	CLA	OBD-CAD	4.49	1.28	1.22
11	2	1226	CLA	CHC-C1C	4.49	1.48	1.35
11	8	1503	CLA	OBD-CAD	4.49	1.28	1.22
11	A	1140	CLA	OBD-CAD	4.49	1.28	1.22
11	a	1139	CLA	C3C-C2C	4.49	1.46	1.36
11	L	1503	CLA	OBD-CAD	4.49	1.28	1.22
11	a	1107	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1101	CLA	CHC-C1C	4.49	1.48	1.35
11	B	1239	CLA	CHC-C1C	4.49	1.48	1.35
11	8	1502	CLA	OBD-CAD	4.49	1.28	1.22
11	2	1209	CLA	CHC-C1C	4.49	1.48	1.35
11	B	1219	CLA	CHC-C1C	4.49	1.48	1.35
11	b	1202	CLA	C3C-C2C	4.49	1.46	1.36
11	1	1109	CLA	OBD-CAD	4.49	1.28	1.22
11	A	1118	CLA	OBD-CAD	4.49	1.28	1.22
11	1	1101	CLA	C3C-C2C	4.49	1.46	1.36
11	1	1801	CLA	CHC-C1C	4.49	1.48	1.35
11	b	1220	CLA	CHC-C1C	4.49	1.48	1.35
11	A	1105	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1105	CLA	CHC-C1C	4.49	1.48	1.35
11	B	1204	CLA	C3B-C2B	4.49	1.46	1.40
11	1	1106	CLA	C3C-C2C	4.49	1.46	1.36
11	a	1138	CLA	C3C-C2C	4.49	1.46	1.36
11	A	1127	CLA	CHC-C1C	4.49	1.48	1.35
11	b	1212	CLA	C3C-C2C	4.49	1.46	1.36
11	B	1207	CLA	OBD-CAD	4.49	1.28	1.22
11	A	1102	CLA	CHC-C1C	4.49	1.48	1.35
11	A	1124	CLA	OBD-CAD	4.49	1.28	1.22
11	B	1220	CLA	OBD-CAD	4.49	1.28	1.22
11	B	1205	CLA	C3B-C2B	4.49	1.46	1.40
11	a	1121	CLA	OBD-CAD	4.49	1.28	1.22
11	a	1106	CLA	CHC-C1C	4.49	1.48	1.35
11	A	1124	CLA	C3B-C2B	4.50	1.46	1.40
11	1	1121	CLA	CHC-C1C	4.50	1.48	1.35
11	A	1122	CLA	C3C-C2C	4.50	1.46	1.36
11	2	1235	CLA	OBD-CAD	4.50	1.28	1.22
11	K	1401	CLA	CHC-C1C	4.50	1.48	1.35
11	1	1125	CLA	C3B-C2B	4.50	1.46	1.40
11	B	1235	CLA	OBD-CAD	4.50	1.28	1.22
11	A	1011	CLA	C3C-C2C	4.50	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	1502	CLA	OBD-CAD	4.50	1.28	1.22
11	2	1238	CLA	OBD-CAD	4.50	1.28	1.22
11	A	1105	CLA	OBD-CAD	4.50	1.28	1.22
11	k	1401	CLA	CHC-C1C	4.50	1.48	1.35
11	1	1120	CLA	CHC-C1C	4.50	1.48	1.35
11	a	1118	CLA	OBD-CAD	4.50	1.28	1.22
11	1	1131	CLA	OBD-CAD	4.50	1.28	1.22
11	b	1221	CLA	OBD-CAD	4.50	1.28	1.22
11	A	1124	CLA	CHC-C1C	4.50	1.48	1.35
11	A	1121	CLA	CHC-C1C	4.50	1.48	1.35
11	b	1215	CLA	CHC-C1C	4.50	1.48	1.35
11	b	1223	CLA	OBD-CAD	4.50	1.28	1.22
11	2	1221	CLA	C3C-C2C	4.50	1.46	1.36
11	1	1011	CLA	C3C-C2C	4.50	1.46	1.36
11	1	1126	CLA	C3C-C2C	4.51	1.46	1.36
11	B	1231	CLA	C3C-C2C	4.51	1.46	1.36
11	2	1214	CLA	C3C-C2C	4.51	1.46	1.36
11	1	1106	CLA	CHC-C1C	4.51	1.48	1.35
11	2	1222	CLA	CHC-C1C	4.51	1.48	1.35
11	B	1234	CLA	OBD-CAD	4.51	1.28	1.22
11	1	1136	CLA	CHC-C1C	4.51	1.48	1.35
11	B	1225	CLA	CHC-C1C	4.51	1.48	1.35
11	A	1109	CLA	CHC-C1C	4.51	1.48	1.35
11	1	1106	CLA	OBD-CAD	4.51	1.28	1.22
11	2	1221	CLA	CHC-C1C	4.51	1.48	1.35
11	B	1013	CLA	C3C-C2C	4.51	1.46	1.36
11	A	1012	CLA	OBD-CAD	4.51	1.28	1.22
11	2	1210	CLA	OBD-CAD	4.51	1.28	1.22
11	1	1119	CLA	CHC-C1C	4.51	1.48	1.35
11	B	1219	CLA	C3C-C2C	4.51	1.46	1.36
11	2	1214	CLA	OBD-CAD	4.51	1.28	1.22
11	A	1128	CLA	CHC-C1C	4.51	1.48	1.35
11	l	1502	CLA	C3C-C2C	4.51	1.46	1.36
11	B	1021	CLA	C3B-C2B	4.51	1.46	1.40
11	b	1219	CLA	C3C-C2C	4.51	1.46	1.36
11	2	1225	CLA	CHC-C1C	4.51	1.48	1.35
11	a	1108	CLA	C3C-C2C	4.51	1.46	1.36
11	a	1130	CLA	OBD-CAD	4.51	1.28	1.22
11	a	1129	CLA	CHC-C1C	4.51	1.48	1.35
11	b	1203	CLA	CHC-C1C	4.51	1.48	1.35
11	a	1113	CLA	CHC-C1C	4.51	1.48	1.35
11	1	1138	CLA	OBD-CAD	4.51	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1209	CLA	OBD-CAD	4.51	1.28	1.22
11	2	1216	CLA	CHC-C1C	4.51	1.48	1.35
11	a	1130	CLA	CHC-C1C	4.52	1.48	1.35
11	2	1225	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1216	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1203	CLA	C3B-C2B	4.52	1.46	1.40
11	B	1229	CLA	C3B-C2B	4.52	1.46	1.40
11	2	1211	CLA	CHC-C1C	4.52	1.48	1.35
11	a	1111	CLA	CHC-C1C	4.52	1.48	1.35
11	2	1211	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1204	CLA	OBD-CAD	4.52	1.28	1.22
11	a	1801	CLA	OBD-CAD	4.52	1.28	1.22
11	B	1209	CLA	OBD-CAD	4.52	1.28	1.22
11	A	1102	CLA	OBD-CAD	4.52	1.28	1.22
11	a	1114	CLA	C3C-C2C	4.52	1.46	1.36
11	A	1134	CLA	OBD-CAD	4.52	1.28	1.22
11	1	1136	CLA	OBD-CAD	4.52	1.28	1.22
11	a	1124	CLA	CHC-C1C	4.52	1.48	1.35
11	1	1137	CLA	CHC-C1C	4.52	1.48	1.35
11	A	1130	CLA	CHC-C1C	4.52	1.48	1.35
11	B	1227	CLA	OBD-CAD	4.52	1.28	1.22
11	1	1134	CLA	OBD-CAD	4.52	1.28	1.22
11	a	1109	CLA	OBD-CAD	4.52	1.28	1.22
11	A	1127	CLA	C3C-C2C	4.52	1.46	1.36
11	2	1230	CLA	C3C-C2C	4.52	1.46	1.36
11	1	1122	CLA	OBD-CAD	4.52	1.28	1.22
11	a	1127	CLA	C3C-C2C	4.52	1.46	1.36
11	1	1134	CLA	CHC-C1C	4.52	1.48	1.35
11	a	1117	CLA	CHC-C1C	4.53	1.48	1.35
11	b	1204	CLA	C3C-C2C	4.53	1.46	1.36
11	B	1216	CLA	CHC-C1C	4.53	1.48	1.35
11	B	1227	CLA	C3B-C2B	4.53	1.46	1.40
11	1	1130	CLA	CHC-C1C	4.53	1.48	1.35
11	1	1113	CLA	CHC-C1C	4.53	1.48	1.35
11	A	1130	CLA	OBD-CAD	4.53	1.28	1.22
11	B	1228	CLA	OBD-CAD	4.53	1.28	1.22
11	2	1206	CLA	OBD-CAD	4.53	1.28	1.22
11	2	1207	CLA	OBD-CAD	4.53	1.28	1.22
11	A	1122	CLA	CHC-C1C	4.53	1.48	1.35
11	a	1109	CLA	CHC-C1C	4.53	1.48	1.35
11	1	1110	CLA	C3C-C2C	4.53	1.46	1.36
11	b	1223	CLA	C3C-C2C	4.53	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1132	CLA	CHC-C1C	4.53	1.48	1.35
11	A	1118	CLA	C3B-C2B	4.53	1.46	1.40
11	0	1401	CLA	CHC-C1C	4.53	1.48	1.35
11	b	1211	CLA	CHC-C1C	4.53	1.48	1.35
11	2	1218	CLA	C3C-C2C	4.53	1.46	1.36
11	B	1208	CLA	OBD-CAD	4.53	1.28	1.22
11	l	1501	CLA	CHC-C1C	4.53	1.48	1.35
11	B	1217	CLA	CHC-C1C	4.53	1.48	1.35
11	K	1402	CLA	OBD-CAD	4.53	1.28	1.22
11	A	1012	CLA	CHC-C1C	4.53	1.48	1.35
11	2	1225	CLA	OBD-CAD	4.53	1.28	1.22
11	1	1131	CLA	C3C-C2C	4.53	1.46	1.36
11	b	1218	CLA	CHC-C1C	4.53	1.48	1.35
11	b	1202	CLA	OBD-CAD	4.53	1.28	1.22
11	A	1123	CLA	OBD-CAD	4.53	1.28	1.22
11	l	1503	CLA	C3C-C2C	4.53	1.46	1.36
11	0	1401	CLA	C3C-C2C	4.53	1.46	1.36
11	A	1126	CLA	OBD-CAD	4.53	1.28	1.22
11	B	1226	CLA	C3C-C2C	4.53	1.46	1.36
11	2	1218	CLA	OBD-CAD	4.54	1.28	1.22
11	a	1102	CLA	OBD-CAD	4.54	1.28	1.22
11	1	1105	CLA	OBD-CAD	4.54	1.28	1.22
11	b	1224	CLA	CHC-C1C	4.54	1.48	1.35
11	A	1137	CLA	C3C-C2C	4.54	1.46	1.36
11	b	1201	CLA	CHC-C1C	4.54	1.48	1.35
11	a	1136	CLA	OBD-CAD	4.54	1.28	1.22
11	B	1224	CLA	OBD-CAD	4.54	1.28	1.22
11	a	1106	CLA	OBD-CAD	4.54	1.28	1.22
11	A	1112	CLA	OBD-CAD	4.54	1.28	1.22
11	B	1225	CLA	C3C-C2C	4.54	1.46	1.36
11	b	1230	CLA	C3C-C2C	4.54	1.46	1.36
11	B	1232	CLA	OBD-CAD	4.54	1.28	1.22
11	1	1110	CLA	OBD-CAD	4.54	1.28	1.22
11	1	1801	CLA	C3B-C2B	4.54	1.46	1.40
11	K	1401	CLA	C3C-C2C	4.54	1.46	1.36
11	8	1502	CLA	CHC-C1C	4.54	1.48	1.35
11	8	1501	CLA	OBD-CAD	4.54	1.28	1.22
11	1	1132	CLA	C3B-C2B	4.54	1.46	1.40
11	a	1104	CLA	C3C-C2C	4.54	1.46	1.36
11	b	1208	CLA	C3C-C2C	4.54	1.46	1.36
11	2	1222	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1131	CLA	OBD-CAD	4.54	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	l	1502	CLA	CHC-C1C	4.54	1.48	1.35
11	A	1113	CLA	C3C-C2C	4.54	1.46	1.36
11	2	1209	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1128	CLA	OBD-CAD	4.54	1.28	1.22
11	b	1201	CLA	OBD-CAD	4.54	1.28	1.22
11	2	1205	CLA	OBD-CAD	4.54	1.28	1.22
11	a	1108	CLA	OBD-CAD	4.54	1.28	1.22
11	a	1011	CLA	C3C-C2C	4.54	1.46	1.36
11	B	1239	CLA	C3C-C2C	4.54	1.46	1.36
11	A	1136	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1121	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1134	CLA	CHC-C1C	4.54	1.48	1.35
11	a	1105	CLA	C3C-C2C	4.54	1.46	1.36
11	2	1218	CLA	CHC-C1C	4.54	1.48	1.35
11	b	1203	CLA	OBD-CAD	4.54	1.28	1.22
11	1	1102	CLA	CHC-C1C	4.54	1.48	1.35
11	2	1212	CLA	C3C-C2C	4.54	1.46	1.36
11	a	1139	CLA	C3B-C2B	4.54	1.46	1.40
11	a	1122	CLA	OBD-CAD	4.55	1.28	1.22
11	B	1221	CLA	CHC-C1C	4.55	1.48	1.35
11	B	1218	CLA	OBD-CAD	4.55	1.28	1.22
11	2	1234	CLA	C3B-C2B	4.55	1.46	1.40
11	A	1125	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1138	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1108	CLA	CHC-C1C	4.55	1.48	1.35
11	b	1206	CLA	C3C-C2C	4.55	1.46	1.36
11	l	1503	CLA	OBD-CAD	4.55	1.28	1.22
11	2	1228	CLA	OBD-CAD	4.55	1.28	1.22
11	a	1104	CLA	C3B-C2B	4.55	1.46	1.40
11	K	1401	CLA	OBD-CAD	4.55	1.28	1.22
11	l	1501	CLA	OBD-CAD	4.55	1.28	1.22
11	b	1229	CLA	OBD-CAD	4.55	1.28	1.22
11	b	1206	CLA	OBD-CAD	4.55	1.28	1.22
11	a	1122	CLA	C3C-C2C	4.55	1.46	1.36
11	B	1215	CLA	OBD-CAD	4.55	1.28	1.22
11	B	1021	CLA	C3C-C2C	4.55	1.46	1.36
11	L	1501	CLA	CHC-C1C	4.55	1.48	1.35
11	A	1107	CLA	O2D-CGD	4.55	1.44	1.33
11	b	1222	CLA	OBD-CAD	4.55	1.28	1.22
11	k	1401	CLA	OBD-CAD	4.55	1.28	1.22
11	b	1212	CLA	OBD-CAD	4.55	1.28	1.22
11	A	1129	CLA	C3C-C2C	4.55	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1112	CLA	OBD-CAD	4.55	1.28	1.22
11	1	1102	CLA	OBD-CAD	4.55	1.28	1.22
11	b	1231	CLA	CHC-C1C	4.55	1.48	1.35
11	b	1232	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1133	CLA	OBD-CAD	4.55	1.28	1.22
11	A	1106	CLA	C3C-C2C	4.55	1.46	1.36
11	A	1135	CLA	C3C-C2C	4.55	1.46	1.36
11	1	1801	CLA	OBD-CAD	4.55	1.28	1.22
11	a	1120	CLA	OBD-CAD	4.55	1.28	1.22
11	B	1204	CLA	OBD-CAD	4.55	1.28	1.22
11	8	1501	CLA	C3C-C2C	4.55	1.46	1.36
11	B	1210	CLA	CHC-C1C	4.55	1.48	1.35
11	a	1132	CLA	OBD-CAD	4.55	1.28	1.22
11	b	1208	CLA	OBD-CAD	4.55	1.28	1.22
11	a	1111	CLA	OBD-CAD	4.55	1.28	1.22
11	a	1140	CLA	OBD-CAD	4.55	1.28	1.22
11	A	1107	CLA	CHC-C1C	4.55	1.48	1.35
11	B	1220	CLA	C3C-C2C	4.55	1.46	1.36
11	b	1225	CLA	CHC-C1C	4.55	1.48	1.35
11	B	1209	CLA	C3C-C2C	4.55	1.46	1.36
11	0	1401	CLA	OBD-CAD	4.55	1.28	1.22
11	A	1114	CLA	OBD-CAD	4.55	1.28	1.22
11	1	1118	CLA	OBD-CAD	4.56	1.28	1.22
11	A	1108	CLA	CHC-C1C	4.56	1.48	1.35
11	a	1133	CLA	OBD-CAD	4.56	1.28	1.22
11	B	1203	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1022	CLA	C3B-C2B	4.56	1.46	1.40
11	1	1116	CLA	CHC-C1C	4.56	1.48	1.35
11	B	1206	CLA	C3B-C2B	4.56	1.46	1.40
11	1	1120	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1135	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1128	CLA	C3B-C2B	4.56	1.46	1.40
11	a	1112	CLA	OBD-CAD	4.56	1.28	1.22
11	b	1225	CLA	C3C-C2C	4.56	1.46	1.36
11	k	1402	CLA	CHC-C1C	4.56	1.48	1.35
11	b	1239	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1131	CLA	C3C-C2C	4.56	1.46	1.36
11	b	1240	CLA	CHC-C1C	4.56	1.48	1.35
11	2	1232	CLA	CHC-C1C	4.56	1.48	1.35
11	b	1013	CLA	CHC-C1C	4.56	1.48	1.35
11	A	1120	CLA	C3C-C2C	4.56	1.46	1.36
11	1	1127	CLA	C3C-C2C	4.56	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1117	CLA	C3C-C2C	4.56	1.46	1.36
11	b	1234	CLA	OBD-CAD	4.56	1.28	1.22
11	2	1221	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1116	CLA	OBD-CAD	4.56	1.28	1.22
11	b	1218	CLA	OBD-CAD	4.56	1.28	1.22
11	A	1132	CLA	OBD-CAD	4.56	1.28	1.22
11	1	1101	CLA	OBD-CAD	4.56	1.28	1.22
11	A	1102	CLA	C3C-C2C	4.56	1.46	1.36
11	1	1022	CLA	CHC-C1C	4.56	1.48	1.35
11	1	1139	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1105	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1138	CLA	OBD-CAD	4.56	1.28	1.22
11	a	1136	CLA	C3C-C2C	4.56	1.46	1.36
11	1	1123	CLA	OBD-CAD	4.56	1.28	1.22
11	A	1114	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1122	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1132	CLA	OBD-CAD	4.57	1.28	1.22
11	2	1229	CLA	OBD-CAD	4.57	1.28	1.22
11	2	1219	CLA	OBD-CAD	4.57	1.28	1.22
11	A	1107	CLA	OBD-CAD	4.57	1.28	1.22
11	2	1021	CLA	C3C-C2C	4.57	1.46	1.36
11	B	1222	CLA	CHC-C1C	4.57	1.48	1.35
11	A	1133	CLA	C3C-C2C	4.57	1.46	1.36
11	2	1215	CLA	C3C-C2C	4.57	1.46	1.36
11	2	1013	CLA	C3C-C2C	4.57	1.46	1.36
11	A	1110	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1227	CLA	OBD-CAD	4.57	1.28	1.22
11	B	1226	CLA	OBD-CAD	4.57	1.28	1.22
11	b	1216	CLA	CHC-C1C	4.57	1.48	1.35
11	B	1013	CLA	CHC-C1C	4.57	1.48	1.35
11	b	1226	CLA	CHC-C1C	4.57	1.48	1.35
11	a	1012	CLA	CHC-C1C	4.57	1.48	1.35
11	a	1118	CLA	C3C-C2C	4.57	1.46	1.36
11	k	1401	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1231	CLA	C3C-C2C	4.57	1.46	1.36
11	2	1230	CLA	OBD-CAD	4.57	1.28	1.22
11	0	1401	CLA	C3B-C2B	4.57	1.46	1.40
11	a	1113	CLA	OBD-CAD	4.57	1.28	1.22
11	b	1210	CLA	OBD-CAD	4.57	1.28	1.22
11	b	1211	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1116	CLA	OBD-CAD	4.57	1.29	1.22
11	1	1113	CLA	OBD-CAD	4.57	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	1402	CLA	OBD-CAD	4.57	1.29	1.22
11	a	1134	CLA	OBD-CAD	4.57	1.29	1.22
11	A	1801	CLA	OBD-CAD	4.57	1.29	1.22
11	a	1128	CLA	OBD-CAD	4.57	1.29	1.22
11	a	1119	CLA	C3C-C2C	4.57	1.46	1.36
11	1	1134	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1021	CLA	OBD-CAD	4.57	1.29	1.22
11	A	1111	CLA	C3B-C2B	4.57	1.46	1.40
11	1	1119	CLA	C3B-C2B	4.57	1.46	1.40
11	b	1235	CLA	CHC-C1C	4.57	1.48	1.35
11	1	1132	CLA	C3C-C2C	4.57	1.46	1.36
11	a	1113	CLA	C3C-C2C	4.57	1.46	1.36
11	K	1401	CLA	C3B-C2B	4.57	1.46	1.40
11	1	1107	CLA	OBD-CAD	4.57	1.29	1.22
11	1	1125	CLA	CHC-C1C	4.57	1.48	1.35
11	a	1117	CLA	C3C-C2C	4.57	1.46	1.36
11	b	1240	CLA	OBD-CAD	4.58	1.29	1.22
11	a	1137	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1105	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1023	CLA	C3B-C2B	4.58	1.46	1.40
11	A	1120	CLA	CHC-C1C	4.58	1.48	1.35
11	B	1224	CLA	CHC-C1C	4.58	1.48	1.35
11	B	1206	CLA	OBD-CAD	4.58	1.29	1.22
11	1	1140	CLA	OBD-CAD	4.58	1.29	1.22
11	1	1103	CLA	OBD-CAD	4.58	1.29	1.22
11	A	1108	CLA	OBD-CAD	4.58	1.29	1.22
11	a	1140	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1012	CLA	OBD-CAD	4.58	1.29	1.22
11	B	1223	CLA	CHC-C1C	4.58	1.48	1.35
11	A	1131	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1112	CLA	C3C-C2C	4.58	1.46	1.36
11	2	1208	CLA	OBD-CAD	4.58	1.29	1.22
11	B	1238	CLA	OBD-CAD	4.58	1.29	1.22
11	B	1229	CLA	OBD-CAD	4.58	1.29	1.22
11	1	1128	CLA	OBD-CAD	4.58	1.29	1.22
11	b	1203	CLA	C3B-C2B	4.58	1.46	1.40
11	A	1139	CLA	CHC-C1C	4.58	1.48	1.35
11	B	1239	CLA	OBD-CAD	4.58	1.29	1.22
11	1	1133	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1238	CLA	C3C-C2C	4.58	1.46	1.36
11	1	1112	CLA	C3C-C2C	4.58	1.46	1.36
11	b	1213	CLA	OBD-CAD	4.58	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1111	CLA	OBD-CAD	4.58	1.29	1.22
11	b	1234	CLA	C3B-C2B	4.58	1.46	1.40
11	a	1134	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1215	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1139	CLA	OBD-CAD	4.58	1.29	1.22
11	a	1110	CLA	OBD-CAD	4.58	1.29	1.22
11	1	1121	CLA	C3C-C2C	4.58	1.46	1.36
11	b	1226	CLA	C3B-C2B	4.58	1.46	1.40
11	B	1221	CLA	C3C-C2C	4.58	1.46	1.36
11	a	1104	CLA	CHC-C1C	4.58	1.48	1.35
11	a	1129	CLA	OBD-CAD	4.58	1.29	1.22
11	A	1103	CLA	OBD-CAD	4.58	1.29	1.22
11	a	1115	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1213	CLA	CHC-C1C	4.58	1.48	1.35
11	2	1013	CLA	CHC-C1C	4.58	1.48	1.35
11	a	1115	CLA	OBD-CAD	4.58	1.29	1.22
11	2	1215	CLA	OBD-CAD	4.58	1.29	1.22
11	b	1215	CLA	C3C-C2C	4.58	1.46	1.36
11	b	1229	CLA	C3B-C2B	4.58	1.46	1.40
11	B	1013	CLA	OBD-CAD	4.58	1.29	1.22
11	a	1012	CLA	C3C-C2C	4.58	1.46	1.36
11	B	1236	CLA	CHC-C1C	4.58	1.48	1.35
11	b	1205	CLA	OBD-CAD	4.58	1.29	1.22
11	1	1116	CLA	C3C-C2C	4.58	1.46	1.36
11	A	1113	CLA	CHC-C1C	4.58	1.48	1.35
11	1	1022	CLA	OBD-CAD	4.59	1.29	1.22
11	b	1207	CLA	OBD-CAD	4.59	1.29	1.22
11	b	1215	CLA	C3B-C2B	4.59	1.46	1.40
11	2	1239	CLA	OBD-CAD	4.59	1.29	1.22
11	2	1231	CLA	C3C-C2C	4.59	1.46	1.36
11	8	1503	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1129	CLA	CHC-C1C	4.59	1.48	1.35
11	B	1235	CLA	CHC-C1C	4.59	1.48	1.35
11	A	1110	CLA	OBD-CAD	4.59	1.29	1.22
11	a	1012	CLA	C3B-C2B	4.59	1.46	1.40
11	2	1224	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1101	CLA	OBD-CAD	4.59	1.29	1.22
11	1	1130	CLA	OBD-CAD	4.59	1.29	1.22
11	A	1011	CLA	OBD-CAD	4.59	1.29	1.22
11	A	1135	CLA	OBD-CAD	4.59	1.29	1.22
11	A	1139	CLA	C3C-C2C	4.59	1.46	1.36
11	a	1133	CLA	C3B-C2B	4.59	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1503	CLA	CHC-C1C	4.59	1.48	1.35
11	A	1138	CLA	OBD-CAD	4.59	1.29	1.22
11	1	1125	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1101	CLA	C3B-C2B	4.59	1.46	1.40
11	B	1227	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1129	CLA	OBD-CAD	4.59	1.29	1.22
11	1	1104	CLA	OBD-CAD	4.59	1.29	1.22
11	2	1218	CLA	C3B-C2B	4.59	1.46	1.40
11	a	1116	CLA	CHC-C1C	4.59	1.48	1.35
11	2	1208	CLA	C3C-C2C	4.59	1.46	1.36
11	2	1216	CLA	C3B-C2B	4.59	1.46	1.40
11	a	1126	CLA	OBD-CAD	4.59	1.29	1.22
11	A	1126	CLA	C3B-C2B	4.59	1.46	1.40
11	1	1126	CLA	OBD-CAD	4.59	1.29	1.22
11	b	1232	CLA	OBD-CAD	4.59	1.29	1.22
11	a	1116	CLA	C3C-C2C	4.59	1.46	1.36
11	B	1218	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1135	CLA	C3B-C2B	4.59	1.46	1.40
11	2	1226	CLA	OBD-CAD	4.59	1.29	1.22
11	B	1240	CLA	OBD-CAD	4.59	1.29	1.22
11	B	1201	CLA	OBD-CAD	4.59	1.29	1.22
11	2	1229	CLA	CHC-C1C	4.59	1.48	1.35
11	A	1022	CLA	CHC-C1C	4.59	1.48	1.35
11	b	1216	CLA	OBD-CAD	4.59	1.29	1.22
11	A	1116	CLA	OBD-CAD	4.59	1.29	1.22
11	k	1401	CLA	C3B-C2B	4.59	1.46	1.40
11	2	1236	CLA	C3C-C2C	4.59	1.46	1.36
11	1	1112	CLA	CHC-C1C	4.59	1.48	1.35
11	2	1023	CLA	OBD-CAD	4.59	1.29	1.22
11	1	1011	CLA	OBD-CAD	4.59	1.29	1.22
11	b	1013	CLA	C3C-C2C	4.59	1.46	1.36
11	A	1124	CLA	C3C-C2C	4.59	1.46	1.36
11	b	1236	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1210	CLA	CHC-C1C	4.60	1.48	1.35
11	A	1117	CLA	OBD-CAD	4.60	1.29	1.22
11	A	1128	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1240	CLA	C3C-C2C	4.60	1.46	1.36
11	A	1131	CLA	OBD-CAD	4.60	1.29	1.22
11	2	1240	CLA	OBD-CAD	4.60	1.29	1.22
11	B	1225	CLA	OBD-CAD	4.60	1.29	1.22
11	B	1231	CLA	OBD-CAD	4.60	1.29	1.22
11	2	1013	CLA	OBD-CAD	4.60	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1203	CLA	C3B-C2B	4.60	1.46	1.40
11	a	1104	CLA	OBD-CAD	4.60	1.29	1.22
11	a	1137	CLA	OBD-CAD	4.60	1.29	1.22
11	2	1204	CLA	C3C-C2C	4.60	1.46	1.36
11	0	1402	CLA	CHC-C1C	4.60	1.48	1.35
11	2	1231	CLA	O2D-CGD	4.60	1.44	1.33
11	L	1502	CLA	C3C-C2C	4.60	1.46	1.36
11	B	1208	CLA	CHC-C1C	4.60	1.48	1.35
11	1	1133	CLA	OBD-CAD	4.60	1.29	1.22
11	B	1240	CLA	CHC-C1C	4.60	1.48	1.35
11	b	1230	CLA	OBD-CAD	4.60	1.29	1.22
11	a	1011	CLA	OBD-CAD	4.60	1.29	1.22
11	2	1021	CLA	OBD-CAD	4.60	1.29	1.22
11	a	1801	CLA	CHC-C1C	4.60	1.48	1.35
11	a	1102	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1227	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1201	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1202	CLA	CHC-C1C	4.60	1.48	1.35
11	a	1114	CLA	OBD-CAD	4.60	1.29	1.22
11	A	1122	CLA	OBD-CAD	4.60	1.29	1.22
11	b	1209	CLA	C3C-C2C	4.60	1.46	1.36
11	b	1214	CLA	CHC-C1C	4.60	1.48	1.35
11	l	1502	CLA	OBD-CAD	4.60	1.29	1.22
11	a	1022	CLA	C3C-C2C	4.60	1.46	1.36
11	2	1232	CLA	OBD-CAD	4.60	1.29	1.22
11	1	1117	CLA	OBD-CAD	4.60	1.29	1.22
11	A	1115	CLA	CHC-C1C	4.60	1.48	1.35
11	b	1220	CLA	OBD-CAD	4.61	1.29	1.22
11	1	1114	CLA	OBD-CAD	4.61	1.29	1.22
11	0	1402	CLA	OBD-CAD	4.61	1.29	1.22
11	2	1236	CLA	CHC-C1C	4.61	1.48	1.35
11	b	1238	CLA	C3C-C2C	4.61	1.46	1.36
11	b	1023	CLA	OBD-CAD	4.61	1.29	1.22
11	B	1235	CLA	C3C-C2C	4.61	1.46	1.36
11	a	1237	CLA	OBD-CAD	4.61	1.29	1.22
11	a	1111	CLA	O2A-C1	4.61	1.59	1.46
11	2	1204	CLA	CHC-C1C	4.61	1.48	1.35
11	a	1125	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1022	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1107	CLA	C3C-C2C	4.61	1.46	1.36
11	a	1101	CLA	OBD-CAD	4.61	1.29	1.22
11	2	1211	CLA	OBD-CAD	4.61	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1011	CLA	C3B-C2B	4.61	1.46	1.40
11	B	1213	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1115	CLA	C3C-C2C	4.61	1.46	1.36
11	B	1202	CLA	OBD-CAD	4.61	1.29	1.22
11	1	1124	CLA	C3C-C2C	4.61	1.46	1.36
11	1	1111	CLA	OBD-CAD	4.61	1.29	1.22
11	b	1225	CLA	OBD-CAD	4.61	1.29	1.22
11	2	1231	CLA	OBD-CAD	4.61	1.29	1.22
11	2	1213	CLA	OBD-CAD	4.61	1.29	1.22
11	1	1136	CLA	C3C-C2C	4.61	1.46	1.36
11	A	1139	CLA	OBD-CAD	4.62	1.29	1.22
11	b	1213	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1137	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1203	CLA	C3C-C2C	4.62	1.46	1.36
11	2	1212	CLA	OBD-CAD	4.62	1.29	1.22
11	B	1212	CLA	OBD-CAD	4.62	1.29	1.22
11	A	1101	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1133	CLA	C3C-C2C	4.62	1.46	1.36
11	b	1231	CLA	OBD-CAD	4.62	1.29	1.22
11	1	1110	CLA	C3B-C2B	4.62	1.46	1.40
11	B	1240	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1129	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1108	CLA	OBD-CAD	4.62	1.29	1.22
11	A	1022	CLA	OBD-CAD	4.62	1.29	1.22
11	1	1113	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1122	CLA	CHC-C1C	4.62	1.48	1.35
11	b	1236	CLA	CHC-C1C	4.62	1.48	1.35
11	B	1213	CLA	OBD-CAD	4.62	1.29	1.22
11	2	1219	CLA	CHC-C1C	4.62	1.48	1.35
11	2	1232	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1119	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1104	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1229	CLA	C3C-C2C	4.62	1.46	1.36
11	a	1106	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1212	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1212	CLA	CHC-C1C	4.62	1.48	1.35
11	1	1121	CLA	C3B-C2B	4.62	1.46	1.40
11	B	1021	CLA	OBD-CAD	4.62	1.29	1.22
11	2	1229	CLA	C3C-C2C	4.62	1.46	1.36
11	A	1132	CLA	C3C-C2C	4.62	1.46	1.36
11	1	1105	CLA	C3B-C2B	4.62	1.46	1.40
11	2	1201	CLA	OBD-CAD	4.62	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1109	CLA	C3C-C2C	4.62	1.46	1.36
11	B	1230	CLA	OBD-CAD	4.62	1.29	1.22
11	B	1216	CLA	C3C-C2C	4.63	1.46	1.36
11	2	1217	CLA	C3C-C2C	4.63	1.46	1.36
11	B	1210	CLA	OBD-CAD	4.63	1.29	1.22
11	B	1202	CLA	C3C-C2C	4.63	1.46	1.36
11	2	1238	CLA	C3C-C2C	4.63	1.46	1.36
11	a	1132	CLA	C3B-C2B	4.63	1.46	1.40
11	B	1205	CLA	OBD-CAD	4.63	1.29	1.22
11	2	1227	CLA	OBD-CAD	4.63	1.29	1.22
11	8	1502	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1201	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1222	CLA	C3C-C2C	4.63	1.46	1.36
11	b	1013	CLA	OBD-CAD	4.63	1.29	1.22
11	b	1224	CLA	C3C-C2C	4.63	1.46	1.36
11	A	1130	CLA	C3C-C2C	4.63	1.46	1.36
11	1	1111	CLA	CHC-C1C	4.63	1.48	1.35
11	b	1215	CLA	OBD-CAD	4.63	1.29	1.22
11	2	1222	CLA	OBD-CAD	4.63	1.29	1.22
11	A	1126	CLA	C3C-C2C	4.63	1.46	1.36
11	a	1101	CLA	C3C-C2C	4.63	1.46	1.36
11	1	1122	CLA	CHC-C1C	4.63	1.48	1.35
11	l	1501	CLA	C3C-C2C	4.63	1.46	1.36
11	2	1226	CLA	C3C-C2C	4.63	1.46	1.36
11	B	1208	CLA	C3C-C2C	4.63	1.46	1.36
11	1	1102	CLA	C3C-C2C	4.63	1.46	1.36
11	B	1222	CLA	OBD-CAD	4.63	1.29	1.22
11	A	1137	CLA	CHC-C1C	4.63	1.48	1.35
11	b	1235	CLA	C3C-C2C	4.63	1.46	1.36
11	a	1130	CLA	C3C-C2C	4.63	1.46	1.36
11	A	1111	CLA	O2A-C1	4.63	1.60	1.46
11	b	1234	CLA	C3C-C2C	4.64	1.46	1.36
11	b	1239	CLA	C3C-C2C	4.64	1.46	1.36
11	1	1114	CLA	C3B-C2B	4.64	1.46	1.40
11	b	1202	CLA	CHC-C1C	4.64	1.48	1.35
11	B	1215	CLA	C3B-C2B	4.64	1.46	1.40
11	1	1139	CLA	C3C-C2C	4.64	1.46	1.36
11	1	1114	CLA	C3C-C2C	4.64	1.46	1.36
11	A	1109	CLA	OBD-CAD	4.64	1.29	1.22
11	1	1129	CLA	C3C-C2C	4.64	1.46	1.36
11	a	1110	CLA	C3C-C2C	4.64	1.46	1.36
11	B	1207	CLA	C3B-C2B	4.64	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	1501	CLA	C3B-C2B	4.64	1.46	1.40
11	b	1203	CLA	C3C-C2C	4.64	1.46	1.36
11	b	1213	CLA	CHC-C1C	4.64	1.48	1.35
11	a	1132	CLA	C3C-C2C	4.64	1.46	1.36
11	b	1204	CLA	O2A-C1	4.64	1.60	1.46
11	a	1112	CLA	C3B-C2B	4.64	1.46	1.40
11	a	1115	CLA	CHC-C1C	4.64	1.48	1.35
11	2	1202	CLA	OBD-CAD	4.65	1.29	1.22
11	a	1109	CLA	C3C-C2C	4.65	1.46	1.36
11	b	1021	CLA	C3C-C2C	4.65	1.46	1.36
11	a	1117	CLA	OBD-CAD	4.65	1.29	1.22
11	2	1235	CLA	CHC-C1C	4.65	1.48	1.35
11	2	1209	CLA	OBD-CAD	4.65	1.29	1.22
11	A	1109	CLA	C3C-C2C	4.65	1.46	1.36
11	B	1214	CLA	CHC-C1C	4.65	1.48	1.35
11	2	1213	CLA	CHC-C1C	4.65	1.48	1.35
11	B	1234	CLA	C3B-C2B	4.65	1.46	1.40
11	b	1023	CLA	C3B-C2B	4.65	1.46	1.40
11	k	1402	CLA	C3C-C2C	4.65	1.46	1.36
11	b	1218	CLA	C3C-C2C	4.65	1.46	1.36
11	L	1501	CLA	C3C-C2C	4.65	1.46	1.36
11	1	1012	CLA	C3C-C2C	4.65	1.46	1.36
11	1	1140	CLA	C3C-C2C	4.65	1.46	1.36
11	1	1108	CLA	C3C-C2C	4.65	1.46	1.36
11	2	1219	CLA	C3C-C2C	4.66	1.46	1.36
11	A	1022	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1226	CLA	C3C-C2C	4.66	1.46	1.36
11	A	1121	CLA	C3C-C2C	4.66	1.46	1.36
11	A	1112	CLA	C3C-C2C	4.66	1.46	1.36
11	a	1124	CLA	C3C-C2C	4.66	1.46	1.36
11	B	1236	CLA	C3C-C2C	4.66	1.46	1.36
11	B	1224	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1221	CLA	CHC-C1C	4.66	1.48	1.35
11	b	1210	CLA	CHC-C1C	4.66	1.48	1.35
11	a	1111	CLA	C3B-C2B	4.66	1.46	1.40
11	b	1228	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1231	CLA	O2D-CGD	4.66	1.45	1.33
11	1	1101	CLA	O2A-C1	4.66	1.60	1.46
11	B	1201	CLA	C3C-C2C	4.66	1.46	1.36
11	b	1216	CLA	C3C-C2C	4.67	1.46	1.36
11	2	1214	CLA	C3B-C2B	4.67	1.46	1.40
11	B	1222	CLA	C3C-C2C	4.67	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1135	CLA	C3C-C2C	4.67	1.46	1.36
11	b	1227	CLA	C3C-C2C	4.67	1.46	1.36
11	a	1138	CLA	C3B-C2B	4.67	1.46	1.40
11	1	1128	CLA	C3C-C2C	4.67	1.46	1.36
11	2	1228	CLA	C3C-C2C	4.67	1.46	1.36
11	1	1126	CLA	CHC-C1C	4.67	1.49	1.35
11	b	1218	CLA	C3B-C2B	4.67	1.46	1.40
11	2	1239	CLA	C3C-C2C	4.67	1.46	1.36
11	a	1114	CLA	C3B-C2B	4.67	1.46	1.40
11	B	1225	CLA	C3B-C2B	4.67	1.46	1.40
11	1	1126	CLA	O2A-C1	4.67	1.60	1.46
11	8	1501	CLA	C3B-C2B	4.67	1.46	1.40
11	A	1111	CLA	CHC-C1C	4.67	1.49	1.35
11	1	1135	CLA	C3C-C2C	4.67	1.46	1.36
11	A	1116	CLA	CHC-C1C	4.68	1.49	1.35
11	a	1121	CLA	C3B-C2B	4.68	1.46	1.40
11	1	1127	CLA	O2A-C1	4.68	1.60	1.46
11	1	1120	CLA	C3C-C2C	4.68	1.46	1.36
11	b	1231	CLA	C3B-C2B	4.68	1.46	1.40
11	2	1215	CLA	C3B-C2B	4.68	1.46	1.40
11	2	1223	CLA	C3B-C2B	4.68	1.46	1.40
11	2	1223	CLA	CHC-C1C	4.68	1.49	1.35
11	A	1132	CLA	C3B-C2B	4.68	1.46	1.40
11	a	1103	CLA	C3C-C2C	4.68	1.46	1.36
11	B	1211	CLA	C3C-C2C	4.68	1.46	1.36
11	A	1117	CLA	CHC-C1C	4.68	1.49	1.35
11	b	1212	CLA	C3B-C2B	4.69	1.46	1.40
11	1	1126	CLA	C3B-C2B	4.69	1.46	1.40
11	a	1112	CLA	CHC-C1C	4.69	1.49	1.35
11	a	1120	CLA	C3C-C2C	4.69	1.46	1.36
11	A	1012	CLA	C3C-C2C	4.69	1.46	1.36
11	B	1223	CLA	C3C-C2C	4.69	1.46	1.36
11	B	1013	CLA	C3B-C2B	4.69	1.46	1.40
11	1	1113	CLA	C3B-C2B	4.70	1.46	1.40
11	a	1128	CLA	C3C-C2C	4.70	1.46	1.36
11	A	1131	CLA	C3B-C2B	4.70	1.46	1.40
11	b	1217	CLA	C3C-C2C	4.70	1.46	1.36
12	B	2002	PQN	C10-C5	4.70	1.48	1.40
11	B	1223	CLA	C3B-C2B	4.70	1.46	1.40
11	b	1220	CLA	C3C-C2C	4.70	1.46	1.36
11	B	1217	CLA	C3C-C2C	4.70	1.46	1.36
11	b	1227	CLA	C3B-C2B	4.70	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	1123	CLA	OBD-CAD	4.70	1.29	1.22
11	B	1202	CLA	CHC-C1C	4.70	1.49	1.35
11	A	1120	CLA	OBD-CAD	4.70	1.29	1.22
11	b	1013	CLA	C3B-C2B	4.70	1.46	1.40
11	A	1104	CLA	C3C-C2C	4.71	1.46	1.36
11	A	1011	CLA	O2A-C1	4.71	1.60	1.46
11	A	1116	CLA	C3B-C2B	4.71	1.46	1.40
11	a	1120	CLA	C3B-C2B	4.71	1.46	1.40
12	1	2001	PQN	C10-C5	4.71	1.48	1.40
11	B	1215	CLA	O2A-C1	4.71	1.60	1.46
11	1	1130	CLA	C3C-C2C	4.71	1.46	1.36
11	1	1012	CLA	C3B-C2B	4.71	1.46	1.40
11	2	1217	CLA	C3B-C2B	4.72	1.46	1.40
11	B	1228	CLA	C3C-C2C	4.72	1.46	1.36
11	0	1402	CLA	C3C-C2C	4.72	1.46	1.36
11	A	1101	CLA	C3B-C2B	4.72	1.46	1.40
11	l	1501	CLA	C3B-C2B	4.72	1.46	1.40
11	1	1117	CLA	C3B-C2B	4.72	1.46	1.40
11	A	1122	CLA	O2D-CGD	4.72	1.45	1.33
11	b	1229	CLA	C3C-C2C	4.72	1.46	1.36
11	A	1104	CLA	C3B-C2B	4.72	1.46	1.40
11	b	1205	CLA	C3B-C2B	4.72	1.46	1.40
11	A	1103	CLA	CHC-C1C	4.72	1.49	1.35
11	A	1117	CLA	C3C-C2C	4.72	1.46	1.36
11	2	1223	CLA	C3C-C2C	4.72	1.46	1.36
11	a	1126	CLA	CHC-C1C	4.72	1.49	1.35
11	a	1109	CLA	C3B-C2B	4.72	1.46	1.40
11	b	1235	CLA	O2A-C1	4.72	1.60	1.46
11	A	1012	CLA	C3B-C2B	4.72	1.46	1.40
11	b	1204	CLA	C3B-C2B	4.72	1.46	1.40
11	2	1219	CLA	O2A-C1	4.72	1.60	1.46
11	A	1120	CLA	C3B-C2B	4.72	1.46	1.40
11	A	1012	CLA	O2A-C1	4.73	1.60	1.46
11	A	1104	CLA	O2A-C1	4.73	1.60	1.46
12	2	2002	PQN	C10-C5	4.73	1.48	1.40
11	a	1126	CLA	O2A-C1	4.73	1.60	1.46
11	A	1129	CLA	C3B-C2B	4.73	1.46	1.40
11	2	1205	CLA	C3B-C2B	4.73	1.46	1.40
11	a	1119	CLA	C3B-C2B	4.73	1.46	1.40
11	B	1231	CLA	O2D-CGD	4.73	1.45	1.33
11	A	1110	CLA	O2D-CGD	4.73	1.45	1.33
11	2	1013	CLA	C3B-C2B	4.73	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1115	CLA	C3C-C2C	4.73	1.46	1.36
11	A	1110	CLA	O2A-C1	4.73	1.60	1.46
11	1	1131	CLA	O2A-C1	4.73	1.60	1.46
11	B	1216	CLA	C3B-C2B	4.74	1.46	1.40
11	A	1130	CLA	C3B-C2B	4.74	1.46	1.40
11	B	1220	CLA	C3B-C2B	4.74	1.46	1.40
11	A	1105	CLA	C3B-C2B	4.74	1.46	1.40
11	1	1123	CLA	C3B-C2B	4.74	1.46	1.40
11	1	1140	CLA	C3B-C2B	4.74	1.46	1.40
12	a	2001	PQN	C10-C5	4.74	1.48	1.40
11	1	1503	CLA	C3B-C2B	4.74	1.46	1.40
11	A	1022	CLA	O2A-C1	4.74	1.60	1.46
11	1	1120	CLA	C3B-C2B	4.74	1.46	1.40
11	a	1102	CLA	C3B-C2B	4.74	1.46	1.40
11	1	1112	CLA	C3B-C2B	4.74	1.46	1.40
11	A	1109	CLA	C3B-C2B	4.74	1.46	1.40
11	2	1021	CLA	C3B-C2B	4.74	1.46	1.40
11	b	1201	CLA	O2A-C1	4.74	1.60	1.46
11	K	1402	CLA	C3C-C2C	4.75	1.46	1.36
11	a	1140	CLA	C3B-C2B	4.75	1.46	1.40
11	b	1208	CLA	C3B-C2B	4.75	1.46	1.40
11	1	1138	CLA	C3B-C2B	4.75	1.46	1.40
11	1	1103	CLA	C3B-C2B	4.75	1.46	1.40
11	2	1205	CLA	O2A-C1	4.75	1.60	1.46
11	1	1133	CLA	C3B-C2B	4.75	1.46	1.40
11	A	1101	CLA	O2A-C1	4.75	1.60	1.46
11	2	1204	CLA	C3B-C2B	4.75	1.46	1.40
11	a	1801	CLA	C3B-C2B	4.75	1.46	1.40
11	A	1127	CLA	O2A-C1	4.75	1.60	1.46
11	1	1111	CLA	C3B-C2B	4.75	1.46	1.40
11	A	1139	CLA	C3B-C2B	4.75	1.46	1.40
11	2	1225	CLA	O2A-C1	4.75	1.60	1.46
11	b	1216	CLA	C3B-C2B	4.75	1.46	1.40
11	B	1023	CLA	C3B-C2B	4.76	1.46	1.40
11	2	1222	CLA	C3B-C2B	4.76	1.46	1.40
11	a	1103	CLA	O2A-C1	4.76	1.60	1.46
11	1	1129	CLA	C3B-C2B	4.76	1.46	1.40
11	B	1221	CLA	C3B-C2B	4.76	1.46	1.40
11	2	1021	CLA	O2A-C1	4.76	1.60	1.46
11	1	1124	CLA	O2A-C1	4.76	1.60	1.46
11	A	1139	CLA	O2A-C1	4.76	1.60	1.46
11	A	1112	CLA	CHC-C1C	4.76	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	8	1502	CLA	O2D-CGD	4.76	1.45	1.33
11	1	1123	CLA	O2A-C1	4.76	1.60	1.46
11	2	1221	CLA	C3B-C2B	4.76	1.46	1.40
11	2	1224	CLA	O2A-C1	4.76	1.60	1.46
11	b	1228	CLA	C3B-C2B	4.76	1.46	1.40
11	2	1209	CLA	C3B-C2B	4.76	1.46	1.40
11	1	1139	CLA	O2A-C1	4.77	1.60	1.46
11	B	1021	CLA	O2A-C1	4.77	1.60	1.46
11	A	1114	CLA	C3B-C2B	4.77	1.46	1.40
11	a	1127	CLA	O2A-C1	4.77	1.60	1.46
11	B	1231	CLA	C3B-C2B	4.77	1.46	1.40
11	1	1103	CLA	O2A-C1	4.77	1.60	1.46
11	A	1103	CLA	O2A-C1	4.77	1.60	1.46
12	b	2002	PQN	C10-C5	4.78	1.48	1.40
11	1	1110	CLA	O2A-C1	4.78	1.60	1.46
11	1	1011	CLA	O2A-C1	4.78	1.60	1.46
11	a	1107	CLA	C3B-C2B	4.78	1.46	1.40
11	a	1125	CLA	O2A-C1	4.78	1.60	1.46
11	1	1132	CLA	O2D-CGD	4.78	1.45	1.33
11	b	1221	CLA	O2A-C1	4.78	1.60	1.46
11	A	1108	CLA	C3B-C2B	4.78	1.46	1.40
11	B	1204	CLA	O2A-C1	4.78	1.60	1.46
11	2	1228	CLA	C3B-C2B	4.78	1.46	1.40
11	b	1203	CLA	O2A-C1	4.79	1.60	1.46
11	a	1134	CLA	C3B-C2B	4.79	1.46	1.40
11	A	1105	CLA	O2D-CGD	4.79	1.45	1.33
11	2	1208	CLA	C3B-C2B	4.79	1.46	1.40
11	B	1023	CLA	O2A-C1	4.79	1.60	1.46
11	8	1501	CLA	O2A-C1	4.79	1.60	1.46
11	A	1136	CLA	C3B-C2B	4.79	1.46	1.40
11	1	1125	CLA	O2A-C1	4.79	1.60	1.46
11	A	1138	CLA	C3B-C2B	4.79	1.46	1.40
11	A	1102	CLA	C3B-C2B	4.79	1.46	1.40
11	a	1104	CLA	O2A-C1	4.79	1.60	1.46
11	a	1124	CLA	C3B-C2B	4.80	1.46	1.40
11	1	1135	CLA	C3B-C2B	4.80	1.46	1.40
11	b	1214	CLA	C3B-C2B	4.80	1.46	1.40
12	A	2001	PQN	C10-C5	4.80	1.48	1.40
11	a	1011	CLA	O2A-C1	4.80	1.60	1.46
11	b	1213	CLA	O2A-C1	4.80	1.60	1.46
11	1	1104	CLA	O2A-C1	4.80	1.60	1.46
11	b	1223	CLA	O2D-CGD	4.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	b	1240	CLA	C3B-C2B	4.81	1.46	1.40
11	2	1229	CLA	O2A-C1	4.81	1.60	1.46
11	a	1127	CLA	C3B-C2B	4.81	1.46	1.40
11	a	1125	CLA	C3B-C2B	4.81	1.46	1.40
11	a	1124	CLA	O2A-C1	4.81	1.60	1.46
11	a	1101	CLA	C3B-C2B	4.81	1.46	1.40
11	B	1203	CLA	O2A-C1	4.81	1.60	1.46
11	1	1136	CLA	C3B-C2B	4.81	1.46	1.40
11	2	1204	CLA	O2A-C1	4.81	1.60	1.46
11	A	1123	CLA	O2A-C1	4.81	1.60	1.46
11	a	1136	CLA	C3B-C2B	4.81	1.46	1.40
11	A	1119	CLA	C3C-C2C	4.81	1.47	1.36
11	0	1401	CLA	O2A-C1	4.81	1.60	1.46
11	B	1218	CLA	C3B-C2B	4.81	1.46	1.40
11	2	1234	CLA	O2A-C1	4.82	1.60	1.46
11	a	1107	CLA	O2D-CGD	4.82	1.45	1.33
11	a	1123	CLA	C3B-C2B	4.82	1.46	1.40
11	A	1137	CLA	O2A-C1	4.82	1.60	1.46
11	b	1203	CLA	O2D-CGD	4.82	1.45	1.33
11	a	1111	CLA	O2D-CGD	4.82	1.45	1.33
11	2	1226	CLA	O2A-C1	4.82	1.60	1.46
11	1	1139	CLA	C3B-C2B	4.82	1.46	1.40
11	B	1229	CLA	O2D-CGD	4.82	1.45	1.33
11	B	1202	CLA	O2A-C1	4.82	1.60	1.46
11	1	1116	CLA	C3B-C2B	4.82	1.46	1.40
11	A	1111	CLA	O2D-CGD	4.82	1.45	1.33
11	B	1220	CLA	O2D-CGD	4.82	1.45	1.33
11	b	1023	CLA	O2A-C1	4.83	1.60	1.46
11	b	1226	CLA	O2D-CGD	4.83	1.45	1.33
11	B	1208	CLA	C3B-C2B	4.83	1.46	1.40
11	B	1023	CLA	O2D-CGD	4.83	1.45	1.33
11	1	1102	CLA	O2D-CGD	4.83	1.45	1.33
11	b	1202	CLA	O2A-C1	4.83	1.60	1.46
11	a	1123	CLA	O2A-C1	4.83	1.60	1.46
11	A	1103	CLA	O2D-CGD	4.83	1.45	1.33
11	b	1222	CLA	O2A-C1	4.83	1.60	1.46
11	b	1232	CLA	C3B-C2B	4.83	1.46	1.40
11	A	1134	CLA	C3B-C2B	4.83	1.46	1.40
11	8	1502	CLA	C3B-C2B	4.83	1.46	1.40
11	B	1213	CLA	O2A-C1	4.83	1.60	1.46
11	2	1205	CLA	O2D-CGD	4.83	1.45	1.33
11	L	1502	CLA	C3B-C2B	4.83	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1118	CLA	C3B-C2B	4.83	1.46	1.40
11	L	1503	CLA	O2A-C1	4.84	1.60	1.46
11	1	1237	CLA	C3B-C2B	4.84	1.46	1.40
11	B	1209	CLA	C3B-C2B	4.84	1.46	1.40
11	a	1118	CLA	C3B-C2B	4.84	1.46	1.40
11	2	1207	CLA	C3B-C2B	4.84	1.46	1.40
11	B	1214	CLA	O2A-C1	4.84	1.60	1.46
11	2	1210	CLA	C3B-C2B	4.84	1.46	1.40
11	b	1238	CLA	O2A-C1	4.84	1.60	1.46
11	B	1214	CLA	C3B-C2B	4.84	1.46	1.40
11	L	1503	CLA	O2D-CGD	4.84	1.45	1.33
11	K	1401	CLA	O2A-C1	4.84	1.60	1.46
11	A	1237	CLA	C3B-C2B	4.84	1.46	1.40
11	B	1205	CLA	O2D-CGD	4.84	1.45	1.33
11	b	1219	CLA	O2A-C1	4.84	1.60	1.46
11	l	1503	CLA	O2A-C1	4.84	1.60	1.46
11	2	1224	CLA	C3B-C2B	4.84	1.46	1.40
11	A	1115	CLA	C3B-C2B	4.84	1.46	1.40
11	A	1126	CLA	O2A-C1	4.84	1.60	1.46
11	L	1503	CLA	C3B-C2B	4.84	1.46	1.40
11	B	1206	CLA	O2A-C1	4.84	1.60	1.46
11	b	1207	CLA	C3B-C2B	4.84	1.46	1.40
11	a	1801	CLA	C3C-C2C	4.85	1.47	1.36
11	1	1128	CLA	O2A-C1	4.85	1.60	1.46
11	a	1124	CLA	O2D-CGD	4.85	1.45	1.33
11	b	1222	CLA	C3B-C2B	4.85	1.46	1.40
11	B	1217	CLA	C3B-C2B	4.85	1.46	1.40
11	b	1226	CLA	O2A-C1	4.85	1.60	1.46
11	a	1101	CLA	O2A-C1	4.85	1.60	1.46
11	2	1225	CLA	C3B-C2B	4.85	1.46	1.40
11	A	1101	CLA	O2D-CGD	4.85	1.45	1.33
11	a	1131	CLA	C3B-C2B	4.85	1.46	1.40
11	b	1234	CLA	O2A-C1	4.85	1.60	1.46
11	B	1238	CLA	O2D-CGD	4.85	1.45	1.33
11	a	1137	CLA	O2D-CGD	4.85	1.45	1.33
11	a	1135	CLA	C3B-C2B	4.85	1.46	1.40
11	2	1213	CLA	O2A-C1	4.85	1.60	1.46
11	B	1238	CLA	C3B-C2B	4.85	1.46	1.40
11	B	1228	CLA	C3B-C2B	4.85	1.46	1.40
11	b	1216	CLA	O2A-C1	4.85	1.60	1.46
11	B	1224	CLA	O2A-C1	4.85	1.60	1.46
11	A	1124	CLA	O2A-C1	4.85	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1205	CLA	O2A-C1	4.85	1.60	1.46
11	A	1105	CLA	O2A-C1	4.86	1.60	1.46
11	1	1132	CLA	O2A-C1	4.86	1.60	1.46
11	a	1129	CLA	C3B-C2B	4.86	1.46	1.40
11	2	1202	CLA	O2A-C1	4.86	1.60	1.46
11	2	1221	CLA	O2D-CGD	4.86	1.45	1.33
11	1	1108	CLA	C3B-C2B	4.86	1.46	1.40
11	B	1239	CLA	C3B-C2B	4.86	1.46	1.40
11	A	1126	CLA	CHC-C1C	4.86	1.49	1.35
11	a	1107	CLA	O2A-C1	4.86	1.60	1.46
11	B	1210	CLA	O2A-C1	4.86	1.60	1.46
11	a	1801	CLA	O2D-CGD	4.86	1.45	1.33
11	A	1140	CLA	C3B-C2B	4.86	1.46	1.40
11	b	1240	CLA	C3C-C2C	4.86	1.47	1.36
11	a	1119	CLA	O2A-C1	4.86	1.60	1.46
11	A	1128	CLA	O2A-C1	4.86	1.60	1.46
11	k	1401	CLA	O2A-C1	4.86	1.60	1.46
11	1	1106	CLA	C3B-C2B	4.86	1.46	1.40
11	2	1238	CLA	O2D-CGD	4.86	1.45	1.33
11	l	1501	CLA	O2A-C1	4.86	1.60	1.46
11	B	1229	CLA	O2A-C1	4.86	1.60	1.46
11	B	1201	CLA	O2A-C1	4.87	1.60	1.46
11	b	1236	CLA	O2D-CGD	4.87	1.45	1.33
11	b	1211	CLA	O2D-CGD	4.87	1.45	1.33
11	1	1110	CLA	O2D-CGD	4.87	1.45	1.33
11	2	1235	CLA	O2A-C1	4.87	1.60	1.46
11	b	1021	CLA	C3B-C2B	4.87	1.46	1.40
11	b	1021	CLA	O2A-C1	4.87	1.60	1.46
11	1	1124	CLA	C3B-C2B	4.87	1.46	1.40
11	a	1135	CLA	O2A-C1	4.87	1.60	1.46
11	A	1127	CLA	C3B-C2B	4.87	1.46	1.40
11	1	1011	CLA	O2D-CGD	4.87	1.45	1.33
11	2	1210	CLA	O2D-CGD	4.87	1.45	1.33
11	2	1203	CLA	O2A-C1	4.87	1.60	1.46
11	b	1238	CLA	O2D-CGD	4.87	1.45	1.33
11	b	1225	CLA	C3B-C2B	4.87	1.46	1.40
11	1	1111	CLA	O2D-CGD	4.87	1.45	1.33
11	B	1234	CLA	O2A-C1	4.88	1.60	1.46
11	1	1102	CLA	C3B-C2B	4.88	1.46	1.40
11	b	1206	CLA	O2A-C1	4.88	1.60	1.46
11	8	1503	CLA	O2A-C1	4.88	1.60	1.46
11	A	1135	CLA	O2D-CGD	4.88	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1201	CLA	O2D-CGD	4.88	1.45	1.33
11	2	1228	CLA	O2A-C1	4.88	1.60	1.46
11	1	1137	CLA	O2D-CGD	4.88	1.45	1.33
11	B	1213	CLA	C3B-C2B	4.88	1.46	1.40
11	2	1207	CLA	O2D-CGD	4.88	1.45	1.33
11	a	1110	CLA	O2A-C1	4.88	1.60	1.46
11	B	1216	CLA	O2A-C1	4.88	1.60	1.46
11	1	1022	CLA	O2A-C1	4.88	1.60	1.46
11	a	1022	CLA	O2A-C1	4.88	1.60	1.46
11	2	1202	CLA	C3B-C2B	4.88	1.46	1.40
11	2	1220	CLA	C3B-C2B	4.88	1.46	1.40
11	2	1223	CLA	O2D-CGD	4.88	1.45	1.33
11	1	1131	CLA	C3B-C2B	4.88	1.46	1.40
11	A	1117	CLA	O2D-CGD	4.88	1.45	1.33
11	1	1109	CLA	C3B-C2B	4.88	1.46	1.40
11	A	1122	CLA	C3B-C2B	4.88	1.46	1.40
11	A	1129	CLA	O2D-CGD	4.88	1.45	1.33
11	2	1210	CLA	O2A-C1	4.88	1.60	1.46
11	1	1012	CLA	O2D-CGD	4.89	1.45	1.33
11	a	1122	CLA	C3B-C2B	4.89	1.46	1.40
11	B	1207	CLA	O2D-CGD	4.89	1.45	1.33
11	B	1236	CLA	C3B-C2B	4.89	1.46	1.40
11	B	1225	CLA	O2A-C1	4.89	1.60	1.46
11	1	1105	CLA	O2A-C1	4.89	1.60	1.46
11	B	1236	CLA	O2D-CGD	4.89	1.45	1.33
11	2	1206	CLA	O2A-C1	4.89	1.60	1.46
11	b	1210	CLA	C3B-C2B	4.89	1.46	1.40
11	a	1106	CLA	O2D-CGD	4.89	1.45	1.33
11	1	1118	CLA	O2A-C1	4.89	1.60	1.46
11	B	1228	CLA	O2A-C1	4.89	1.60	1.46
11	B	1234	CLA	O2D-CGD	4.89	1.45	1.33
11	a	1103	CLA	C3B-C2B	4.89	1.46	1.40
11	b	1239	CLA	C3B-C2B	4.89	1.46	1.40
11	B	1238	CLA	O2A-C1	4.89	1.60	1.46
11	1	1130	CLA	C3B-C2B	4.89	1.46	1.40
11	1	1111	CLA	O2A-C1	4.89	1.60	1.46
11	1	1137	CLA	O2A-C1	4.89	1.60	1.46
11	2	1231	CLA	C3B-C2B	4.89	1.46	1.40
11	b	1221	CLA	C3B-C2B	4.89	1.46	1.40
11	B	1021	CLA	O2D-CGD	4.89	1.45	1.33
11	b	1221	CLA	O2D-CGD	4.89	1.45	1.33
11	b	1205	CLA	O2A-C1	4.89	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1140	CLA	O2A-C1	4.89	1.60	1.46
11	b	1229	CLA	O2A-C1	4.89	1.60	1.46
11	B	1203	CLA	O2D-CGD	4.89	1.45	1.33
11	a	1106	CLA	C3B-C2B	4.89	1.46	1.40
11	2	1214	CLA	O2A-C1	4.89	1.60	1.46
11	b	1225	CLA	O2A-C1	4.89	1.60	1.46
11	A	1120	CLA	O2D-CGD	4.89	1.45	1.33
11	A	1134	CLA	O2D-CGD	4.89	1.45	1.33
11	l	1502	CLA	O2D-CGD	4.89	1.45	1.33
11	2	1216	CLA	O2A-C1	4.89	1.60	1.46
11	B	1221	CLA	O2D-CGD	4.89	1.45	1.33
11	B	1223	CLA	O2A-C1	4.90	1.60	1.46
11	2	1229	CLA	O2D-CGD	4.90	1.45	1.33
11	B	1013	CLA	O2D-CGD	4.90	1.45	1.33
11	A	1125	CLA	O2A-C1	4.90	1.60	1.46
11	1	1237	CLA	O2D-CGD	4.90	1.45	1.33
11	B	1226	CLA	O2D-CGD	4.90	1.45	1.33
11	A	1022	CLA	O2D-CGD	4.90	1.45	1.33
11	B	1211	CLA	O2D-CGD	4.90	1.45	1.33
11	B	1212	CLA	C3B-C2B	4.90	1.46	1.40
11	2	1201	CLA	O2D-CGD	4.90	1.45	1.33
11	2	1226	CLA	O2D-CGD	4.90	1.45	1.33
11	B	1212	CLA	O2D-CGD	4.90	1.45	1.33
11	a	1139	CLA	O2A-C1	4.90	1.60	1.46
11	B	1235	CLA	C3B-C2B	4.91	1.46	1.40
11	B	1239	CLA	O2D-CGD	4.91	1.45	1.33
11	a	1125	CLA	O2D-CGD	4.91	1.45	1.33
11	1	1107	CLA	O2D-CGD	4.91	1.45	1.33
11	1	1104	CLA	C3B-C2B	4.91	1.46	1.40
11	a	1237	CLA	O2D-CGD	4.91	1.45	1.33
11	B	1219	CLA	O2A-C1	4.91	1.60	1.46
11	2	1023	CLA	O2A-C1	4.91	1.60	1.46
11	2	1224	CLA	O2D-CGD	4.91	1.45	1.33
11	2	1214	CLA	O2D-CGD	4.91	1.45	1.33
11	b	1211	CLA	C3B-C2B	4.91	1.46	1.40
11	K	1402	CLA	O2D-CGD	4.91	1.45	1.33
11	a	1140	CLA	O2D-CGD	4.91	1.45	1.33
11	A	1113	CLA	C3B-C2B	4.91	1.46	1.40
11	A	1237	CLA	O2A-C1	4.91	1.60	1.46
11	b	1214	CLA	O2D-CGD	4.91	1.45	1.33
11	2	1201	CLA	C3B-C2B	4.92	1.46	1.40
11	b	1210	CLA	O2D-CGD	4.92	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1210	CLA	C3B-C2B	4.92	1.46	1.40
11	b	1224	CLA	O2A-C1	4.92	1.60	1.46
11	B	1215	CLA	O2D-CGD	4.92	1.45	1.33
11	B	1226	CLA	O2A-C1	4.92	1.60	1.46
11	b	1222	CLA	O2D-CGD	4.92	1.45	1.33
11	2	1222	CLA	O2D-CGD	4.92	1.45	1.33
11	1	1103	CLA	O2D-CGD	4.92	1.45	1.33
11	B	1202	CLA	O2D-CGD	4.92	1.45	1.33
11	b	1229	CLA	O2D-CGD	4.92	1.45	1.33
11	B	1209	CLA	O2D-CGD	4.92	1.45	1.33
11	A	1122	CLA	O2A-C1	4.92	1.60	1.46
11	L	1501	CLA	O2A-C1	4.92	1.60	1.46
11	1	1131	CLA	O2D-CGD	4.92	1.45	1.33
11	1	1237	CLA	O2A-C1	4.92	1.60	1.46
11	B	1224	CLA	O2D-CGD	4.92	1.45	1.33
11	a	1117	CLA	O2D-CGD	4.92	1.45	1.33
11	2	1206	CLA	O2D-CGD	4.92	1.45	1.33
11	L	1502	CLA	O2D-CGD	4.92	1.45	1.33
11	A	1132	CLA	O2D-CGD	4.92	1.45	1.33
11	2	1239	CLA	C3B-C2B	4.92	1.46	1.40
11	b	1220	CLA	O2D-CGD	4.93	1.45	1.33
11	2	1223	CLA	O2A-C1	4.93	1.60	1.46
11	B	1206	CLA	O2D-CGD	4.93	1.45	1.33
11	2	1013	CLA	O2A-C1	4.93	1.60	1.46
11	a	1116	CLA	C3B-C2B	4.93	1.46	1.40
11	b	1239	CLA	O2D-CGD	4.93	1.45	1.33
11	2	1240	CLA	O2D-CGD	4.93	1.45	1.33
11	a	1112	CLA	O2D-CGD	4.93	1.45	1.33
11	A	1121	CLA	O2D-CGD	4.93	1.45	1.33
11	2	1222	CLA	O2A-C1	4.93	1.60	1.46
11	B	1222	CLA	O2D-CGD	4.93	1.45	1.33
11	a	1135	CLA	O2D-CGD	4.93	1.45	1.33
11	a	1106	CLA	O2A-C1	4.93	1.60	1.46
11	B	1227	CLA	O2D-CGD	4.93	1.45	1.33
11	a	1104	CLA	O2D-CGD	4.93	1.45	1.33
11	a	1022	CLA	O2D-CGD	4.93	1.45	1.33
11	a	1012	CLA	O2A-C1	4.93	1.60	1.46
11	2	1236	CLA	C3B-C2B	4.93	1.46	1.40
11	B	1201	CLA	C3B-C2B	4.93	1.46	1.40
11	A	1135	CLA	O2A-C1	4.93	1.60	1.46
11	B	1222	CLA	O2A-C1	4.93	1.60	1.46
11	a	1131	CLA	O2A-C1	4.93	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1115	CLA	C3B-C2B	4.93	1.46	1.40
11	b	1228	CLA	O2A-C1	4.93	1.60	1.46
11	2	1212	CLA	C3B-C2B	4.93	1.46	1.40
11	b	1238	CLA	C3B-C2B	4.93	1.46	1.40
11	A	1118	CLA	O2D-CGD	4.93	1.45	1.33
11	b	1223	CLA	O2A-C1	4.93	1.60	1.46
11	2	1218	CLA	O2D-CGD	4.94	1.45	1.33
11	a	1122	CLA	O2D-CGD	4.94	1.45	1.33
11	2	1240	CLA	C3B-C2B	4.94	1.46	1.40
11	2	1212	CLA	O2D-CGD	4.94	1.45	1.33
11	a	1113	CLA	O2D-CGD	4.94	1.45	1.33
11	a	1113	CLA	C3B-C2B	4.94	1.46	1.40
11	A	1130	CLA	O2D-CGD	4.94	1.45	1.33
11	A	1109	CLA	O2A-C1	4.94	1.60	1.46
11	b	1215	CLA	O2A-C1	4.94	1.60	1.46
11	1	1134	CLA	C3B-C2B	4.94	1.46	1.40
11	0	1402	CLA	O2A-C1	4.94	1.60	1.46
11	A	1127	CLA	O2D-CGD	4.94	1.45	1.33
11	2	1232	CLA	O2D-CGD	4.94	1.45	1.33
11	B	1225	CLA	O2D-CGD	4.94	1.45	1.33
11	1	1116	CLA	O2A-C1	4.94	1.60	1.46
11	2	1230	CLA	C3B-C2B	4.94	1.46	1.40
11	2	1209	CLA	O2D-CGD	4.94	1.45	1.33
11	B	1235	CLA	O2A-C1	4.94	1.60	1.46
11	A	1131	CLA	O2D-CGD	4.94	1.45	1.33
11	1	1124	CLA	O2D-CGD	4.94	1.45	1.33
11	1	1135	CLA	O2D-CGD	4.95	1.45	1.33
11	A	1012	CLA	O2D-CGD	4.95	1.45	1.33
11	1	1122	CLA	O2A-C1	4.95	1.60	1.46
11	a	1132	CLA	O2D-CGD	4.95	1.45	1.33
11	l	1502	CLA	C3B-C2B	4.95	1.46	1.40
11	1	1140	CLA	O2A-C1	4.95	1.60	1.46
11	1	1135	CLA	O2A-C1	4.95	1.60	1.46
11	A	1137	CLA	O2D-CGD	4.95	1.45	1.33
11	A	1107	CLA	O2A-C1	4.95	1.60	1.46
11	2	1221	CLA	O2A-C1	4.95	1.60	1.46
11	1	1109	CLA	O2A-C1	4.95	1.60	1.46
11	A	1113	CLA	O2D-CGD	4.95	1.45	1.33
11	1	1116	CLA	O2D-CGD	4.95	1.45	1.33
11	B	1223	CLA	O2D-CGD	4.95	1.45	1.33
11	a	1134	CLA	O2D-CGD	4.95	1.45	1.33
11	a	1126	CLA	C3B-C2B	4.95	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	1	1123	CLA	O2D-CGD	4.95	1.45	1.33
11	L	1501	CLA	O2D-CGD	4.95	1.45	1.33
11	A	1118	CLA	O2A-C1	4.95	1.60	1.46
11	2	1217	CLA	O2D-CGD	4.95	1.45	1.33
11	A	1114	CLA	O2D-CGD	4.95	1.45	1.33
11	8	1501	CLA	O2D-CGD	4.95	1.45	1.33
11	1	1122	CLA	C3B-C2B	4.95	1.46	1.40
11	1	1127	CLA	O2D-CGD	4.95	1.45	1.33
11	2	1225	CLA	O2D-CGD	4.96	1.45	1.33
11	b	1214	CLA	O2A-C1	4.96	1.60	1.46
11	1	1127	CLA	OBD-CAD	4.96	1.29	1.22
11	2	1234	CLA	O2D-CGD	4.96	1.45	1.33
11	a	1128	CLA	O2A-C1	4.96	1.60	1.46
11	1	1022	CLA	O2D-CGD	4.96	1.45	1.33
11	0	1402	CLA	O2D-CGD	4.96	1.45	1.33
11	1	1104	CLA	O2D-CGD	4.96	1.45	1.33
11	1	1012	CLA	O2A-C1	4.96	1.60	1.46
11	a	1118	CLA	O2D-CGD	4.96	1.45	1.33
11	l	1503	CLA	O2D-CGD	4.96	1.45	1.33
11	a	1102	CLA	O2A-C1	4.96	1.60	1.46
11	1	1126	CLA	O2D-CGD	4.96	1.45	1.33
11	K	1402	CLA	O2A-C1	4.96	1.60	1.46
11	a	1133	CLA	O2D-CGD	4.96	1.45	1.33
11	1	1129	CLA	O2D-CGD	4.96	1.45	1.33
11	a	1116	CLA	O2D-CGD	4.96	1.45	1.33
11	a	1121	CLA	O2D-CGD	4.96	1.45	1.33
11	a	1110	CLA	C3B-C2B	4.97	1.46	1.40
11	1	1102	CLA	O2A-C1	4.97	1.61	1.46
11	2	1219	CLA	O2D-CGD	4.97	1.45	1.33
11	1	1801	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1225	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1209	CLA	C3B-C2B	4.97	1.46	1.40
11	b	1204	CLA	O2D-CGD	4.97	1.45	1.33
11	B	1013	CLA	O2A-C1	4.97	1.61	1.46
11	b	1220	CLA	C3B-C2B	4.97	1.46	1.40
11	A	1102	CLA	O2A-C1	4.97	1.61	1.46
11	b	1205	CLA	O2D-CGD	4.97	1.45	1.33
11	B	1210	CLA	O2D-CGD	4.97	1.45	1.33
11	a	1110	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1227	CLA	O2D-CGD	4.97	1.45	1.33
11	a	1012	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1023	CLA	O2D-CGD	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1224	CLA	C3B-C2B	4.97	1.46	1.40
11	1	1106	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1232	CLA	O2D-CGD	4.97	1.45	1.33
11	b	1217	CLA	O2D-CGD	4.98	1.45	1.33
11	b	1217	CLA	C3B-C2B	4.98	1.46	1.40
11	B	1230	CLA	C3B-C2B	4.98	1.46	1.40
11	b	1240	CLA	O2D-CGD	4.98	1.45	1.33
11	a	1237	CLA	O2A-C1	4.98	1.61	1.46
11	b	1212	CLA	O2D-CGD	4.98	1.45	1.33
11	1	1140	CLA	O2D-CGD	4.98	1.45	1.33
11	A	1124	CLA	O2D-CGD	4.98	1.45	1.33
11	b	1208	CLA	O2D-CGD	4.98	1.45	1.33
11	B	1204	CLA	O2D-CGD	4.98	1.45	1.33
11	A	1123	CLA	O2D-CGD	4.98	1.45	1.33
11	A	1131	CLA	O2A-C1	4.98	1.61	1.46
11	1	1120	CLA	O2D-CGD	4.98	1.45	1.33
11	a	1118	CLA	O2A-C1	4.98	1.61	1.46
11	B	1216	CLA	O2D-CGD	4.98	1.45	1.33
11	1	1134	CLA	O2D-CGD	4.98	1.45	1.33
11	k	1401	CLA	O2D-CGD	4.98	1.45	1.33
11	B	1221	CLA	O2A-C1	4.98	1.61	1.46
11	1	1118	CLA	O2D-CGD	4.98	1.45	1.33
11	A	1108	CLA	O2D-CGD	4.98	1.45	1.33
11	a	1108	CLA	C3B-C2B	4.98	1.46	1.40
11	a	1129	CLA	O2D-CGD	4.98	1.45	1.33
11	a	1140	CLA	O2A-C1	4.98	1.61	1.46
11	1	1127	CLA	C3B-C2B	4.98	1.46	1.40
11	A	1121	CLA	C3B-C2B	4.98	1.46	1.40
11	a	1105	CLA	C3B-C2B	4.98	1.46	1.40
11	b	1013	CLA	O2A-C1	4.98	1.61	1.46
11	b	1234	CLA	O2D-CGD	4.98	1.45	1.33
11	A	1126	CLA	O2D-CGD	4.98	1.45	1.33
11	K	1401	CLA	O2D-CGD	4.98	1.45	1.33
11	1	1117	CLA	O2D-CGD	4.98	1.45	1.33
11	a	1109	CLA	O2A-C1	4.98	1.61	1.46
11	l	1501	CLA	O2D-CGD	4.98	1.45	1.33
11	a	1123	CLA	O2D-CGD	4.98	1.45	1.33
11	2	1215	CLA	O2D-CGD	4.99	1.45	1.33
11	1	1117	CLA	O2A-C1	4.99	1.61	1.46
11	A	1112	CLA	O2D-CGD	4.99	1.45	1.33
11	2	1215	CLA	O2A-C1	4.99	1.61	1.46
11	a	1128	CLA	O2D-CGD	4.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	2	1213	CLA	O2D-CGD	4.99	1.45	1.33
11	b	1202	CLA	O2D-CGD	4.99	1.45	1.33
11	b	1230	CLA	C3B-C2B	4.99	1.46	1.40
11	b	1230	CLA	O2D-CGD	4.99	1.45	1.33
11	b	1210	CLA	O2A-C1	4.99	1.61	1.46
11	b	1201	CLA	O2D-CGD	4.99	1.45	1.33
11	B	1240	CLA	O2D-CGD	4.99	1.45	1.33
11	A	1102	CLA	O2D-CGD	4.99	1.45	1.33
11	A	1103	CLA	C3B-C2B	4.99	1.46	1.40
11	1	1119	CLA	O2A-C1	4.99	1.61	1.46
11	0	1401	CLA	O2D-CGD	4.99	1.45	1.33
11	b	1224	CLA	C3B-C2B	4.99	1.46	1.40
11	B	1219	CLA	C3B-C2B	4.99	1.46	1.40
11	B	1207	CLA	O2A-C1	4.99	1.61	1.46
11	A	1104	CLA	O2D-CGD	4.99	1.45	1.33
11	1	1139	CLA	O2D-CGD	4.99	1.45	1.33
11	b	1209	CLA	O2D-CGD	5.00	1.45	1.33
11	b	1013	CLA	O2D-CGD	5.00	1.45	1.33
11	1	1105	CLA	O2D-CGD	5.00	1.45	1.33
11	1	1119	CLA	O2D-CGD	5.00	1.45	1.33
11	A	1138	CLA	O2D-CGD	5.00	1.45	1.33
11	2	1226	CLA	C3B-C2B	5.00	1.47	1.40
11	2	1202	CLA	O2D-CGD	5.00	1.45	1.33
11	b	1235	CLA	O2D-CGD	5.00	1.45	1.33
11	B	1214	CLA	O2D-CGD	5.00	1.45	1.33
11	2	1235	CLA	O2D-CGD	5.00	1.45	1.33
11	k	1402	CLA	O2D-CGD	5.00	1.45	1.33
11	1	1113	CLA	O2D-CGD	5.00	1.45	1.33
11	a	1115	CLA	C3B-C2B	5.00	1.47	1.40
11	B	1211	CLA	C3B-C2B	5.00	1.47	1.40
11	2	1220	CLA	O2D-CGD	5.00	1.45	1.33
11	a	1237	CLA	C3B-C2B	5.00	1.47	1.40
11	2	1203	CLA	O2D-CGD	5.00	1.45	1.33
11	1	1101	CLA	O2D-CGD	5.00	1.45	1.33
11	a	1130	CLA	O2D-CGD	5.00	1.45	1.33
11	A	1801	CLA	O2D-CGD	5.00	1.45	1.33
11	B	1228	CLA	O2D-CGD	5.01	1.45	1.33
11	1	1115	CLA	O2D-CGD	5.01	1.45	1.33
11	1	1128	CLA	O2D-CGD	5.01	1.45	1.33
11	1	1107	CLA	C3B-C2B	5.01	1.47	1.40
11	2	1236	CLA	O2D-CGD	5.01	1.45	1.33
11	2	1227	CLA	O2D-CGD	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1208	CLA	O2D-CGD	5.01	1.45	1.33
11	2	1211	CLA	C3B-C2B	5.01	1.47	1.40
11	A	1128	CLA	O2D-CGD	5.01	1.45	1.33
11	A	1136	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1801	CLA	O2A-C1	5.01	1.61	1.46
11	b	1206	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1117	CLA	C3B-C2B	5.01	1.47	1.40
11	1	1133	CLA	O2D-CGD	5.01	1.45	1.33
11	A	1140	CLA	O2D-CGD	5.01	1.45	1.33
11	A	1125	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1117	CLA	O2A-C1	5.01	1.61	1.46
11	A	1801	CLA	O2A-C1	5.01	1.61	1.46
11	A	1106	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1102	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1138	CLA	O2D-CGD	5.01	1.45	1.33
11	a	1136	CLA	O2D-CGD	5.02	1.45	1.33
11	a	1137	CLA	O2A-C1	5.02	1.61	1.46
11	B	1217	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1801	CLA	O2A-C1	5.02	1.61	1.46
11	b	1213	CLA	C3B-C2B	5.02	1.47	1.40
11	b	1215	CLA	O2D-CGD	5.02	1.45	1.33
11	b	1216	CLA	O2D-CGD	5.02	1.45	1.33
11	2	1021	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1122	CLA	O2D-CGD	5.02	1.45	1.33
11	A	1139	CLA	O2D-CGD	5.02	1.45	1.33
11	2	1013	CLA	O2D-CGD	5.02	1.45	1.33
11	a	1126	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1114	CLA	O2D-CGD	5.02	1.45	1.33
11	B	1219	CLA	O2D-CGD	5.02	1.45	1.33
11	B	1235	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1130	CLA	O2D-CGD	5.02	1.45	1.33
11	1	1136	CLA	O2D-CGD	5.03	1.45	1.33
11	1	1801	CLA	C3C-C2C	5.03	1.47	1.36
11	B	1232	CLA	O2D-CGD	5.03	1.45	1.33
11	A	1116	CLA	O2D-CGD	5.03	1.45	1.33
11	b	1228	CLA	O2D-CGD	5.03	1.45	1.33
11	8	1503	CLA	O2D-CGD	5.03	1.46	1.33
11	a	1103	CLA	O2D-CGD	5.03	1.46	1.33
11	b	1207	CLA	O2A-C1	5.03	1.61	1.46
11	1	1108	CLA	O2D-CGD	5.03	1.46	1.33
11	a	1131	CLA	O2D-CGD	5.03	1.46	1.33
11	B	1230	CLA	O2D-CGD	5.03	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1218	CLA	O2D-CGD	5.03	1.46	1.33
11	a	1120	CLA	O2D-CGD	5.03	1.46	1.33
11	a	1109	CLA	O2D-CGD	5.03	1.46	1.33
11	2	1211	CLA	O2D-CGD	5.03	1.46	1.33
11	A	1237	CLA	O2D-CGD	5.04	1.46	1.33
11	a	1114	CLA	O2D-CGD	5.04	1.46	1.33
11	a	1139	CLA	O2D-CGD	5.04	1.46	1.33
11	a	1115	CLA	O2D-CGD	5.04	1.46	1.33
11	2	1204	CLA	O2D-CGD	5.04	1.46	1.33
11	b	1219	CLA	O2D-CGD	5.04	1.46	1.33
11	1	1125	CLA	O2D-CGD	5.04	1.46	1.33
11	2	1238	CLA	C3B-C2B	5.04	1.47	1.40
11	2	1238	CLA	O2A-C1	5.04	1.61	1.46
11	a	1116	CLA	O2A-C1	5.04	1.61	1.46
11	A	1119	CLA	O2D-CGD	5.04	1.46	1.33
11	A	1119	CLA	O2A-C1	5.04	1.61	1.46
11	A	1125	CLA	C3B-C2B	5.05	1.47	1.40
11	2	1230	CLA	O2A-C1	5.05	1.61	1.46
11	a	1105	CLA	O2D-CGD	5.05	1.46	1.33
11	2	1208	CLA	O2D-CGD	5.05	1.46	1.33
11	1	1109	CLA	O2D-CGD	5.05	1.46	1.33
11	A	1011	CLA	O2D-CGD	5.05	1.46	1.33
11	b	1207	CLA	O2D-CGD	5.05	1.46	1.33
11	k	1402	CLA	O2A-C1	5.05	1.61	1.46
11	2	1239	CLA	O2D-CGD	5.05	1.46	1.33
11	a	1119	CLA	O2D-CGD	5.05	1.46	1.33
11	a	1137	CLA	C3B-C2B	5.05	1.47	1.40
11	b	1021	CLA	O2D-CGD	5.06	1.46	1.33
11	2	1201	CLA	O2A-C1	5.06	1.61	1.46
11	A	1132	CLA	O2A-C1	5.06	1.61	1.46
11	1	1112	CLA	O2D-CGD	5.06	1.46	1.33
11	b	1213	CLA	O2D-CGD	5.06	1.46	1.33
11	b	1224	CLA	O2D-CGD	5.06	1.46	1.33
11	b	1202	CLA	C3B-C2B	5.06	1.47	1.40
11	2	1023	CLA	O2D-CGD	5.07	1.46	1.33
11	b	1218	CLA	O2D-CGD	5.07	1.46	1.33
11	B	1213	CLA	O2D-CGD	5.07	1.46	1.33
11	a	1108	CLA	O2D-CGD	5.07	1.46	1.33
11	a	1105	CLA	O2A-C1	5.07	1.61	1.46
11	2	1216	CLA	O2D-CGD	5.07	1.46	1.33
11	2	1228	CLA	O2D-CGD	5.07	1.46	1.33
11	2	1230	CLA	O2D-CGD	5.08	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1116	CLA	O2A-C1	5.08	1.61	1.46
11	A	1115	CLA	O2D-CGD	5.08	1.46	1.33
11	1	1121	CLA	O2D-CGD	5.08	1.46	1.33
11	a	1132	CLA	O2A-C1	5.08	1.61	1.46
11	a	1130	CLA	C3B-C2B	5.08	1.47	1.40
11	A	1107	CLA	C3B-C2B	5.09	1.47	1.40
11	b	1236	CLA	C3B-C2B	5.09	1.47	1.40
11	a	1122	CLA	O2A-C1	5.11	1.61	1.46
11	1	1107	CLA	O2A-C1	5.11	1.61	1.46
11	A	1133	CLA	O2D-CGD	5.11	1.46	1.33
11	2	1207	CLA	O2A-C1	5.12	1.61	1.46
11	2	1213	CLA	C3B-C2B	5.12	1.47	1.40
11	k	1402	CLA	C3B-C2B	5.12	1.47	1.40
11	1	1138	CLA	O2D-CGD	5.13	1.46	1.33
11	a	1101	CLA	O2D-CGD	5.13	1.46	1.33
11	a	1127	CLA	O2D-CGD	5.14	1.46	1.33
11	A	1109	CLA	O2D-CGD	5.15	1.46	1.33
11	K	1402	CLA	C3B-C2B	5.15	1.47	1.40
11	b	1230	CLA	O2A-C1	5.15	1.61	1.46
11	A	1117	CLA	O2A-C1	5.16	1.61	1.46
11	0	1402	CLA	C3B-C2B	5.16	1.47	1.40
11	2	1213	CLA	C3C-C2C	5.17	1.47	1.36
11	1	1137	CLA	C3B-C2B	5.17	1.47	1.40
11	1	1106	CLA	O2A-C1	5.17	1.61	1.46
11	A	1106	CLA	O2A-C1	5.17	1.61	1.46
11	2	1235	CLA	C3B-C2B	5.18	1.47	1.40
11	B	1230	CLA	O2A-C1	5.18	1.61	1.46
11	B	1240	CLA	C3B-C2B	5.21	1.47	1.40
11	A	1110	CLA	C3B-C2B	5.22	1.47	1.40
11	A	1801	CLA	C3C-C2C	5.22	1.47	1.36
11	a	1011	CLA	O2D-CGD	5.23	1.46	1.33
11	a	1011	CLA	C3B-C2B	5.23	1.47	1.40
11	b	1223	CLA	C3B-C2B	5.28	1.47	1.40
11	8	1503	CLA	C3B-C2B	5.30	1.47	1.40
11	A	1117	CLA	C3B-C2B	5.40	1.47	1.40
11	b	1235	CLA	C3B-C2B	5.46	1.47	1.40
11	b	1201	CLA	C3B-C2B	5.53	1.47	1.40
11	b	1219	CLA	C3B-C2B	5.53	1.47	1.40
11	B	1202	CLA	C3B-C2B	5.54	1.47	1.40
11	A	1137	CLA	C3B-C2B	5.59	1.47	1.40
11	B	1222	CLA	C3B-C2B	5.63	1.47	1.40
11	2	1219	CLA	C3B-C2B	5.70	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	1220	CLA	O2A-C1	6.20	1.60	1.45
11	a	1134	CLA	O2A-C1	6.22	1.60	1.45
11	B	1239	CLA	O2A-C1	6.23	1.60	1.45
11	A	1133	CLA	O2A-C1	6.26	1.60	1.45
11	1	1129	CLA	O2A-C1	6.26	1.60	1.45
11	b	1239	CLA	O2A-C1	6.26	1.60	1.45
11	8	1502	CLA	O2A-C1	6.27	1.60	1.45
11	a	1136	CLA	O2A-C1	6.27	1.60	1.45
11	A	1115	CLA	O2A-C1	6.27	1.60	1.45
11	A	1136	CLA	O2A-C1	6.28	1.60	1.45
11	B	1211	CLA	O2A-C1	6.28	1.60	1.45
11	a	1129	CLA	O2A-C1	6.28	1.60	1.45
11	b	1211	CLA	O2A-C1	6.28	1.60	1.45
11	1	1115	CLA	O2A-C1	6.28	1.60	1.45
11	A	1130	CLA	O2A-C1	6.28	1.60	1.45
11	1	1114	CLA	O2A-C1	6.29	1.60	1.45
11	l	1502	CLA	O2A-C1	6.29	1.60	1.45
11	A	1114	CLA	O2A-C1	6.29	1.60	1.45
11	A	1138	CLA	O2A-C1	6.29	1.60	1.45
11	2	1220	CLA	O2A-C1	6.29	1.60	1.45
11	a	1114	CLA	O2A-C1	6.30	1.60	1.45
11	b	1220	CLA	O2A-C1	6.30	1.60	1.45
11	1	1120	CLA	O2A-C1	6.30	1.60	1.45
11	A	1120	CLA	O2A-C1	6.30	1.60	1.45
11	1	1138	CLA	O2A-C1	6.30	1.60	1.45
11	1	1136	CLA	O2A-C1	6.31	1.60	1.45
11	a	1115	CLA	O2A-C1	6.31	1.60	1.45
11	a	1138	CLA	O2A-C1	6.31	1.60	1.45
11	1	1121	CLA	O2A-C1	6.31	1.60	1.45
11	2	1239	CLA	O2A-C1	6.31	1.60	1.45
11	1	1133	CLA	O2A-C1	6.31	1.60	1.45
11	a	1133	CLA	O2A-C1	6.31	1.60	1.45
11	a	1130	CLA	O2A-C1	6.32	1.60	1.45
11	1	1134	CLA	O2A-C1	6.32	1.60	1.45
11	L	1502	CLA	O2A-C1	6.33	1.60	1.45
11	A	1129	CLA	O2A-C1	6.33	1.60	1.45
11	A	1134	CLA	O2A-C1	6.33	1.60	1.45
11	1	1130	CLA	O2A-C1	6.33	1.60	1.45
11	A	1121	CLA	O2A-C1	6.34	1.60	1.45
11	2	1211	CLA	O2A-C1	6.36	1.60	1.45
11	a	1120	CLA	O2A-C1	6.36	1.60	1.45
12	a	2001	PQN	C3-C2	6.38	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	2002	PQN	C3-C2	6.40	1.49	1.35
11	a	1121	CLA	O2A-C1	6.42	1.60	1.45
12	A	2001	PQN	C3-C2	6.43	1.49	1.35
12	2	2002	PQN	C3-C2	6.44	1.49	1.35
12	B	2002	PQN	C3-C2	6.49	1.49	1.35
12	1	2001	PQN	C3-C2	6.55	1.49	1.35

All (5490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4003	BCR	C24-C23-C22	-7.24	115.34	126.21
14	6	4018	BCR	C24-C23-C22	-7.00	115.70	126.21
14	L	4019	BCR	C24-C23-C22	-6.91	115.83	126.21
14	f	4018	BCR	C24-C23-C22	-6.62	116.26	126.21
14	b	4017	BCR	C34-C9-C10	-6.48	113.84	122.92
14	7	4021	BCR	C7-C8-C9	-6.43	116.55	126.21
14	2	4011	BCR	C7-C8-C9	-6.35	116.67	126.21
14	B	4014	BCR	C7-C8-C9	-6.32	116.72	126.21
14	B	4011	BCR	C7-C8-C9	-6.27	116.79	126.21
14	6	4020	BCR	C7-C8-C9	-6.25	116.82	126.21
14	A	4003	BCR	C24-C23-C22	-6.24	116.84	126.21
14	A	4001	BCR	C24-C23-C22	-6.11	117.03	126.21
14	B	4014	BCR	C24-C23-C22	-6.09	117.06	126.21
11	A	1012	CLA	O2A-CGA-O1A	-6.03	108.56	123.55
14	L	4022	BCR	C24-C23-C22	-5.96	117.26	126.21
14	m	4021	BCR	C7-C8-C9	-5.87	117.39	126.21
11	2	1205	CLA	O2A-CGA-O1A	-5.85	109.01	123.55
11	A	1012	CLA	OBD-CAD-CBD	-5.85	117.12	125.94
14	F	4013	BCR	C15-C14-C13	-5.84	118.97	127.31
14	F	4018	BCR	C24-C23-C22	-5.82	117.46	126.21
11	1	1140	CLA	O2A-CGA-O1A	-5.75	109.28	123.55
11	1	1011	CLA	C3D-CAD-CBD	-5.72	99.51	107.60
14	f	4013	BCR	C24-C23-C22	-5.70	117.66	126.21
11	1	1012	CLA	O2A-CGA-O1A	-5.69	109.42	123.55
14	1	4003	BCR	C37-C22-C21	-5.66	115.00	122.92
11	1	1119	CLA	O2A-CGA-O1A	-5.66	109.50	123.55
11	B	1207	CLA	O2A-CGA-O1A	-5.64	109.56	123.55
11	b	1207	CLA	O2A-CGA-O1A	-5.63	109.57	123.55
11	a	1119	CLA	O2A-CGA-O1A	-5.63	109.57	123.55
11	L	1503	CLA	C1C-C2C-C3C	-5.58	100.73	106.92
11	B	1013	CLA	O2A-CGA-O1A	-5.57	109.72	123.55
11	2	1224	CLA	O2A-CGA-O1A	-5.57	109.73	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4014	BCR	C24-C23-C22	-5.56	117.85	126.21
11	2	1207	CLA	O2A-CGA-O1A	-5.56	109.75	123.55
11	B	1224	CLA	O2A-CGA-O1A	-5.56	109.75	123.55
14	A	4003	BCR	C7-C8-C9	-5.55	117.87	126.21
11	b	1013	CLA	O2A-CGA-O1A	-5.55	109.77	123.55
14	a	4001	BCR	C24-C23-C22	-5.53	117.90	126.21
14	b	4017	BCR	C7-C8-C9	-5.53	117.90	126.21
14	l	4022	BCR	C24-C23-C22	-5.53	117.91	126.21
11	2	1013	CLA	O2A-CGA-O1A	-5.52	109.83	123.55
11	2	1023	CLA	O2A-CGA-O1A	-5.49	109.91	123.55
11	l	1501	CLA	O2A-CGA-O1A	-5.49	109.93	123.55
11	a	1102	CLA	O2A-CGA-O1A	-5.47	109.96	123.55
11	8	1501	CLA	O2A-CGA-O1A	-5.46	109.98	123.55
11	A	1011	CLA	C1C-C2C-C3C	-5.46	100.86	106.92
11	B	1021	CLA	C1C-C2C-C3C	-5.46	100.86	106.92
11	B	1234	CLA	O2A-CGA-O1A	-5.46	109.99	123.55
14	1	4008	BCR	C15-C14-C13	-5.45	119.53	127.31
11	B	1021	CLA	O2A-CGA-O1A	-5.45	110.03	123.55
11	b	1224	CLA	O2A-CGA-O1A	-5.44	110.04	123.55
11	1	1109	CLA	O2A-CGA-O1A	-5.44	110.04	123.55
11	b	1205	CLA	O2A-CGA-O1A	-5.43	110.06	123.55
11	A	1135	CLA	O2A-CGA-O1A	-5.42	110.08	123.55
11	A	1801	CLA	O2A-CGA-O1A	-5.41	110.11	123.55
11	1	1110	CLA	O2A-CGA-O1A	-5.41	110.11	123.55
11	a	1109	CLA	O2A-CGA-O1A	-5.40	110.14	123.55
11	b	1234	CLA	O2A-CGA-O1A	-5.39	110.17	123.55
11	1	1022	CLA	O2A-CGA-O1A	-5.38	110.19	123.55
11	b	1021	CLA	O2A-CGA-O1A	-5.38	110.19	123.55
14	A	4008	BCR	C34-C9-C10	-5.37	115.40	122.92
11	1	1137	CLA	O2A-CGA-O1A	-5.37	110.21	123.55
14	a	4003	BCR	C24-C23-C22	-5.37	118.14	126.21
11	A	1137	CLA	O2A-CGA-O1A	-5.37	110.22	123.55
11	A	1133	CLA	C1C-C2C-C3C	-5.37	100.97	106.92
11	1	1104	CLA	C1C-C2C-C3C	-5.37	100.97	106.92
11	L	1501	CLA	O2A-CGA-O1A	-5.36	110.23	123.55
11	a	1139	CLA	C1C-C2C-C3C	-5.36	100.97	106.92
11	B	1205	CLA	O2A-CGA-O1A	-5.36	110.24	123.55
11	b	1239	CLA	C1C-C2C-C3C	-5.35	100.99	106.92
11	1	1011	CLA	C1C-C2C-C3C	-5.34	100.99	106.92
14	1	4002	BCR	C33-C5-C6	-5.34	118.53	124.51
11	B	1023	CLA	O2A-CGA-O1A	-5.34	110.30	123.55
11	a	1103	CLA	C1C-C2C-C3C	-5.33	101.01	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	4013	BCR	C7-C8-C9	-5.32	118.21	126.21
11	A	1118	CLA	C1C-C2C-C3C	-5.32	101.02	106.92
11	b	1222	CLA	O2A-CGA-O1A	-5.32	110.34	123.55
11	a	1801	CLA	O2A-CGA-O1A	-5.32	110.35	123.55
11	A	1102	CLA	O2A-CGA-O1A	-5.31	110.36	123.55
11	A	1104	CLA	O2A-CGA-O1A	-5.30	110.38	123.55
11	2	1213	CLA	C1C-C2C-C3C	-5.30	101.04	106.92
14	B	4017	BCR	C24-C23-C22	-5.30	118.25	126.21
11	b	1023	CLA	O2A-CGA-O1A	-5.30	110.40	123.55
14	2	4005	BCR	C24-C23-C22	-5.29	118.27	126.21
11	b	1217	CLA	O2A-CGA-O1A	-5.29	110.42	123.55
11	l	1503	CLA	C1C-C2C-C3C	-5.28	101.06	106.92
11	B	1236	CLA	C1C-C2C-C3C	-5.27	101.07	106.92
11	0	1402	CLA	O2A-CGA-O1A	-5.27	110.46	123.55
11	B	1202	CLA	O2A-CGA-O1A	-5.27	110.47	123.55
14	a	4008	BCR	C24-C23-C22	-5.26	118.30	126.21
11	a	1118	CLA	C1C-C2C-C3C	-5.26	101.08	106.92
11	A	1104	CLA	C1C-C2C-C3C	-5.25	101.09	106.92
11	A	1801	CLA	C1C-C2C-C3C	-5.25	101.09	106.92
11	B	1205	CLA	C1C-C2C-C3C	-5.25	101.09	106.92
14	8	4022	BCR	C24-C23-C22	-5.25	118.33	126.21
11	a	1122	CLA	O2A-CGA-O1A	-5.25	110.52	123.55
11	a	1011	CLA	C1C-C2C-C3C	-5.24	101.11	106.92
11	b	1230	CLA	O2A-CGA-O1A	-5.23	110.57	123.55
14	b	4014	BCR	C24-C23-C22	-5.22	118.36	126.21
11	A	1122	CLA	O2A-CGA-O1A	-5.22	110.59	123.55
11	a	1011	CLA	O2A-CGA-O1A	-5.22	110.59	123.55
11	2	1228	CLA	O2A-CGA-O1A	-5.22	110.60	123.55
11	1	1133	CLA	C1C-C2C-C3C	-5.21	101.14	106.92
11	2	1206	CLA	C1C-C2C-C3C	-5.21	101.14	106.92
11	B	1234	CLA	C1C-C2C-C3C	-5.21	101.14	106.92
11	a	1105	CLA	O2A-CGA-O1A	-5.21	110.62	123.55
11	1	1115	CLA	C1C-C2C-C3C	-5.20	101.15	106.92
11	1	1111	CLA	O2A-CGA-O1A	-5.19	110.66	123.55
11	0	1401	CLA	O2A-CGA-O1A	-5.19	110.66	123.55
11	2	1215	CLA	C1C-C2C-C3C	-5.19	101.16	106.92
11	K	1401	CLA	O2A-CGA-O1A	-5.19	110.67	123.55
11	A	1011	CLA	O2A-CGA-O1A	-5.18	110.68	123.55
11	k	1401	CLA	O2A-CGA-O1A	-5.18	110.68	123.55
11	A	1107	CLA	O2A-CGA-O1A	-5.18	110.69	123.55
11	A	1110	CLA	O2A-CGA-O1A	-5.18	110.69	123.55
11	1	1102	CLA	O2A-CGA-O1A	-5.18	110.69	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1118	CLA	O2A-CGA-O1A	-5.17	110.71	123.55
11	b	1212	CLA	C1C-C2C-C3C	-5.17	101.18	106.92
11	k	1402	CLA	O2A-CGA-O1A	-5.17	110.72	123.55
11	2	1225	CLA	C1C-C2C-C3C	-5.17	101.19	106.92
14	A	4008	BCR	C15-C14-C13	-5.16	119.95	127.31
11	b	1021	CLA	C1C-C2C-C3C	-5.16	101.20	106.92
11	A	1106	CLA	C1C-C2C-C3C	-5.16	101.20	106.92
11	B	1231	CLA	C1C-C2C-C3C	-5.15	101.20	106.92
11	B	1217	CLA	O2A-CGA-O1A	-5.15	110.76	123.55
11	2	1234	CLA	O2A-CGA-O1A	-5.15	110.76	123.55
11	2	1236	CLA	O2A-CGA-O1A	-5.15	110.76	123.55
11	B	1239	CLA	C1C-C2C-C3C	-5.15	101.21	106.92
11	b	1222	CLA	C1C-C2C-C3C	-5.15	101.21	106.92
11	1	1139	CLA	O2A-CGA-O1A	-5.15	110.77	123.55
11	A	1109	CLA	C1C-C2C-C3C	-5.14	101.21	106.92
11	1	1127	CLA	O2A-CGA-O1A	-5.14	110.78	123.55
14	B	4005	BCR	C24-C23-C22	-5.14	118.48	126.21
11	2	1021	CLA	C1C-C2C-C3C	-5.14	101.21	106.92
11	A	1111	CLA	O2A-CGA-O1A	-5.14	110.78	123.55
11	a	1133	CLA	C1C-C2C-C3C	-5.14	101.22	106.92
11	2	1222	CLA	O2A-CGA-O1A	-5.14	110.79	123.55
11	B	1204	CLA	C1C-C2C-C3C	-5.14	101.22	106.92
11	b	1203	CLA	C1C-C2C-C3C	-5.14	101.22	106.92
11	1	1801	CLA	C1C-C2C-C3C	-5.13	101.22	106.92
11	B	1203	CLA	C1C-C2C-C3C	-5.13	101.22	106.92
11	b	1215	CLA	O2A-CGA-O1A	-5.13	110.80	123.55
14	1	4003	BCR	C15-C14-C13	-5.13	119.99	127.31
11	b	1227	CLA	C1C-C2C-C3C	-5.13	101.23	106.92
11	1	1116	CLA	O2A-CGA-O1A	-5.13	110.82	123.55
11	A	1134	CLA	C1C-C2C-C3C	-5.12	101.23	106.92
11	a	1105	CLA	C1C-C2C-C3C	-5.12	101.23	106.92
14	b	4011	BCR	C7-C8-C9	-5.12	118.52	126.21
11	1	1102	CLA	C1C-C2C-C3C	-5.12	101.24	106.92
11	a	1137	CLA	O2A-CGA-O1A	-5.12	110.83	123.55
11	a	1104	CLA	O2A-CGA-O1A	-5.12	110.85	123.55
11	a	1012	CLA	O2A-CGA-O1A	-5.11	110.85	123.55
11	1	1106	CLA	O2A-CGA-O1A	-5.11	110.86	123.55
11	1	1124	CLA	O2A-CGA-O1A	-5.11	110.86	123.55
11	B	1210	CLA	O2A-CGA-O1A	-5.11	110.86	123.55
11	B	1222	CLA	O2A-CGA-O1A	-5.11	110.86	123.55
11	B	1232	CLA	C1C-C2C-C3C	-5.11	101.25	106.92
11	b	1219	CLA	C1C-C2C-C3C	-5.11	101.25	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1502	CLA	C1C-C2C-C3C	-5.10	101.26	106.92
11	l	1502	CLA	C1C-C2C-C3C	-5.10	101.26	106.92
11	A	1138	CLA	C1C-C2C-C3C	-5.10	101.26	106.92
11	2	1211	CLA	C1C-C2C-C3C	-5.10	101.26	106.92
11	A	1109	CLA	O2A-CGA-O1A	-5.10	110.89	123.55
14	6	4013	BCR	C7-C8-C9	-5.10	118.55	126.21
11	2	1205	CLA	C1C-C2C-C3C	-5.10	101.26	106.92
11	a	1129	CLA	C1C-C2C-C3C	-5.10	101.26	106.92
14	b	4011	BCR	C34-C9-C10	-5.10	115.78	122.92
11	B	1226	CLA	O2A-CGA-O1A	-5.10	110.89	123.55
11	1	1011	CLA	O2A-CGA-O1A	-5.09	110.90	123.55
11	1	1114	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	a	1101	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	2	1212	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	2	1202	CLA	O2A-CGA-O1A	-5.09	110.91	123.55
11	a	1109	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	a	1127	CLA	O2A-CGA-O1A	-5.09	110.91	123.55
14	f	4013	BCR	C15-C14-C13	-5.09	120.05	127.31
11	2	1208	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	2	1227	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	b	1207	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
11	b	1219	CLA	O2A-CGA-O1A	-5.09	110.91	123.55
11	B	1226	CLA	C1C-C2C-C3C	-5.09	101.28	106.92
11	b	1206	CLA	C1C-C2C-C3C	-5.09	101.28	106.92
11	2	1226	CLA	C1C-C2C-C3C	-5.09	101.28	106.92
11	2	1216	CLA	O2A-CGA-O1A	-5.08	110.92	123.55
11	b	1201	CLA	O2A-CGA-O1A	-5.08	110.93	123.55
11	B	1214	CLA	O2A-CGA-O1A	-5.08	110.93	123.55
11	b	1203	CLA	O2A-CGA-O1A	-5.08	110.93	123.55
14	A	4003	BCR	C37-C22-C21	-5.08	115.81	122.92
11	a	1124	CLA	O2A-CGA-O1A	-5.08	110.94	123.55
11	B	1211	CLA	C1C-C2C-C3C	-5.08	101.29	106.92
11	b	1236	CLA	O2A-CGA-O1A	-5.08	110.94	123.55
11	1	1105	CLA	O2A-CGA-O1A	-5.08	110.94	123.55
11	A	1127	CLA	O2A-CGA-O1A	-5.07	110.95	123.55
11	a	1114	CLA	C1C-C2C-C3C	-5.07	101.29	106.92
11	a	1110	CLA	C1C-C2C-C3C	-5.07	101.29	106.92
11	2	1234	CLA	C1C-C2C-C3C	-5.07	101.29	106.92
11	2	1203	CLA	C1C-C2C-C3C	-5.07	101.29	106.92
11	2	1224	CLA	C1C-C2C-C3C	-5.07	101.30	106.92
11	a	1137	CLA	C1C-C2C-C3C	-5.07	101.30	106.92
11	B	1215	CLA	C1C-C2C-C3C	-5.06	101.30	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1107	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
11	2	1239	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
11	2	1222	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
11	B	1213	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
11	a	1135	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
11	a	1123	CLA	O2A-CGA-O1A	-5.06	110.98	123.55
11	1	1801	CLA	O2A-CGA-O1A	-5.06	110.99	123.55
11	A	1121	CLA	C1C-C2C-C3C	-5.05	101.31	106.92
11	A	1114	CLA	C1C-C2C-C3C	-5.05	101.31	106.92
11	2	1204	CLA	C1C-C2C-C3C	-5.05	101.32	106.92
11	b	1229	CLA	C1C-C2C-C3C	-5.05	101.32	106.92
11	B	1219	CLA	O2A-CGA-O1A	-5.05	111.02	123.55
11	A	1022	CLA	OBD-CAD-CBD	-5.05	118.32	125.94
11	b	1228	CLA	O2A-CGA-O1A	-5.05	111.02	123.55
11	2	1226	CLA	O2A-CGA-O1A	-5.05	111.02	123.55
11	a	1127	CLA	C1C-C2C-C3C	-5.04	101.33	106.92
11	B	1208	CLA	C1C-C2C-C3C	-5.04	101.33	106.92
14	7	4021	BCR	C33-C5-C6	-5.04	118.87	124.51
11	l	1503	CLA	O2A-CGA-O1A	-5.04	111.04	123.55
11	A	1125	CLA	C1C-NC-C4C	-5.04	104.16	107.06
11	a	1101	CLA	O2A-CGA-O1A	-5.04	111.04	123.55
11	8	1501	CLA	C1C-C2C-C3C	-5.04	101.33	106.92
11	a	1107	CLA	C1C-C2C-C3C	-5.04	101.33	106.92
11	B	1227	CLA	C1C-C2C-C3C	-5.03	101.34	106.92
11	a	1106	CLA	C1C-C2C-C3C	-5.03	101.34	106.92
11	b	1208	CLA	C1C-C2C-C3C	-5.03	101.34	106.92
11	2	1223	CLA	O2A-CGA-O1A	-5.03	111.06	123.55
11	A	1140	CLA	O2A-CGA-O1A	-5.03	111.06	123.55
11	b	1223	CLA	O2A-CGA-O1A	-5.03	111.07	123.55
11	2	1238	CLA	C1C-C2C-C3C	-5.03	101.34	106.92
11	A	1124	CLA	O2A-CGA-O1A	-5.03	111.07	123.55
11	1	1108	CLA	C1C-C2C-C3C	-5.02	101.34	106.92
11	1	1118	CLA	C1C-C2C-C3C	-5.02	101.34	106.92
11	1	1134	CLA	C1C-C2C-C3C	-5.02	101.34	106.92
11	K	1402	CLA	O2A-CGA-O1A	-5.02	111.07	123.55
11	a	1120	CLA	C1C-C2C-C3C	-5.02	101.35	106.92
11	b	1202	CLA	O2A-CGA-O1A	-5.02	111.08	123.55
11	A	1136	CLA	C1C-C2C-C3C	-5.02	101.35	106.92
11	b	1236	CLA	C1C-C2C-C3C	-5.02	101.35	106.92
11	1	1012	CLA	C1C-C2C-C3C	-5.02	101.35	106.92
11	1	1103	CLA	C1C-C2C-C3C	-5.02	101.35	106.92
11	A	1237	CLA	C1C-C2C-C3C	-5.02	101.35	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1130	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	B	1225	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	A	1110	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	B	1222	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	a	1022	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	1	1109	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	1	1132	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	A	1102	CLA	C1C-C2C-C3C	-5.01	101.36	106.92
11	B	1238	CLA	C1C-C2C-C3C	-5.01	101.37	106.92
11	1	1117	CLA	O2A-CGA-O1A	-5.01	111.12	123.55
11	a	1125	CLA	C1C-C2C-C3C	-5.00	101.37	106.92
11	A	1139	CLA	C1C-C2C-C3C	-5.00	101.37	106.92
11	b	1213	CLA	C1C-C2C-C3C	-5.00	101.37	106.92
11	1	1121	CLA	C1C-C2C-C3C	-5.00	101.37	106.92
11	L	1503	CLA	O2A-CGA-O1A	-5.00	111.14	123.55
11	b	1205	CLA	C1C-C2C-C3C	-5.00	101.38	106.92
11	a	1022	CLA	O2A-CGA-O1A	-4.99	111.15	123.55
11	1	1124	CLA	C1C-C2C-C3C	-4.99	101.38	106.92
11	B	1235	CLA	C1C-C2C-C3C	-4.99	101.38	106.92
11	A	1137	CLA	C1C-C2C-C3C	-4.99	101.38	106.92
11	b	1215	CLA	C1C-C2C-C3C	-4.99	101.39	106.92
14	2	4014	BCR	C15-C14-C13	-4.99	120.19	127.31
11	1	1139	CLA	C1C-C2C-C3C	-4.99	101.39	106.92
11	1	1129	CLA	C1C-C2C-C3C	-4.99	101.39	106.92
11	a	1131	CLA	C1C-C2C-C3C	-4.98	101.39	106.92
11	1	1117	CLA	C1C-C2C-C3C	-4.98	101.39	106.92
11	1	1130	CLA	C1C-C2C-C3C	-4.98	101.39	106.92
11	b	1235	CLA	C1C-C2C-C3C	-4.98	101.39	106.92
11	B	1217	CLA	C1C-C2C-C3C	-4.98	101.39	106.92
14	M	4021	BCR	C33-C5-C6	-4.98	118.93	124.51
11	a	1139	CLA	O2A-CGA-O1A	-4.98	111.18	123.55
11	B	1216	CLA	O2A-CGA-O1A	-4.98	111.19	123.55
11	2	1210	CLA	O2A-CGA-O1A	-4.98	111.19	123.55
11	k	1401	CLA	C1C-C2C-C3C	-4.97	101.40	106.92
11	B	1215	CLA	O2A-CGA-O1A	-4.97	111.21	123.55
11	1	1012	CLA	C1C-NC-C4C	-4.97	104.20	107.06
11	a	1237	CLA	O2A-CGA-O1A	-4.97	111.21	123.55
11	a	1136	CLA	C1C-C2C-C3C	-4.97	101.41	106.92
11	a	1237	CLA	C1C-C2C-C3C	-4.97	101.41	106.92
11	b	1232	CLA	C1C-C2C-C3C	-4.97	101.41	106.92
14	b	4006	BCR	C7-C8-C9	-4.97	118.75	126.21
11	B	1216	CLA	C1C-C2C-C3C	-4.97	101.41	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1140	CLA	C1C-C2C-C3C	-4.97	101.41	106.92
11	B	1236	CLA	O2A-CGA-O1A	-4.97	111.21	123.55
11	a	1111	CLA	O2A-CGA-O1A	-4.97	111.22	123.55
11	a	1140	CLA	O2A-CGA-O1A	-4.97	111.22	123.55
14	6	4020	BCR	C24-C23-C22	-4.97	118.75	126.21
11	2	1203	CLA	O2A-CGA-O1A	-4.96	111.22	123.55
11	A	1135	CLA	C1C-C2C-C3C	-4.96	101.41	106.92
14	m	4021	BCR	C33-C5-C6	-4.96	118.95	124.51
14	M	4021	BCR	C7-C8-C9	-4.96	118.75	126.21
11	0	1401	CLA	C1C-C2C-C3C	-4.96	101.42	106.92
11	b	1207	CLA	C1C-NC-C4C	-4.96	104.20	107.06
11	a	1121	CLA	C1C-C2C-C3C	-4.96	101.42	106.92
11	a	1116	CLA	O2A-CGA-O1A	-4.96	111.23	123.55
11	1	1104	CLA	O2A-CGA-O1A	-4.96	111.24	123.55
11	1	1106	CLA	C1C-C2C-C3C	-4.96	101.42	106.92
11	b	1226	CLA	C1C-C2C-C3C	-4.96	101.42	106.92
11	a	1108	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
11	1	1119	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
11	a	1130	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
11	a	1125	CLA	O2A-CGA-O1A	-4.95	111.25	123.55
11	b	1204	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
11	A	1132	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
11	1	1131	CLA	C1C-C2C-C3C	-4.95	101.42	106.92
11	b	1211	CLA	C1C-C2C-C3C	-4.95	101.43	106.92
11	2	1221	CLA	C1C-C2C-C3C	-4.95	101.43	106.92
11	8	1503	CLA	O2A-CGA-O1A	-4.95	111.26	123.55
11	8	1503	CLA	C1C-C2C-C3C	-4.95	101.43	106.92
14	7	4021	BCR	C38-C26-C25	-4.95	118.97	124.51
14	6	4020	BCR	C34-C9-C10	-4.94	116.00	122.92
11	K	1401	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	B	1206	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	1	1135	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	2	1236	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	8	1502	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	1	1122	CLA	O2A-CGA-O1A	-4.94	111.28	123.55
14	1	4002	BCR	C36-C18-C17	-4.94	116.00	122.92
11	A	1131	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	A	1115	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	b	1217	CLA	C1C-C2C-C3C	-4.94	101.44	106.92
11	A	1117	CLA	O2A-CGA-O1A	-4.94	111.29	123.55
14	2	4014	BCR	C7-C8-C9	-4.94	118.80	126.21
11	b	1226	CLA	O2A-CGA-O1A	-4.94	111.29	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4004	BCR	C7-C8-C9	-4.94	118.80	126.21
11	b	1210	CLA	O2A-CGA-O1A	-4.93	111.30	123.55
11	2	1228	CLA	C1C-C2C-C3C	-4.93	101.45	106.92
11	a	1022	CLA	OBD-CAD-CBD	-4.93	118.50	125.94
11	b	1225	CLA	C1C-C2C-C3C	-4.93	101.45	106.92
11	1	1110	CLA	C1C-C2C-C3C	-4.93	101.45	106.92
11	2	1213	CLA	O2A-CGA-O1A	-4.93	111.31	123.55
11	l	1501	CLA	C1C-C2C-C3C	-4.92	101.46	106.92
11	a	1102	CLA	C1C-C2C-C3C	-4.92	101.46	106.92
11	A	1123	CLA	C1C-C2C-C3C	-4.92	101.46	106.92
11	1	1120	CLA	C1C-C2C-C3C	-4.92	101.46	106.92
11	B	1228	CLA	O2A-CGA-O1A	-4.92	111.33	123.55
11	1	1137	CLA	C1C-C2C-C3C	-4.92	101.47	106.92
11	1	1101	CLA	O2A-CGA-O1A	-4.92	111.34	123.55
11	2	1214	CLA	C1C-C2C-C3C	-4.92	101.47	106.92
11	2	1202	CLA	C1C-C2C-C3C	-4.92	101.47	106.92
11	2	1231	CLA	C1C-C2C-C3C	-4.91	101.47	106.92
11	a	1113	CLA	C1C-C2C-C3C	-4.91	101.47	106.92
11	2	1229	CLA	O2A-CGA-O1A	-4.91	111.35	123.55
11	A	1101	CLA	C1C-C2C-C3C	-4.91	101.47	106.92
11	A	1116	CLA	O2A-CGA-O1A	-4.91	111.36	123.55
11	1	1011	CLA	C1C-NC-C4C	-4.91	104.23	107.06
14	6	4018	BCR	C7-C8-C9	-4.91	118.84	126.21
11	a	1118	CLA	O2A-CGA-O1A	-4.91	111.37	123.55
11	B	1235	CLA	O2A-CGA-O1A	-4.90	111.37	123.55
11	B	1229	CLA	C1C-C2C-C3C	-4.90	101.48	106.92
11	b	1238	CLA	C1C-C2C-C3C	-4.90	101.48	106.92
14	1	4007	BCR	C24-C23-C22	-4.90	118.85	126.21
11	b	1201	CLA	C1C-C2C-C3C	-4.90	101.48	106.92
11	a	1119	CLA	C1C-C2C-C3C	-4.90	101.49	106.92
11	A	1107	CLA	C1C-C2C-C3C	-4.90	101.49	106.92
11	a	1012	CLA	C1C-C2C-C3C	-4.90	101.49	106.92
11	a	1801	CLA	C1C-C2C-C3C	-4.90	101.49	106.92
11	A	1105	CLA	C1C-C2C-C3C	-4.90	101.49	106.92
11	a	1124	CLA	C1C-C2C-C3C	-4.89	101.49	106.92
11	a	1134	CLA	C1C-C2C-C3C	-4.89	101.49	106.92
11	b	1216	CLA	C1C-C2C-C3C	-4.89	101.49	106.92
11	b	1228	CLA	C1C-C2C-C3C	-4.89	101.49	106.92
11	2	1021	CLA	O2A-CGA-O1A	-4.89	111.41	123.55
11	a	1140	CLA	C1C-C2C-C3C	-4.89	101.50	106.92
11	1	1022	CLA	C1C-C2C-C3C	-4.89	101.50	106.92
14	B	4004	BCR	C33-C5-C6	-4.88	119.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1501	CLA	C1C-C2C-C3C	-4.88	101.51	106.92
11	1	1101	CLA	C1C-C2C-C3C	-4.88	101.51	106.92
11	A	1237	CLA	O2A-CGA-O1A	-4.88	111.44	123.55
14	a	4002	BCR	C7-C8-C9	-4.88	118.88	126.21
11	B	1223	CLA	O2A-CGA-O1A	-4.87	111.45	123.55
11	A	1106	CLA	O2A-CGA-O1A	-4.87	111.45	123.55
11	B	1221	CLA	C1C-C2C-C3C	-4.87	101.52	106.92
11	1	1127	CLA	C1C-C2C-C3C	-4.87	101.52	106.92
11	b	1213	CLA	O2A-CGA-O1A	-4.87	111.46	123.55
11	1	1116	CLA	C1C-C2C-C3C	-4.87	101.52	106.92
11	2	1217	CLA	O2A-CGA-O1A	-4.86	111.47	123.55
11	2	1201	CLA	O2A-CGA-O1A	-4.86	111.47	123.55
11	1	1123	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	A	1022	CLA	O2A-CGA-O1A	-4.86	111.48	123.55
11	B	1202	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	B	1212	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	a	1104	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	B	1240	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	A	1125	CLA	O2A-CGA-O1A	-4.86	111.49	123.55
11	0	1402	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	A	1127	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	2	1207	CLA	C1C-C2C-C3C	-4.86	101.53	106.92
11	b	1238	CLA	O2A-CGA-O1A	-4.85	111.50	123.55
11	2	1206	CLA	O2A-CGA-O1A	-4.85	111.50	123.55
11	2	1216	CLA	C1C-C2C-C3C	-4.85	101.54	106.92
11	a	1107	CLA	C1C-NC-C4C	-4.85	104.27	107.06
11	b	1231	CLA	C1C-C2C-C3C	-4.85	101.54	106.92
11	1	1237	CLA	C1C-C2C-C3C	-4.85	101.54	106.92
11	B	1221	CLA	O2A-CGA-O1A	-4.84	111.52	123.55
11	1	1128	CLA	C1C-C2C-C3C	-4.84	101.55	106.92
11	1	1113	CLA	C1C-C2C-C3C	-4.84	101.55	106.92
11	a	1128	CLA	C1C-C2C-C3C	-4.84	101.55	106.92
11	b	1218	CLA	C1C-C2C-C3C	-4.84	101.55	106.92
14	b	4004	BCR	C7-C8-C9	-4.84	118.95	126.21
11	A	1022	CLA	C1C-C2C-C3C	-4.83	101.56	106.92
11	2	1216	CLA	C1C-NC-C4C	-4.83	104.28	107.06
11	a	1106	CLA	O2A-CGA-O1A	-4.83	111.56	123.55
11	a	1117	CLA	O2A-CGA-O1A	-4.83	111.56	123.55
11	a	1123	CLA	C1C-C2C-C3C	-4.83	101.56	106.92
11	a	1135	CLA	O2A-CGA-O1A	-4.83	111.56	123.55
14	A	4008	BCR	C24-C23-C22	-4.82	118.96	126.21
14	b	4014	BCR	C7-C8-C9	-4.82	118.96	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4002	BCR	C33-C5-C6	-4.82	119.11	124.51
11	A	1120	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	b	1209	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	1	1105	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	B	1220	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	a	1132	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	A	1117	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	b	1023	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
14	2	4004	BCR	C33-C5-C6	-4.82	119.11	124.51
11	1	1122	CLA	C1C-C2C-C3C	-4.82	101.57	106.92
11	1	1118	CLA	O2A-CGA-O1A	-4.82	111.58	123.55
11	A	1139	CLA	O2A-CGA-O1A	-4.81	111.60	123.55
11	1	1126	CLA	O2A-CGA-O1A	-4.81	111.60	123.55
11	b	1240	CLA	C1C-C2C-C3C	-4.81	101.59	106.92
11	B	1213	CLA	O2A-CGA-O1A	-4.80	111.62	123.55
11	A	1124	CLA	C1C-C2C-C3C	-4.80	101.59	106.92
11	A	1113	CLA	C1C-C2C-C3C	-4.80	101.59	106.92
11	b	1224	CLA	C1C-C2C-C3C	-4.80	101.59	106.92
11	A	1105	CLA	O2A-CGA-O1A	-4.80	111.62	123.55
14	B	4010	BCR	C33-C5-C6	-4.80	119.13	124.51
11	A	1012	CLA	C1C-C2C-C3C	-4.80	101.59	106.92
11	b	1216	CLA	O2A-CGA-O1A	-4.80	111.63	123.55
11	2	1215	CLA	O2A-CGA-O1A	-4.80	111.63	123.55
11	a	1103	CLA	O2A-CGA-O1A	-4.80	111.63	123.55
11	a	1126	CLA	O2A-CGA-O1A	-4.80	111.63	123.55
11	2	1232	CLA	C1C-C2C-C3C	-4.80	101.60	106.92
11	B	1207	CLA	C1C-C2C-C3C	-4.80	101.60	106.92
11	b	1234	CLA	C1C-C2C-C3C	-4.80	101.60	106.92
14	A	4008	BCR	C33-C5-C6	-4.79	119.14	124.51
11	a	1131	CLA	O2A-CGA-O1A	-4.79	111.64	123.55
11	B	1224	CLA	C1C-C2C-C3C	-4.79	101.60	106.92
11	A	1128	CLA	O2A-CGA-O1A	-4.79	111.66	123.55
11	a	1117	CLA	C1C-C2C-C3C	-4.79	101.61	106.92
14	a	4007	BCR	C33-C5-C6	-4.79	119.15	124.51
11	A	1128	CLA	C1C-C2C-C3C	-4.79	101.61	106.92
11	2	1217	CLA	C1C-C2C-C3C	-4.79	101.61	106.92
11	a	1110	CLA	O2A-CGA-O1A	-4.78	111.67	123.55
11	1	1112	CLA	C1C-C2C-C3C	-4.78	101.61	106.92
14	2	4011	BCR	C34-C9-C10	-4.78	116.22	122.92
11	A	1132	CLA	O2A-CGA-O1A	-4.78	111.68	123.55
14	A	4002	BCR	C24-C23-C22	-4.78	119.03	126.21
11	2	1240	CLA	C1C-C2C-C3C	-4.78	101.62	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1219	CLA	O2A-CGA-O1A	-4.78	111.69	123.55
11	b	1221	CLA	O2A-CGA-O1A	-4.77	111.70	123.55
11	A	1108	CLA	C1C-C2C-C3C	-4.77	101.63	106.92
11	A	1122	CLA	C1C-C2C-C3C	-4.76	101.64	106.92
14	A	4008	BCR	C7-C8-C9	-4.76	119.06	126.21
14	F	4020	BCR	C33-C5-C6	-4.76	119.18	124.51
14	F	4018	BCR	C7-C8-C9	-4.76	119.06	126.21
11	2	1219	CLA	C1C-C2C-C3C	-4.76	101.64	106.92
11	B	1209	CLA	C1C-C2C-C3C	-4.76	101.64	106.92
11	b	1223	CLA	C1C-C2C-C3C	-4.76	101.64	106.92
11	2	1229	CLA	C1C-C2C-C3C	-4.75	101.65	106.92
14	b	4010	BCR	C7-C8-C9	-4.75	119.07	126.21
11	B	1225	CLA	O2A-CGA-O1A	-4.75	111.76	123.55
11	2	1213	CLA	C1C-NC-C4C	-4.74	104.33	107.06
11	B	1230	CLA	C1C-NC-C4C	-4.74	104.33	107.06
11	B	1219	CLA	C1C-C2C-C3C	-4.74	101.66	106.92
14	2	4006	BCR	C1-C6-C5	-4.74	115.93	122.59
11	a	1128	CLA	O2A-CGA-O1A	-4.74	111.78	123.55
11	2	1209	CLA	C1C-C2C-C3C	-4.74	101.66	106.92
11	2	1225	CLA	O2A-CGA-O1A	-4.74	111.79	123.55
11	B	1228	CLA	C1C-C2C-C3C	-4.73	101.67	106.92
11	A	1125	CLA	C1C-C2C-C3C	-4.73	101.67	106.92
11	B	1203	CLA	O2A-CGA-O1A	-4.73	111.81	123.55
11	1	1123	CLA	O2A-CGA-O1A	-4.73	111.81	123.55
14	f	4020	BCR	C7-C8-C9	-4.73	119.11	126.21
11	2	1201	CLA	C1C-C2C-C3C	-4.73	101.68	106.92
11	A	1129	CLA	C1C-C2C-C3C	-4.72	101.69	106.92
14	f	4018	BCR	C7-C8-C9	-4.71	119.13	126.21
14	F	4013	BCR	C24-C23-C22	-4.71	119.13	126.21
14	b	4010	BCR	C38-C26-C25	-4.71	119.24	124.51
11	B	1223	CLA	C1C-C2C-C3C	-4.71	101.70	106.92
11	a	1116	CLA	C1C-C2C-C3C	-4.71	101.70	106.92
11	B	1230	CLA	C1C-C2C-C3C	-4.70	101.71	106.92
11	1	1107	CLA	O2A-CGA-O1A	-4.70	111.89	123.55
11	B	1229	CLA	O2A-CGA-O1A	-4.70	111.89	123.55
14	1	4007	BCR	C33-C5-C6	-4.69	119.25	124.51
14	a	4002	BCR	C33-C5-C6	-4.69	119.26	124.51
11	1	1135	CLA	O2A-CGA-O1A	-4.69	111.91	123.55
11	B	1201	CLA	C1C-C2C-C3C	-4.68	101.72	106.92
14	B	4005	BCR	C7-C8-C9	-4.68	119.18	126.21
11	1	1138	CLA	C1C-C2C-C3C	-4.68	101.73	106.92
11	b	1230	CLA	C1C-NC-C4C	-4.68	104.36	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1128	CLA	O2A-CGA-O1A	-4.68	111.93	123.55
11	1	1131	CLA	O2A-CGA-O1A	-4.67	111.95	123.55
11	a	1107	CLA	O2A-CGA-O1A	-4.67	111.96	123.55
11	B	1204	CLA	O2A-CGA-O1A	-4.67	111.96	123.55
11	K	1402	CLA	C1C-C2C-C3C	-4.67	101.74	106.92
11	2	1220	CLA	C1C-C2C-C3C	-4.67	101.74	106.92
14	8	4019	BCR	C15-C14-C13	-4.65	120.67	127.31
11	1	1022	CLA	OBD-CAD-CBD	-4.65	118.91	125.94
11	2	1221	CLA	O2A-CGA-O1A	-4.65	112.00	123.55
11	A	1801	CLA	C1C-NC-C4C	-4.65	104.38	107.06
11	B	1206	CLA	O2A-CGA-O1A	-4.65	112.01	123.55
11	2	1230	CLA	O2A-CGA-O1A	-4.65	112.01	123.55
11	b	1230	CLA	C1C-C2C-C3C	-4.65	101.77	106.92
14	b	4005	BCR	C24-C23-C22	-4.64	119.23	126.21
11	B	1218	CLA	C1C-C2C-C3C	-4.64	101.77	106.92
11	2	1206	CLA	C1C-NC-C4C	-4.64	104.38	107.06
11	1	1125	CLA	O2A-CGA-O1A	-4.64	112.02	123.55
11	A	1126	CLA	O2A-CGA-O1A	-4.64	112.02	123.55
11	k	1402	CLA	C1C-C2C-C3C	-4.64	101.77	106.92
11	b	1220	CLA	C1C-C2C-C3C	-4.64	101.77	106.92
11	A	1237	CLA	C1C-NC-C4C	-4.63	104.39	107.06
11	a	1122	CLA	C1C-C2C-C3C	-4.63	101.79	106.92
11	2	1204	CLA	O2A-CGA-O1A	-4.63	112.06	123.55
11	b	1221	CLA	C1C-C2C-C3C	-4.62	101.79	106.92
11	b	1013	CLA	C1C-C2C-C3C	-4.62	101.79	106.92
11	A	1126	CLA	C1C-C2C-C3C	-4.61	101.80	106.92
11	1	1126	CLA	C1C-C2C-C3C	-4.61	101.80	106.92
11	A	1123	CLA	C1C-NC-C4C	-4.61	104.40	107.06
11	b	1204	CLA	O2A-CGA-O1A	-4.61	112.10	123.55
11	2	1023	CLA	C1C-C2C-C3C	-4.61	101.81	106.92
11	1	1136	CLA	C1C-C2C-C3C	-4.60	101.81	106.92
11	A	1140	CLA	C1C-C2C-C3C	-4.60	101.81	106.92
11	a	1138	CLA	C1C-C2C-C3C	-4.60	101.82	106.92
11	2	1013	CLA	C1C-C2C-C3C	-4.60	101.82	106.92
11	1	1237	CLA	O2A-CGA-O1A	-4.60	112.14	123.55
11	8	1502	CLA	C1C-NC-C4C	-4.59	104.41	107.06
14	A	4002	BCR	C38-C26-C25	-4.59	119.36	124.51
11	L	1503	CLA	C1C-NC-C4C	-4.59	104.41	107.06
11	a	1012	CLA	C1C-NC-C4C	-4.59	104.42	107.06
11	b	1234	CLA	C1C-NC-C4C	-4.58	104.42	107.06
11	b	1202	CLA	C1C-C2C-C3C	-4.58	101.84	106.92
11	B	1023	CLA	C1C-C2C-C3C	-4.57	101.85	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1123	CLA	O2A-CGA-O1A	-4.57	112.20	123.55
14	1	4002	BCR	C24-C23-C22	-4.57	119.35	126.21
14	f	4013	BCR	C38-C26-C25	-4.57	119.40	124.51
11	A	1133	CLA	C1C-NC-C4C	-4.57	104.43	107.06
14	A	4007	BCR	C38-C26-C25	-4.56	119.40	124.51
11	1	1132	CLA	O2A-CGA-O1A	-4.56	112.22	123.55
11	1	1107	CLA	C1C-NC-C4C	-4.56	104.43	107.06
11	a	1111	CLA	C1C-C2C-C3C	-4.56	101.86	106.92
11	A	1103	CLA	C1C-C2C-C3C	-4.56	101.86	106.92
11	b	1235	CLA	O2A-CGA-O1A	-4.56	112.23	123.55
11	1	1122	CLA	C1C-NC-C4C	-4.56	104.43	107.06
11	a	1112	CLA	C1C-C2C-C3C	-4.56	101.87	106.92
11	B	1201	CLA	O2A-CGA-O1A	-4.55	112.24	123.55
11	B	1230	CLA	O2A-CGA-O1A	-4.55	112.25	123.55
11	l	1502	CLA	C1C-NC-C4C	-4.54	104.44	107.06
11	b	1219	CLA	C1C-NC-C4C	-4.54	104.44	107.06
11	2	1223	CLA	C1C-C2C-C3C	-4.54	101.88	106.92
14	1	4008	BCR	C33-C5-C6	-4.54	119.42	124.51
14	1	4002	BCR	C7-C8-C9	-4.54	119.39	126.21
14	2	4010	BCR	C7-C8-C9	-4.54	119.39	126.21
11	1	1103	CLA	O2A-CGA-O1A	-4.54	112.27	123.55
11	B	1225	CLA	C1C-NC-C4C	-4.54	104.44	107.06
11	b	1214	CLA	O2A-CGA-O1A	-4.54	112.29	123.55
11	A	1119	CLA	O2A-CGA-O1A	-4.53	112.29	123.55
14	F	4013	BCR	C7-C8-C9	-4.53	119.40	126.21
11	b	1225	CLA	O2A-CGA-O1A	-4.53	112.30	123.55
11	2	1238	CLA	O2A-CGA-O1A	-4.53	112.30	123.55
14	l	4019	BCR	C15-C14-C13	-4.53	120.85	127.31
14	B	4010	BCR	C7-C8-C9	-4.52	119.41	126.21
11	b	1220	CLA	C1C-NC-C4C	-4.52	104.45	107.06
11	B	1206	CLA	C1C-NC-C4C	-4.52	104.45	107.06
11	A	1137	CLA	C1C-NC-C4C	-4.52	104.45	107.06
14	A	4007	BCR	C33-C5-C6	-4.52	119.45	124.51
11	a	1132	CLA	O2A-CGA-O1A	-4.52	112.33	123.55
14	8	4019	BCR	C33-C5-C6	-4.51	119.45	124.51
11	b	1223	CLA	C1C-NC-C4C	-4.51	104.46	107.06
11	A	1131	CLA	O2A-CGA-O1A	-4.51	112.35	123.55
11	2	1230	CLA	C1C-C2C-C3C	-4.51	101.92	106.92
11	2	1214	CLA	O2A-CGA-O1A	-4.51	112.36	123.55
11	A	1112	CLA	C1C-C2C-C3C	-4.50	101.92	106.92
11	a	1237	CLA	C1C-NC-C4C	-4.50	104.47	107.06
11	B	1221	CLA	C1C-NC-C4C	-4.50	104.47	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	4013	BCR	C38-C26-C25	-4.50	119.47	124.51
14	f	4020	BCR	C33-C5-C6	-4.50	119.47	124.51
11	1	1110	CLA	C1C-NC-C4C	-4.50	104.47	107.06
11	a	1011	CLA	C1C-NC-C4C	-4.49	104.47	107.06
11	a	1126	CLA	C1C-C2C-C3C	-4.49	101.94	106.92
11	B	1013	CLA	C1C-C2C-C3C	-4.49	101.94	106.92
11	2	1235	CLA	C1C-C2C-C3C	-4.49	101.94	106.92
11	B	1214	CLA	C1C-C2C-C3C	-4.49	101.94	106.92
14	2	4010	BCR	C37-C22-C21	-4.49	116.64	122.92
11	B	1238	CLA	O2A-CGA-O1A	-4.49	112.41	123.55
14	2	4010	BCR	C38-C26-C25	-4.48	119.49	124.51
11	1	1115	CLA	C1C-NC-C4C	-4.48	104.48	107.06
14	b	4010	BCR	C33-C5-C6	-4.48	119.50	124.51
11	a	1135	CLA	C1C-NC-C4C	-4.47	104.48	107.06
14	1	4008	BCR	C34-C9-C10	-4.46	116.67	122.92
11	b	1229	CLA	O2A-CGA-O1A	-4.45	112.49	123.55
11	b	1214	CLA	C1C-C2C-C3C	-4.45	101.98	106.92
11	B	1226	CLA	C1C-NC-C4C	-4.45	104.50	107.06
14	a	4003	BCR	C7-C8-C9	-4.44	119.54	126.21
14	6	4013	BCR	C33-C5-C6	-4.44	119.54	124.51
14	L	4019	BCR	C33-C5-C6	-4.44	119.54	124.51
11	b	1206	CLA	O2A-CGA-O1A	-4.43	112.55	123.55
14	a	4002	BCR	C24-C23-C22	-4.43	119.56	126.21
11	A	1129	CLA	C1C-NC-C4C	-4.42	104.51	107.06
11	2	1234	CLA	C1C-NC-C4C	-4.42	104.52	107.06
11	a	1012	CLA	OBD-CAD-CBD	-4.41	119.28	125.94
11	A	1116	CLA	C1C-C2C-C3C	-4.41	102.03	106.92
14	2	4006	BCR	C38-C26-C25	-4.41	119.57	124.51
11	A	1134	CLA	C1C-NC-C4C	-4.41	104.52	107.06
11	B	1234	CLA	C1C-NC-C4C	-4.40	104.52	107.06
11	a	1022	CLA	C1C-NC-C4C	-4.40	104.53	107.06
11	1	1135	CLA	C1C-NC-C4C	-4.40	104.53	107.06
11	a	1114	CLA	C1C-NC-C4C	-4.39	104.53	107.06
14	F	4013	BCR	C38-C26-C25	-4.38	119.60	124.51
11	1	1125	CLA	C1C-C2C-C3C	-4.38	102.06	106.92
14	6	4013	BCR	C24-C23-C22	-4.38	119.64	126.21
14	6	4020	BCR	C33-C5-C6	-4.38	119.61	124.51
11	2	1221	CLA	C1C-NC-C4C	-4.38	104.54	107.06
11	A	1111	CLA	C1C-C2C-C3C	-4.38	102.07	106.92
14	A	4001	BCR	C15-C14-C13	-4.37	121.07	127.31
11	1	1123	CLA	C1C-NC-C4C	-4.37	104.54	107.06
11	a	1139	CLA	C1C-NC-C4C	-4.37	104.54	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1115	CLA	C1C-C2C-C3C	-4.37	102.07	106.92
11	A	1103	CLA	O2A-CGA-O1A	-4.36	112.72	123.55
11	2	1239	CLA	C1C-NC-C4C	-4.35	104.55	107.06
11	2	1212	CLA	C1C-NC-C4C	-4.35	104.55	107.06
14	2	4017	BCR	C24-C23-C22	-4.35	119.67	126.21
14	1	4001	BCR	C24-C23-C22	-4.35	119.68	126.21
11	1	1133	CLA	C1C-NC-C4C	-4.34	104.56	107.06
11	a	1133	CLA	C1C-NC-C4C	-4.34	104.56	107.06
14	b	4014	BCR	C15-C14-C13	-4.34	121.12	127.31
11	1	1137	CLA	C1C-NC-C4C	-4.34	104.56	107.06
11	2	1235	CLA	O2A-CGA-O1A	-4.33	112.81	123.55
11	A	1127	CLA	C1C-NC-C4C	-4.33	104.57	107.06
14	b	4010	BCR	C15-C14-C13	-4.31	121.15	127.31
11	2	1218	CLA	C1C-C2C-C3C	-4.31	102.14	106.92
14	B	4006	BCR	C7-C8-C9	-4.31	119.74	126.21
11	a	1101	CLA	C1C-NC-C4C	-4.30	104.58	107.06
11	a	1125	CLA	C1C-NC-C4C	-4.30	104.58	107.06
11	A	1110	CLA	C1C-NC-C4C	-4.29	104.58	107.06
14	2	4006	BCR	C7-C8-C9	-4.29	119.76	126.21
11	b	1226	CLA	C1C-NC-C4C	-4.29	104.59	107.06
11	A	1140	CLA	C1C-NC-C4C	-4.28	104.59	107.06
14	a	4002	BCR	C38-C26-C25	-4.28	119.72	124.51
11	b	1221	CLA	C1C-NC-C4C	-4.28	104.59	107.06
11	a	1121	CLA	C1C-NC-C4C	-4.28	104.59	107.06
11	b	1021	CLA	C1C-NC-C4C	-4.27	104.60	107.06
14	A	4001	BCR	C1-C6-C5	-4.27	116.59	122.59
11	2	1230	CLA	C1C-NC-C4C	-4.27	104.60	107.06
14	B	4011	BCR	C34-C9-C10	-4.26	116.95	122.92
11	a	1129	CLA	C1C-NC-C4C	-4.26	104.61	107.06
14	b	4017	BCR	C24-C23-C22	-4.26	119.82	126.21
11	2	1224	CLA	C1C-NC-C4C	-4.25	104.61	107.06
11	1	1113	CLA	C1C-NC-C4C	-4.24	104.62	107.06
11	2	1240	CLA	C1C-NC-C4C	-4.24	104.62	107.06
14	2	4009	BCR	C15-C14-C13	-4.23	121.27	127.31
11	B	1023	CLA	C1C-NC-C4C	-4.23	104.62	107.06
11	A	1114	CLA	C1C-NC-C4C	-4.23	104.62	107.06
14	L	4022	BCR	C33-C5-C6	-4.23	119.78	124.51
11	L	1502	CLA	C1C-NC-C4C	-4.22	104.62	107.06
11	2	1226	CLA	C1C-NC-C4C	-4.22	104.62	107.06
11	B	1222	CLA	C1C-NC-C4C	-4.22	104.63	107.06
11	1	1237	CLA	C1C-NC-C4C	-4.22	104.63	107.06
11	b	1211	CLA	C1C-NC-C4C	-4.22	104.63	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4018	BCR	C34-C9-C10	-4.22	117.02	122.92
11	b	1239	CLA	C1C-NC-C4C	-4.21	104.63	107.06
11	a	1127	CLA	C1C-NC-C4C	-4.21	104.63	107.06
11	b	1224	CLA	C1C-NC-C4C	-4.21	104.63	107.06
11	A	1101	CLA	O2A-CGA-O1A	-4.21	113.09	123.55
11	A	1113	CLA	C1C-NC-C4C	-4.21	104.63	107.06
14	b	4004	BCR	C33-C5-C6	-4.21	119.80	124.51
11	A	1122	CLA	C1C-NC-C4C	-4.21	104.64	107.06
14	L	4022	BCR	C38-C26-C25	-4.21	119.80	124.51
11	A	1107	CLA	C1C-NC-C4C	-4.20	104.64	107.06
14	f	4018	BCR	C3-C4-C5	-4.20	106.55	113.78
14	2	4014	BCR	C36-C18-C17	-4.20	117.04	122.92
11	1	1111	CLA	C1C-C2C-C3C	-4.20	102.26	106.92
11	B	1223	CLA	C1C-NC-C4C	-4.20	104.64	107.06
11	1	1011	CLA	O1D-CGD-CBD	-4.20	117.06	124.60
11	b	1210	CLA	C1C-C2C-C3C	-4.20	102.27	106.92
11	A	1012	CLA	C1C-NC-C4C	-4.19	104.64	107.06
11	A	1131	CLA	C1C-NC-C4C	-4.19	104.65	107.06
11	A	1119	CLA	C1C-C2C-C3C	-4.19	102.28	106.92
11	A	1101	CLA	C1C-NC-C4C	-4.18	104.65	107.06
14	a	4003	BCR	C3-C4-C5	-4.18	106.60	113.78
14	L	4019	BCR	C15-C14-C13	-4.18	121.35	127.31
14	f	4018	BCR	C15-C14-C13	-4.17	121.36	127.31
11	B	1232	CLA	C1C-NC-C4C	-4.17	104.66	107.06
11	B	1229	CLA	C1C-NC-C4C	-4.17	104.66	107.06
14	A	4007	BCR	C24-C23-C22	-4.17	119.95	126.21
11	2	1220	CLA	C1C-NC-C4C	-4.17	104.66	107.06
14	l	4022	BCR	C38-C26-C25	-4.17	119.84	124.51
14	L	4019	BCR	C7-C8-C9	-4.17	119.95	126.21
11	a	1123	CLA	C1C-NC-C4C	-4.16	104.66	107.06
14	m	4021	BCR	C28-C27-C26	-4.16	106.63	113.78
11	1	1129	CLA	C1C-NC-C4C	-4.16	104.66	107.06
14	b	4009	BCR	C38-C26-C25	-4.16	119.86	124.51
11	2	1207	CLA	C1C-NC-C4C	-4.16	104.67	107.06
11	a	1120	CLA	C1C-NC-C4C	-4.15	104.67	107.06
11	2	1211	CLA	C1C-NC-C4C	-4.15	104.67	107.06
14	a	4002	BCR	C34-C9-C10	-4.14	117.12	122.92
14	6	4018	BCR	C3-C4-C5	-4.14	106.66	113.78
11	b	1225	CLA	C1C-NC-C4C	-4.13	104.68	107.06
11	b	1208	CLA	C1C-NC-C4C	-4.13	104.68	107.06
11	k	1401	CLA	C1C-NC-C4C	-4.13	104.68	107.06
11	2	1021	CLA	C1C-NC-C4C	-4.13	104.68	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1113	CLA	C1C-NC-C4C	-4.13	104.68	107.06
11	B	1209	CLA	C1C-NC-C4C	-4.12	104.68	107.06
11	1	1101	CLA	C1C-NC-C4C	-4.12	104.68	107.06
11	B	1215	CLA	C1C-NC-C4C	-4.12	104.69	107.06
11	B	1205	CLA	C1C-NC-C4C	-4.12	104.69	107.06
11	1	1134	CLA	C1C-NC-C4C	-4.11	104.69	107.06
14	1	4001	BCR	C15-C14-C13	-4.11	121.44	127.31
11	a	1136	CLA	C1C-NC-C4C	-4.11	104.69	107.06
11	B	1240	CLA	C1C-NC-C4C	-4.11	104.69	107.06
11	1	1140	CLA	C1C-NC-C4C	-4.10	104.70	107.06
11	2	1209	CLA	C1C-NC-C4C	-4.10	104.70	107.06
14	8	4019	BCR	C24-C23-C22	-4.10	120.06	126.21
14	8	4019	BCR	C7-C8-C9	-4.09	120.07	126.21
11	2	1210	CLA	C1C-C2C-C3C	-4.09	102.38	106.92
11	a	1108	CLA	C1C-NC-C4C	-4.09	104.70	107.06
11	0	1401	CLA	C1C-NC-C4C	-4.08	104.71	107.06
11	1	1801	CLA	C1C-NC-C4C	-4.08	104.71	107.06
11	b	1023	CLA	C1C-NC-C4C	-4.08	104.71	107.06
14	f	4013	BCR	C33-C5-C6	-4.08	119.94	124.51
11	K	1401	CLA	C1C-NC-C4C	-4.08	104.71	107.06
11	1	1108	CLA	C1C-NC-C4C	-4.08	104.71	107.06
14	a	4008	BCR	C15-C14-C13	-4.08	121.49	127.31
14	B	4014	BCR	C33-C5-C6	-4.07	119.95	124.51
11	B	1220	CLA	C1C-NC-C4C	-4.07	104.71	107.06
11	1	1121	CLA	C1C-NC-C4C	-4.07	104.72	107.06
14	F	4020	BCR	C7-C8-C9	-4.07	120.10	126.21
11	B	1231	CLA	C1C-NC-C4C	-4.06	104.72	107.06
14	B	4011	BCR	C15-C14-C13	-4.06	121.52	127.31
14	L	4019	BCR	C37-C22-C21	-4.05	117.25	122.92
14	F	4013	BCR	C33-C5-C6	-4.05	119.97	124.51
14	l	4022	BCR	C37-C22-C21	-4.05	117.25	122.92
14	1	4003	BCR	C7-C8-C9	-4.05	120.13	126.21
14	b	4006	BCR	C38-C26-C25	-4.05	119.98	124.51
14	2	4010	BCR	C15-C14-C13	-4.04	121.54	127.31
11	1	1120	CLA	C1C-NC-C4C	-4.04	104.73	107.06
11	a	1110	CLA	C1C-NC-C4C	-4.04	104.73	107.06
11	l	1501	CLA	C1C-NC-C4C	-4.03	104.74	107.06
11	L	1501	CLA	C1C-NC-C4C	-4.03	104.74	107.06
11	l	1503	CLA	C1C-NC-C4C	-4.03	104.74	107.06
14	b	4009	BCR	C36-C18-C17	-4.02	117.29	122.92
11	B	1021	CLA	C1C-NC-C4C	-4.02	104.74	107.06
14	1	4007	BCR	C38-C26-C25	-4.02	120.01	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1217	CLA	C1C-NC-C4C	-4.01	104.75	107.06
11	a	1103	CLA	C1C-NC-C4C	-4.00	104.75	107.06
11	1	1102	CLA	C1C-NC-C4C	-4.00	104.75	107.06
11	B	1207	CLA	C1C-NC-C4C	-4.00	104.75	107.06
14	6	4018	BCR	C15-C14-C13	-4.00	121.60	127.31
11	2	1215	CLA	C1C-NC-C4C	-4.00	104.76	107.06
14	L	4022	BCR	C7-C8-C9	-4.00	120.21	126.21
11	1	1139	CLA	C1-C2-C3	-4.00	120.37	126.68
11	2	1232	CLA	C1C-NC-C4C	-3.99	104.76	107.06
11	A	1130	CLA	C1C-NC-C4C	-3.99	104.76	107.06
11	a	1137	CLA	C1C-NC-C4C	-3.99	104.76	107.06
11	b	1216	CLA	C1C-NC-C4C	-3.98	104.76	107.06
14	6	4018	BCR	C33-C5-C6	-3.98	120.05	124.51
11	2	1023	CLA	C1C-NC-C4C	-3.98	104.77	107.06
11	A	1136	CLA	C1C-NC-C4C	-3.97	104.77	107.06
11	b	1203	CLA	C1C-NC-C4C	-3.97	104.77	107.06
11	A	1116	CLA	C1C-NC-C4C	-3.97	104.77	107.06
14	B	4006	BCR	C1-C6-C5	-3.96	117.02	122.59
14	B	4011	BCR	C28-C27-C26	-3.96	106.97	113.78
11	B	1213	CLA	C1C-NC-C4C	-3.96	104.78	107.06
11	B	1219	CLA	C1C-NC-C4C	-3.95	104.78	107.06
11	b	1206	CLA	C1C-NC-C4C	-3.95	104.78	107.06
14	1	4002	BCR	C38-C26-C25	-3.95	120.09	124.51
11	b	1212	CLA	C1C-NC-C4C	-3.95	104.78	107.06
14	a	4003	BCR	C37-C22-C21	-3.95	117.40	122.92
11	1	1012	CLA	OBD-CAD-CBD	-3.94	120.00	125.94
14	8	4022	BCR	C34-C9-C10	-3.93	117.41	122.92
11	b	1227	CLA	C1C-NC-C4C	-3.93	104.79	107.06
11	2	1210	CLA	C1C-NC-C4C	-3.93	104.79	107.06
14	2	4014	BCR	C33-C5-C6	-3.93	120.11	124.51
14	2	4005	BCR	C7-C8-C9	-3.93	120.31	126.21
14	F	4018	BCR	C3-C4-C5	-3.93	107.02	113.78
11	1	1121	CLA	O2A-CGA-O1A	-3.93	110.11	123.12
14	m	4021	BCR	C24-C23-C22	-3.93	120.31	126.21
14	l	4019	BCR	C33-C5-C6	-3.93	120.11	124.51
14	2	4014	BCR	C37-C22-C21	-3.93	117.42	122.92
11	B	1223	CLA	OBD-CAD-C3D	-3.92	120.80	128.03
14	A	4001	BCR	C36-C18-C17	-3.92	117.43	122.92
11	A	1132	CLA	C1C-NC-C4C	-3.92	104.80	107.06
11	2	1222	CLA	C1C-NC-C4C	-3.92	104.80	107.06
11	b	1205	CLA	C1C-NC-C4C	-3.92	104.80	107.06
11	A	1011	CLA	C1-C2-C3	-3.91	118.76	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4003	BCR	C3-C4-C5	-3.91	107.06	113.78
11	a	1115	CLA	O2A-CGA-O1A	-3.90	110.19	123.12
11	a	1122	CLA	C1C-NC-C4C	-3.90	104.81	107.06
11	a	1140	CLA	C1C-NC-C4C	-3.90	104.81	107.06
11	B	1224	CLA	C1C-NC-C4C	-3.90	104.81	107.06
11	a	1102	CLA	C1C-NC-C4C	-3.90	104.81	107.06
11	b	1222	CLA	C1C-NC-C4C	-3.90	104.81	107.06
11	A	1120	CLA	O2A-CGA-O1A	-3.90	110.21	123.12
11	8	1503	CLA	C1C-NC-C4C	-3.90	104.81	107.06
11	a	1105	CLA	C1C-NC-C4C	-3.89	104.81	107.06
14	a	4007	BCR	C38-C26-C25	-3.89	120.16	124.51
14	2	4017	BCR	C36-C18-C17	-3.89	117.48	122.92
11	2	1227	CLA	C1C-NC-C4C	-3.89	104.82	107.06
11	a	1124	CLA	C1C-NC-C4C	-3.88	104.82	107.06
14	l	4019	BCR	C38-C26-C25	-3.88	120.17	124.51
14	A	4001	BCR	C37-C22-C21	-3.88	117.49	122.92
11	B	1210	CLA	C1C-C2C-C3C	-3.87	102.62	106.92
11	1	1132	CLA	C1C-NC-C4C	-3.87	104.83	107.06
11	A	1124	CLA	C1C-NC-C4C	-3.87	104.83	107.06
14	2	4006	BCR	C34-C9-C10	-3.86	117.51	122.92
11	8	1501	CLA	C1C-NC-C4C	-3.86	104.83	107.06
11	B	1227	CLA	C1C-NC-C4C	-3.86	104.83	107.06
14	a	4003	BCR	C15-C14-C13	-3.86	121.80	127.31
11	A	1115	CLA	O2A-CGA-O1A	-3.86	110.33	123.12
14	2	4011	BCR	C38-C26-C25	-3.85	120.20	124.51
11	b	1217	CLA	C1C-NC-C4C	-3.85	104.84	107.06
11	B	1211	CLA	C1C-NC-C4C	-3.84	104.84	107.06
11	a	1126	CLA	C1C-NC-C4C	-3.84	104.85	107.06
11	a	1111	CLA	C1C-NC-C4C	-3.84	104.85	107.06
11	B	1236	CLA	C1C-NC-C4C	-3.84	104.85	107.06
11	b	1204	CLA	C1C-NC-C4C	-3.83	104.85	107.06
14	f	4018	BCR	C33-C5-C6	-3.83	120.22	124.51
11	B	1235	CLA	C1C-NC-C4C	-3.83	104.85	107.06
14	B	4009	BCR	C38-C26-C25	-3.83	120.22	124.51
11	2	1236	CLA	C1C-NC-C4C	-3.83	104.85	107.06
11	2	1201	CLA	C1C-NC-C4C	-3.82	104.86	107.06
11	B	1217	CLA	C1C-NC-C4C	-3.82	104.86	107.06
14	A	4003	BCR	C15-C14-C13	-3.82	121.86	127.31
11	B	1214	CLA	C1C-NC-C4C	-3.82	104.86	107.06
11	b	1213	CLA	C1C-NC-C4C	-3.82	104.86	107.06
14	a	4007	BCR	C24-C23-C22	-3.82	120.48	126.21
14	l	4019	BCR	C24-C23-C22	-3.82	120.48	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4017	BCR	C15-C14-C13	-3.81	121.87	127.31
11	a	1801	CLA	C1C-NC-C4C	-3.81	104.86	107.06
11	2	1228	CLA	C1-C2-C3	-3.81	120.66	126.68
14	l	4022	BCR	C33-C5-C6	-3.81	120.25	124.51
14	B	4009	BCR	C34-C9-C10	-3.81	117.59	122.92
14	b	4006	BCR	C3-C4-C5	-3.80	107.24	113.78
11	b	1232	CLA	C1C-NC-C4C	-3.80	104.87	107.06
11	a	1106	CLA	C1C-NC-C4C	-3.80	104.87	107.06
11	2	1223	CLA	C1C-NC-C4C	-3.80	104.87	107.06
11	1	1131	CLA	C1C-NC-C4C	-3.80	104.87	107.06
11	1	1128	CLA	C1C-NC-C4C	-3.80	104.87	107.06
14	F	4020	BCR	C38-C26-C25	-3.79	120.26	124.51
11	a	1131	CLA	C1C-NC-C4C	-3.79	104.87	107.06
14	f	4020	BCR	C24-C23-C22	-3.79	120.52	126.21
14	b	4009	BCR	C37-C22-C21	-3.79	117.61	122.92
11	1	1022	CLA	C1C-NC-C4C	-3.79	104.88	107.06
11	b	1229	CLA	C1C-NC-C4C	-3.79	104.88	107.06
11	1	1125	CLA	C1C-NC-C4C	-3.79	104.88	107.06
11	1	1112	CLA	C1C-NC-C4C	-3.79	104.88	107.06
11	a	1120	CLA	O2A-CGA-O1A	-3.79	110.57	123.12
14	B	4006	BCR	C38-C26-C25	-3.78	120.27	124.51
14	A	4008	BCR	C36-C18-C17	-3.78	117.62	122.92
14	a	4003	BCR	C38-C26-C25	-3.78	120.28	124.51
14	2	4009	BCR	C38-C26-C25	-3.78	120.28	124.51
14	2	4014	BCR	C30-C25-C26	-3.78	117.28	122.59
11	a	1119	CLA	C1C-NC-C4C	-3.78	104.88	107.06
11	B	1239	CLA	C1C-NC-C4C	-3.77	104.88	107.06
11	A	1108	CLA	C1C-NC-C4C	-3.77	104.89	107.06
11	2	1239	CLA	O2A-CGA-O1A	-3.77	110.63	123.12
11	1	1116	CLA	C1C-NC-C4C	-3.77	104.89	107.06
11	A	1022	CLA	OBD-CAD-C3D	-3.77	121.08	128.03
11	2	1228	CLA	C1C-NC-C4C	-3.76	104.89	107.06
14	2	4010	BCR	C33-C5-C6	-3.76	120.30	124.51
11	2	1219	CLA	C1C-NC-C4C	-3.76	104.89	107.06
11	A	1105	CLA	C1C-NC-C4C	-3.76	104.89	107.06
14	f	4020	BCR	C38-C26-C25	-3.76	120.30	124.51
14	1	4001	BCR	C1-C6-C5	-3.76	117.31	122.59
11	8	1502	CLA	O2A-CGA-O1A	-3.76	110.68	123.12
11	a	1022	CLA	OBD-CAD-C3D	-3.76	121.11	128.03
11	2	1225	CLA	C1C-NC-C4C	-3.75	104.90	107.06
14	B	4009	BCR	C15-C14-C13	-3.75	121.97	127.31
14	B	4014	BCR	C15-C14-C13	-3.74	121.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1102	CLA	C1C-NC-C4C	-3.74	104.90	107.06
14	8	4019	BCR	C38-C26-C25	-3.74	120.32	124.51
14	F	4018	BCR	C15-C14-C13	-3.74	121.98	127.31
11	2	1229	CLA	C1C-NC-C4C	-3.73	104.91	107.06
11	1	1114	CLA	C1C-NC-C4C	-3.73	104.91	107.06
11	2	1203	CLA	C1C-NC-C4C	-3.73	104.91	107.06
11	B	1203	CLA	C1C-NC-C4C	-3.73	104.91	107.06
11	A	1011	CLA	C1C-NC-C4C	-3.73	104.91	107.06
11	1	1120	CLA	O2A-CGA-O1A	-3.73	110.78	123.12
11	b	1240	CLA	C1C-NC-C4C	-3.73	104.91	107.06
11	A	1133	CLA	O2A-CGA-O1A	-3.72	110.79	123.12
11	1	1139	CLA	C1C-NC-C4C	-3.72	104.92	107.06
14	1	4003	BCR	C3-C4-C5	-3.72	107.39	113.78
11	2	1238	CLA	C1C-NC-C4C	-3.72	104.92	107.06
11	b	1238	CLA	C1C-NC-C4C	-3.71	104.92	107.06
11	1	1022	CLA	OBD-CAD-C3D	-3.71	121.19	128.03
11	A	1121	CLA	O2A-CGA-O1A	-3.71	110.83	123.12
11	2	1205	CLA	C1C-NC-C4C	-3.71	104.92	107.06
14	B	4017	BCR	C7-C8-C9	-3.71	120.64	126.21
11	a	1134	CLA	O2A-CGA-O1A	-3.70	110.85	123.12
11	a	1121	CLA	O2A-CGA-O1A	-3.70	110.86	123.12
11	b	1214	CLA	C1C-NC-C4C	-3.69	104.93	107.06
14	7	4021	BCR	C24-C23-C22	-3.69	120.67	126.21
11	a	1130	CLA	O2A-CGA-O1A	-3.69	110.89	123.12
11	a	1107	CLA	CAA-C2A-C3A	-3.68	102.71	112.81
14	6	4013	BCR	C37-C22-C21	-3.68	117.76	122.92
11	b	1210	CLA	C1C-NC-C4C	-3.68	104.94	107.06
11	B	1239	CLA	O2A-CGA-O1A	-3.68	110.92	123.12
11	A	1139	CLA	C1C-NC-C4C	-3.68	104.94	107.06
14	1	4001	BCR	C37-C22-C21	-3.68	117.77	122.92
14	B	4009	BCR	C7-C8-C9	-3.68	120.69	126.21
11	1	1106	CLA	C1C-NC-C4C	-3.68	104.94	107.06
11	A	1128	CLA	C1C-NC-C4C	-3.68	104.94	107.06
11	a	1134	CLA	C1C-NC-C4C	-3.67	104.94	107.06
14	1	4007	BCR	C15-C14-C13	-3.67	122.07	127.31
11	2	1220	CLA	O2A-CGA-O1A	-3.67	110.97	123.12
14	a	4008	BCR	C38-C26-C25	-3.67	120.40	124.51
14	2	4017	BCR	C34-C9-C10	-3.67	117.79	122.92
14	6	4020	BCR	C15-C14-C13	-3.66	122.08	127.31
14	B	4004	BCR	C38-C26-C25	-3.66	120.41	124.51
11	a	1133	CLA	O2A-CGA-O1A	-3.66	110.99	123.12
11	1	1124	CLA	C1C-NC-C4C	-3.66	104.95	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1212	CLA	C1C-NC-C4C	-3.66	104.95	107.06
11	1	1134	CLA	O2A-CGA-O1A	-3.66	111.00	123.12
14	F	4018	BCR	C38-C26-C25	-3.65	120.42	124.51
11	2	1235	CLA	C1C-NC-C4C	-3.65	104.95	107.06
11	1	1104	CLA	C1C-NC-C4C	-3.65	104.95	107.06
14	1	4007	BCR	C7-C8-C9	-3.65	120.72	126.21
11	1	1136	CLA	C1C-NC-C4C	-3.65	104.96	107.06
11	b	1215	CLA	C1C-NC-C4C	-3.65	104.96	107.06
11	A	1135	CLA	C1C-NC-C4C	-3.65	104.96	107.06
14	b	4014	BCR	C36-C18-C17	-3.65	117.82	122.92
14	B	4011	BCR	C33-C5-C6	-3.64	120.43	124.51
14	B	4006	BCR	C3-C4-C5	-3.64	107.52	113.78
14	B	4017	BCR	C1-C6-C5	-3.64	117.47	122.59
14	1	4008	BCR	C7-C8-C9	-3.64	120.74	126.21
11	B	1210	CLA	C1C-NC-C4C	-3.64	104.96	107.06
14	2	4009	BCR	C24-C23-C22	-3.64	120.75	126.21
11	1	1136	CLA	O2A-CGA-O1A	-3.64	111.07	123.12
11	a	1115	CLA	C1C-NC-C4C	-3.64	104.96	107.06
11	1	1133	CLA	O2A-CGA-O1A	-3.63	111.08	123.12
11	b	1209	CLA	C1C-NC-C4C	-3.63	104.97	107.06
14	b	4011	BCR	C38-C26-C25	-3.63	120.44	124.51
14	6	4020	BCR	C38-C26-C25	-3.63	120.44	124.51
11	B	1204	CLA	C1C-NC-C4C	-3.63	104.97	107.06
14	a	4001	BCR	C33-C5-C6	-3.63	120.44	124.51
11	1	1119	CLA	C1C-NC-C4C	-3.63	104.97	107.06
11	a	1114	CLA	O2A-CGA-O1A	-3.63	111.10	123.12
14	2	4004	BCR	C38-C26-C25	-3.63	120.45	124.51
11	1	1103	CLA	C1C-NC-C4C	-3.62	104.97	107.06
11	b	1235	CLA	C1C-NC-C4C	-3.62	104.97	107.06
14	b	4014	BCR	C33-C5-C6	-3.61	120.46	124.51
14	M	4021	BCR	C38-C26-C25	-3.61	120.46	124.51
11	a	1136	CLA	O2A-CGA-O1A	-3.61	111.15	123.12
11	B	1220	CLA	O2A-CGA-O1A	-3.61	111.15	123.12
14	B	4005	BCR	C33-C5-C6	-3.61	120.47	124.51
11	A	1121	CLA	C1C-NC-C4C	-3.61	104.98	107.06
14	m	4021	BCR	C36-C18-C17	-3.61	117.87	122.92
14	B	4010	BCR	C37-C22-C21	-3.61	117.87	122.92
11	b	1228	CLA	C1C-NC-C4C	-3.61	104.98	107.06
11	B	1201	CLA	C1C-NC-C4C	-3.61	104.98	107.06
14	2	4009	BCR	C33-C5-C6	-3.61	120.47	124.51
11	b	1218	CLA	C1C-NC-C4C	-3.61	104.98	107.06
11	1	1117	CLA	C1C-NC-C4C	-3.60	104.98	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1129	CLA	O2A-CGA-O1A	-3.60	111.18	123.12
14	1	4003	BCR	C33-C5-C6	-3.60	120.48	124.51
11	B	1216	CLA	C1C-NC-C4C	-3.59	104.99	107.06
14	2	4005	BCR	C33-C5-C6	-3.59	120.49	124.51
14	a	4001	BCR	C37-C22-C21	-3.59	117.90	122.92
11	1	1237	CLA	C1-C2-C3	-3.59	119.35	125.96
11	a	1138	CLA	O2A-CGA-O1A	-3.59	111.24	123.12
11	b	1239	CLA	O2A-CGA-O1A	-3.59	111.24	123.12
11	a	1129	CLA	O2A-CGA-O1A	-3.59	111.24	123.12
14	A	4002	BCR	C7-C8-C9	-3.58	120.83	126.21
14	b	4017	BCR	C27-C26-C25	-3.58	117.48	122.74
11	2	1204	CLA	C1C-NC-C4C	-3.57	105.00	107.06
11	a	1128	CLA	C1C-NC-C4C	-3.57	105.00	107.06
14	F	4018	BCR	C33-C5-C6	-3.57	120.51	124.51
11	2	1214	CLA	C1C-NC-C4C	-3.57	105.00	107.06
11	a	1116	CLA	C1C-NC-C4C	-3.57	105.00	107.06
11	A	1138	CLA	O2A-CGA-O1A	-3.57	111.31	123.12
14	b	4011	BCR	C33-C5-C6	-3.57	120.52	124.51
11	A	1136	CLA	O2A-CGA-O1A	-3.56	111.33	123.12
14	8	4022	BCR	C33-C5-C6	-3.56	120.53	124.51
14	B	4014	BCR	C36-C18-C17	-3.56	117.94	122.92
11	b	1220	CLA	O2A-CGA-O1A	-3.56	111.34	123.12
11	A	1114	CLA	O2A-CGA-O1A	-3.55	111.35	123.12
11	A	1106	CLA	C1C-NC-C4C	-3.55	105.01	107.06
14	a	4008	BCR	C34-C9-C10	-3.55	117.95	122.92
14	A	4003	BCR	C33-C5-C6	-3.55	120.53	124.51
14	B	4011	BCR	C24-C23-C22	-3.55	120.88	126.21
11	1	1138	CLA	O2A-CGA-O1A	-3.55	111.37	123.12
11	B	1238	CLA	C1C-NC-C4C	-3.55	105.02	107.06
14	b	4005	BCR	C15-C14-C13	-3.55	122.25	127.31
14	B	4014	BCR	C37-C22-C21	-3.54	117.96	122.92
14	2	4011	BCR	C33-C5-C6	-3.54	120.54	124.51
11	1	1140	CLA	C1-C2-C3	-3.54	119.43	125.96
11	A	1112	CLA	C1C-NC-C4C	-3.54	105.02	107.06
14	B	4010	BCR	C38-C26-C25	-3.54	120.55	124.51
15	A	5003	LHG	C5-O7-C7	-3.54	109.52	117.88
11	A	1134	CLA	O2A-CGA-O1A	-3.54	111.40	123.12
11	K	1402	CLA	C1C-NC-C4C	-3.54	105.02	107.06
11	1	1130	CLA	O2A-CGA-O1A	-3.53	111.41	123.12
14	a	4003	BCR	C33-C5-C6	-3.53	120.55	124.51
11	1	1127	CLA	C1C-NC-C4C	-3.53	105.02	107.06
11	a	1117	CLA	C1C-NC-C4C	-3.53	105.03	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4003	BCR	C38-C26-C25	-3.53	120.56	124.51
11	2	1208	CLA	C1C-NC-C4C	-3.52	105.03	107.06
14	b	4009	BCR	C24-C23-C22	-3.52	120.92	126.21
11	1	1105	CLA	C1C-NC-C4C	-3.52	105.03	107.06
14	b	4005	BCR	C33-C5-C6	-3.52	120.57	124.51
14	b	4009	BCR	C33-C5-C6	-3.51	120.58	124.51
11	1	1114	CLA	O2A-CGA-O1A	-3.51	111.49	123.12
14	L	4019	BCR	C34-C9-C10	-3.51	118.01	122.92
11	1	1011	CLA	O2D-CGD-O1D	-3.51	116.77	123.82
14	b	4005	BCR	C38-C26-C25	-3.51	120.58	124.51
11	A	1012	CLA	OBD-CAD-C3D	-3.50	121.57	128.03
14	B	4004	BCR	C15-C14-C13	-3.50	122.32	127.31
11	A	1130	CLA	O2A-CGA-O1A	-3.50	111.54	123.12
11	b	1231	CLA	C1C-NC-C4C	-3.49	105.05	107.06
11	b	1211	CLA	O2A-CGA-O1A	-3.49	111.55	123.12
14	M	4021	BCR	C34-C9-C10	-3.49	118.03	122.92
11	b	1201	CLA	C1C-NC-C4C	-3.49	105.05	107.06
11	1	1129	CLA	O2A-CGA-O1A	-3.49	111.57	123.12
11	a	1104	CLA	C1C-NC-C4C	-3.48	105.05	107.06
11	l	1502	CLA	O2A-CGA-O1A	-3.48	111.58	123.12
11	b	1236	CLA	C1C-NC-C4C	-3.48	105.05	107.06
14	b	4004	BCR	C38-C26-C25	-3.48	120.61	124.51
14	b	4004	BCR	C15-C14-C13	-3.48	122.34	127.31
14	L	4019	BCR	C38-C26-C25	-3.48	120.61	124.51
11	1	1115	CLA	O2A-CGA-O1A	-3.47	111.61	123.12
11	L	1502	CLA	O2A-CGA-O1A	-3.47	111.63	123.12
14	a	4008	BCR	C7-C8-C9	-3.47	121.00	126.21
14	2	4017	BCR	C1-C6-C5	-3.47	117.72	122.59
11	2	1211	CLA	O2A-CGA-O1A	-3.47	111.63	123.12
11	a	1132	CLA	C1C-NC-C4C	-3.46	105.06	107.06
14	M	4021	BCR	C36-C18-C17	-3.46	118.07	122.92
11	a	1118	CLA	C1C-NC-C4C	-3.46	105.06	107.06
11	2	1205	CLA	O1D-CGD-CBD	-3.46	118.39	124.60
14	2	4006	BCR	C3-C4-C5	-3.46	107.84	113.78
14	b	4006	BCR	C1-C6-C5	-3.46	117.73	122.59
11	1	1130	CLA	C1C-NC-C4C	-3.46	105.07	107.06
14	b	4009	BCR	C15-C14-C13	-3.45	122.38	127.31
14	2	4004	BCR	C37-C22-C21	-3.45	118.09	122.92
11	A	1125	CLA	OBD-CAD-C3D	-3.45	121.67	128.03
14	B	4017	BCR	C34-C9-C10	-3.45	118.09	122.92
11	B	1211	CLA	O2A-CGA-O1A	-3.45	111.70	123.12
14	B	4009	BCR	C33-C5-C6	-3.45	120.65	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4006	BCR	C34-C9-C10	-3.44	118.10	122.92
11	k	1402	CLA	C1C-NC-C4C	-3.44	105.08	107.06
14	2	4006	BCR	C4-C5-C6	-3.44	117.69	122.74
11	1	1118	CLA	C1C-NC-C4C	-3.44	105.08	107.06
14	6	4018	BCR	C27-C26-C25	-3.44	117.70	122.74
11	0	1402	CLA	C1C-NC-C4C	-3.44	105.08	107.06
11	1	1126	CLA	C1C-NC-C4C	-3.42	105.08	107.06
14	2	4014	BCR	C27-C26-C25	-3.42	117.71	122.74
14	A	4002	BCR	C34-C9-C10	-3.42	118.13	122.92
14	B	4009	BCR	C24-C23-C22	-3.42	121.07	126.21
11	B	1228	CLA	C1C-NC-C4C	-3.41	105.09	107.06
14	a	4008	BCR	C33-C5-C6	-3.40	120.70	124.51
11	a	1130	CLA	C1C-NC-C4C	-3.40	105.10	107.06
14	a	4002	BCR	C37-C22-C21	-3.40	118.17	122.92
11	b	1228	CLA	C1-C2-C3	-3.40	121.31	126.68
11	k	1402	CLA	C1-C2-C3	-3.39	121.33	126.68
14	a	4001	BCR	C36-C18-C17	-3.39	118.18	122.92
11	B	1218	CLA	C1C-NC-C4C	-3.38	105.11	107.06
11	2	1021	CLA	C1-C2-C3	-3.38	119.73	125.96
11	B	1208	CLA	C1C-NC-C4C	-3.38	105.11	107.06
11	A	1107	CLA	CAA-C2A-C3A	-3.37	103.56	112.81
14	A	4003	BCR	C30-C25-C26	-3.37	117.85	122.59
14	B	4017	BCR	C27-C26-C25	-3.37	117.79	122.74
11	b	1202	CLA	C1C-NC-C4C	-3.36	105.12	107.06
14	f	4013	BCR	C37-C22-C21	-3.36	118.21	122.92
14	1	4001	BCR	C36-C18-C17	-3.36	118.21	122.92
11	b	1013	CLA	C1C-NC-C4C	-3.36	105.12	107.06
14	b	4017	BCR	C1-C6-C5	-3.35	117.88	122.59
14	8	4022	BCR	C38-C26-C25	-3.35	120.76	124.51
14	b	4004	BCR	C30-C25-C26	-3.35	117.89	122.59
11	A	1119	CLA	C1C-NC-C4C	-3.34	105.13	107.06
14	6	4018	BCR	C34-C9-C10	-3.34	118.25	122.92
11	A	1103	CLA	C1-C2-C3	-3.34	119.81	125.96
14	2	4009	BCR	C3-C4-C5	-3.34	108.04	113.78
11	2	1202	CLA	C1C-NC-C4C	-3.33	105.14	107.06
11	A	1115	CLA	C1C-NC-C4C	-3.33	105.14	107.06
14	B	4006	BCR	C4-C5-C6	-3.33	117.85	122.74
11	a	1112	CLA	C1C-NC-C4C	-3.32	105.14	107.06
11	2	1231	CLA	C1C-NC-C4C	-3.32	105.14	107.06
14	m	4021	BCR	C38-C26-C25	-3.32	120.79	124.51
11	A	1022	CLA	C1C-NC-C4C	-3.32	105.15	107.06
14	b	4006	BCR	C33-C5-C6	-3.32	120.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4004	BCR	C34-C9-C10	-3.32	118.28	122.92
11	A	1111	CLA	C1C-NC-C4C	-3.32	105.15	107.06
11	a	1138	CLA	C1C-NC-C4C	-3.31	105.15	107.06
14	b	4006	BCR	C34-C9-C10	-3.31	118.28	122.92
11	A	1104	CLA	C1-C2-C3	-3.31	119.87	125.96
14	b	4006	BCR	C4-C5-C6	-3.30	117.89	122.74
14	2	4011	BCR	C28-C27-C26	-3.30	108.11	113.78
14	1	4001	BCR	C33-C5-C6	-3.30	120.82	124.51
14	2	4010	BCR	C36-C18-C17	-3.29	118.31	122.92
14	b	4011	BCR	C28-C27-C26	-3.29	108.13	113.78
11	1	1109	CLA	C1C-NC-C4C	-3.28	105.17	107.06
14	b	4009	BCR	C34-C9-C10	-3.28	118.32	122.92
11	2	1236	CLA	O2D-CGD-O1D	-3.28	117.23	123.82
14	a	4007	BCR	C7-C8-C9	-3.27	121.30	126.21
14	m	4021	BCR	C37-C22-C21	-3.27	118.34	122.92
14	A	4003	BCR	C34-C9-C10	-3.27	118.35	122.92
11	1	1138	CLA	C1C-NC-C4C	-3.26	105.18	107.06
14	2	4004	BCR	C7-C8-C9	-3.26	121.31	126.21
14	F	4013	BCR	C36-C18-C17	-3.25	118.37	122.92
14	B	4014	BCR	C30-C25-C26	-3.25	118.02	122.59
14	L	4022	BCR	C34-C9-C10	-3.25	118.37	122.92
14	2	4006	BCR	C23-C24-C25	-3.24	118.18	127.25
11	B	1205	CLA	O1D-CGD-CBD	-3.24	118.78	124.60
11	A	1104	CLA	C1C-NC-C4C	-3.24	105.19	107.06
14	6	4020	BCR	C28-C27-C26	-3.23	108.22	113.78
14	A	4001	BCR	C30-C25-C26	-3.23	118.05	122.59
11	2	1013	CLA	C1C-NC-C4C	-3.23	105.20	107.06
14	1	4001	BCR	C35-C13-C14	-3.23	118.40	122.92
11	B	1013	CLA	C1C-NC-C4C	-3.23	105.20	107.06
14	A	4001	BCR	C4-C5-C6	-3.22	118.01	122.74
11	A	1120	CLA	C1C-NC-C4C	-3.21	105.21	107.06
14	L	4022	BCR	C37-C22-C21	-3.21	118.43	122.92
11	a	1109	CLA	C1C-NC-C4C	-3.21	105.21	107.06
14	b	4009	BCR	C7-C8-C9	-3.20	121.40	126.21
11	A	1124	CLA	C1-C2-C3	-3.19	120.08	125.96
14	b	4014	BCR	C30-C25-C26	-3.18	118.12	122.59
11	A	1135	CLA	C1-C2-C3	-3.17	120.11	125.96
14	A	4008	BCR	C27-C26-C25	-3.17	118.08	122.74
11	a	1124	CLA	C1-C2-C3	-3.17	120.11	125.96
14	b	4014	BCR	C38-C26-C25	-3.17	120.96	124.51
11	1	1111	CLA	C1C-NC-C4C	-3.17	105.23	107.06
11	a	1012	CLA	OBD-CAD-C3D	-3.17	122.19	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4010	BCR	C23-C24-C25	-3.16	118.40	127.25
14	A	4008	BCR	C35-C13-C14	-3.16	118.50	122.92
14	2	4004	BCR	C30-C25-C26	-3.16	118.16	122.59
14	f	4020	BCR	C36-C18-C17	-3.16	118.50	122.92
11	A	1125	CLA	O2D-CGD-O1D	-3.15	117.47	123.82
14	2	4004	BCR	C24-C23-C22	-3.15	121.48	126.21
11	1	1137	CLA	C4-C3-C2	-3.15	115.28	123.69
11	A	1139	CLA	C1-C2-C3	-3.15	121.70	126.68
14	1	4008	BCR	C24-C23-C22	-3.15	121.48	126.21
14	2	4009	BCR	C1-C6-C5	-3.14	118.17	122.59
14	B	4009	BCR	C37-C22-C21	-3.13	118.53	122.92
11	A	1138	CLA	C1C-NC-C4C	-3.13	105.25	107.06
14	B	4017	BCR	C15-C14-C13	-3.13	122.84	127.31
14	1	4008	BCR	C30-C25-C26	-3.13	118.19	122.59
14	B	4010	BCR	C36-C18-C17	-3.13	118.54	122.92
11	2	1231	CLA	CMA-C3A-C4A	-3.13	103.36	111.77
15	A	5001	LHG	C5-O7-C7	-3.13	110.49	117.88
14	B	4004	BCR	C30-C25-C26	-3.13	118.20	122.59
11	b	1202	CLA	O2D-CGD-O1D	-3.12	117.54	123.82
14	2	4004	BCR	C36-C18-C17	-3.12	118.55	122.92
11	2	1213	CLA	O1D-CGD-CBD	-3.12	119.00	124.60
11	a	1127	CLA	C1-C2-C3	-3.11	120.22	125.96
11	B	1222	CLA	C4-C3-C2	-3.11	115.39	123.69
14	b	4004	BCR	C34-C9-C10	-3.11	118.57	122.92
14	l	4022	BCR	C7-C8-C9	-3.11	121.54	126.21
14	A	4008	BCR	C38-C26-C25	-3.11	121.03	124.51
11	2	1234	CLA	C1-C2-C3	-3.10	120.24	125.96
11	A	1110	CLA	O1D-CGD-CBD	-3.10	119.04	124.60
11	2	1202	CLA	C1-C2-C3	-3.09	120.26	125.96
11	A	1118	CLA	C1C-NC-C4C	-3.09	105.28	107.06
11	A	1127	CLA	OBD-CAD-CBD	-3.09	121.28	125.94
11	A	1111	CLA	C1-C2-C3	-3.09	120.27	125.96
11	2	1210	CLA	C1-C2-C3	-3.09	120.27	125.96
14	F	4020	BCR	C23-C24-C25	-3.08	118.62	127.25
14	8	4022	BCR	C37-C22-C21	-3.08	118.60	122.92
11	1	1124	CLA	C1-C2-C3	-3.08	120.28	125.96
14	6	4020	BCR	C27-C26-C25	-3.08	118.22	122.74
14	L	4022	BCR	C3-C4-C5	-3.07	108.50	113.78
11	B	1205	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
11	A	1110	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
11	a	1137	CLA	C4-C3-C2	-3.07	115.50	123.69
11	a	1103	CLA	C11-C12-C13	-3.07	105.66	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4008	BCR	C27-C26-C25	-3.07	118.24	122.74
14	b	4010	BCR	C28-C27-C26	-3.07	108.51	113.78
14	M	4021	BCR	C37-C22-C21	-3.07	118.63	122.92
14	B	4005	BCR	C36-C18-C17	-3.06	118.63	122.92
11	A	1132	CLA	O2D-CGD-O1D	-3.06	117.66	123.82
11	A	1140	CLA	C1-C2-C3	-3.06	120.32	125.96
11	a	1107	CLA	C4-C3-C2	-3.06	115.53	123.69
11	B	1221	CLA	O1D-CGD-CBD	-3.06	119.11	124.60
14	F	4020	BCR	C24-C23-C22	-3.06	121.62	126.21
14	b	4017	BCR	C4-C5-C6	-3.06	118.25	122.74
14	2	4017	BCR	C27-C26-C25	-3.05	118.26	122.74
11	1	1110	CLA	O2D-CGD-O1D	-3.05	117.68	123.82
11	B	1202	CLA	C1C-NC-C4C	-3.05	105.30	107.06
14	b	4017	BCR	C36-C18-C17	-3.05	118.65	122.92
11	b	1221	CLA	O2D-CGD-O1D	-3.05	117.68	123.82
11	A	1126	CLA	C1C-NC-C4C	-3.05	105.30	107.06
14	F	4020	BCR	C36-C18-C17	-3.04	118.66	122.92
11	a	1106	CLA	O1D-CGD-CBD	-3.04	119.15	124.60
14	A	4002	BCR	C31-C1-C6	-3.03	105.39	110.31
11	B	1206	CLA	OBD-CAD-C3D	-3.03	122.44	128.03
14	1	4003	BCR	C36-C18-C17	-3.03	118.67	122.92
14	1	4002	BCR	C3-C4-C5	-3.03	108.57	113.78
14	b	4006	BCR	C37-C22-C21	-3.03	118.68	122.92
14	2	4011	BCR	C37-C22-C21	-3.02	118.69	122.92
14	B	4004	BCR	C24-C23-C22	-3.02	121.67	126.21
14	B	4006	BCR	C23-C24-C25	-3.02	118.79	127.25
14	B	4011	BCR	C38-C26-C25	-3.02	121.13	124.51
14	2	4006	BCR	C36-C18-C17	-3.02	118.69	122.92
15	B	5004	LHG	C5-O7-C7	-3.02	110.74	117.88
11	2	1218	CLA	C1C-NC-C4C	-3.02	105.32	107.06
11	B	1221	CLA	O2D-CGD-O1D	-3.02	117.74	123.82
11	a	1106	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
14	7	4021	BCR	C37-C22-C21	-3.01	118.71	122.92
14	1	4003	BCR	C30-C25-C26	-3.00	118.37	122.59
11	8	1501	CLA	O2D-CGD-O1D	-3.00	117.78	123.82
14	B	4014	BCR	C38-C26-C25	-3.00	121.15	124.51
14	A	4002	BCR	C37-C22-C21	-3.00	118.72	122.92
11	B	1236	CLA	OBD-CAD-C3D	-3.00	122.50	128.03
14	a	4008	BCR	C1-C6-C5	-3.00	118.38	122.59
14	1	4008	BCR	C23-C24-C25	-2.99	118.87	127.25
11	b	1234	CLA	C1-C2-C3	-2.99	120.44	125.96
11	1	1137	CLA	O2D-CGD-O1D	-2.99	117.80	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	4022	BCR	C34-C9-C10	-2.99	118.74	122.92
11	A	1126	CLA	O1D-CGD-CBD	-2.99	119.24	124.60
11	A	1012	CLA	C1-C2-C3	-2.98	120.46	125.96
14	B	4014	BCR	C3-C4-C5	-2.98	108.65	113.78
14	7	4021	BCR	C36-C18-C17	-2.98	118.74	122.92
14	2	4010	BCR	C34-C9-C10	-2.98	118.75	122.92
14	2	4017	BCR	C7-C8-C9	-2.98	121.73	126.21
14	b	4005	BCR	C36-C18-C17	-2.98	118.75	122.92
14	2	4006	BCR	C33-C5-C6	-2.98	121.17	124.51
14	f	4018	BCR	C38-C26-C25	-2.97	121.18	124.51
14	1	4001	BCR	C38-C26-C25	-2.96	121.19	124.51
11	2	1205	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
14	b	4004	BCR	C24-C23-C22	-2.96	121.77	126.21
14	B	4005	BCR	C27-C26-C25	-2.95	118.41	122.74
11	a	1012	CLA	O2D-CGD-O1D	-2.95	117.89	123.82
14	B	4011	BCR	C37-C22-C21	-2.95	118.80	122.92
14	B	4011	BCR	C27-C26-C25	-2.94	118.42	122.74
14	b	4017	BCR	C30-C25-C26	-2.94	118.46	122.59
11	b	1210	CLA	C1-C2-C3	-2.94	120.54	125.96
14	2	4017	BCR	C33-C5-C6	-2.94	121.22	124.51
11	2	1217	CLA	O2D-CGD-O1D	-2.94	117.90	123.82
11	B	1222	CLA	O1D-CGD-CBD	-2.94	119.32	124.60
14	1	4008	BCR	C38-C26-C25	-2.94	121.22	124.51
14	1	4003	BCR	C38-C26-C25	-2.94	121.22	124.51
11	1	1103	CLA	C1-C2-C3	-2.93	120.55	125.96
14	6	4018	BCR	C37-C22-C21	-2.93	118.81	122.92
14	a	4001	BCR	C15-C14-C13	-2.93	123.13	127.31
11	1	1110	CLA	O1D-CGD-CBD	-2.93	119.34	124.60
15	1	5001	LHG	C5-O7-C7	-2.93	110.96	117.88
14	B	4006	BCR	C36-C18-C17	-2.92	118.83	122.92
14	B	4006	BCR	C15-C14-C13	-2.92	123.14	127.31
14	2	4014	BCR	C3-C4-C5	-2.92	108.76	113.78
11	A	1132	CLA	O1D-CGD-CBD	-2.92	119.35	124.60
14	A	4003	BCR	C36-C18-C17	-2.92	118.84	122.92
14	A	4008	BCR	C30-C25-C26	-2.91	118.50	122.59
11	B	1214	CLA	C1-C2-C3	-2.91	120.60	125.96
11	B	1201	CLA	O2D-CGD-O1D	-2.90	117.98	123.82
14	B	4010	BCR	C15-C14-C13	-2.90	123.17	127.31
11	A	1137	CLA	C4-C3-C2	-2.90	115.95	123.69
14	a	4001	BCR	C1-C6-C5	-2.90	118.52	122.59
14	a	4002	BCR	C3-C4-C5	-2.89	108.80	113.78
11	B	1201	CLA	O1D-CGD-CBD	-2.89	119.41	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1103	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
14	B	4004	BCR	C37-C22-C21	-2.88	118.89	122.92
14	b	4010	BCR	C24-C23-C22	-2.88	121.89	126.21
14	b	4004	BCR	C3-C4-C5	-2.88	108.83	113.78
11	B	1214	CLA	O2D-CGD-O1D	-2.87	118.04	123.82
14	A	4001	BCR	C7-C8-C9	-2.87	121.89	126.21
14	A	4008	BCR	C3-C4-C5	-2.87	108.84	113.78
14	F	4020	BCR	C28-C27-C26	-2.87	108.85	113.78
14	8	4019	BCR	C28-C27-C26	-2.87	108.85	113.78
11	A	1117	CLA	C1C-NC-C4C	-2.87	105.41	107.06
14	b	4014	BCR	C37-C22-C21	-2.87	118.91	122.92
14	6	4013	BCR	C15-C14-C13	-2.87	123.22	127.31
14	F	4020	BCR	C34-C9-C10	-2.86	118.92	122.92
11	1	1126	CLA	O1D-CGD-CBD	-2.86	119.47	124.60
14	b	4005	BCR	C37-C22-C21	-2.86	118.92	122.92
11	1	1123	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
11	a	1129	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
16	2	5002	LMG	C8-O7-C10	-2.85	111.14	117.88
11	B	1224	CLA	O1D-CGD-CBD	-2.85	119.48	124.60
11	B	1215	CLA	C4-C3-C2	-2.85	116.08	123.69
14	2	4009	BCR	C34-C9-C10	-2.85	118.93	122.92
11	B	1227	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
14	b	4004	BCR	C36-C18-C17	-2.84	118.94	122.92
11	B	1226	CLA	O2D-CGD-O1D	-2.84	118.10	123.82
11	8	1501	CLA	C1-C2-C3	-2.84	120.73	125.96
14	a	4008	BCR	C4-C5-C6	-2.84	118.57	122.74
11	2	1211	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
14	b	4005	BCR	C30-C25-C26	-2.83	118.61	122.59
11	B	1226	CLA	O1D-CGD-CBD	-2.83	119.52	124.60
14	b	4011	BCR	C37-C22-C21	-2.83	118.96	122.92
14	2	4005	BCR	C36-C18-C17	-2.83	118.96	122.92
14	2	4004	BCR	C3-C4-C5	-2.82	108.92	113.78
11	1	1137	CLA	O1D-CGD-CBD	-2.82	119.54	124.60
14	a	4003	BCR	C36-C18-C17	-2.82	118.98	122.92
11	b	1222	CLA	O1D-CGD-CBD	-2.81	119.55	124.60
14	F	4013	BCR	C37-C22-C21	-2.81	118.98	122.92
11	L	1502	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
11	2	1226	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
11	1	1115	CLA	OBD-CAD-C3D	-2.81	122.84	128.03
11	a	1137	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
11	b	1221	CLA	O1D-CGD-CBD	-2.81	119.56	124.60
11	a	1135	CLA	C1-C2-C3	-2.81	120.78	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	8	4019	BCR	C36-C18-C17	-2.81	118.99	122.92
11	a	1126	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
11	B	1222	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
11	8	1502	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
14	M	4021	BCR	C24-C23-C22	-2.80	122.00	126.21
11	1	1123	CLA	O1D-CGD-CBD	-2.80	119.57	124.60
11	1	1129	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
11	a	1138	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
14	b	4011	BCR	C24-C23-C22	-2.80	122.00	126.21
14	a	4001	BCR	C7-C8-C9	-2.79	122.01	126.21
14	B	4010	BCR	C30-C25-C26	-2.79	118.67	122.59
14	a	4003	BCR	C30-C25-C26	-2.79	118.67	122.59
14	l	4019	BCR	C36-C18-C17	-2.79	119.02	122.92
14	B	4006	BCR	C37-C22-C21	-2.78	119.03	122.92
11	A	1012	CLA	O2D-CGD-O1D	-2.78	118.22	123.82
11	1	1011	CLA	CHA-C1A-NA	-2.78	119.72	126.18
11	b	1222	CLA	O2D-CGD-O1D	-2.78	118.23	123.82
11	2	1226	CLA	O1D-CGD-CBD	-2.78	119.61	124.60
11	B	1207	CLA	O2D-CGD-O1D	-2.78	118.23	123.82
14	2	4009	BCR	C36-C18-C17	-2.78	119.03	122.92
14	8	4022	BCR	C3-C4-C5	-2.78	109.01	113.78
11	2	1224	CLA	C1-C2-C3	-2.77	120.84	125.96
11	b	1227	CLA	O1D-CGD-CBD	-2.77	119.62	124.60
14	b	4006	BCR	C23-C24-C25	-2.77	119.48	127.25
14	a	4001	BCR	C38-C26-C25	-2.77	121.40	124.51
11	A	1103	CLA	C1C-NC-C4C	-2.77	105.46	107.06
11	B	1227	CLA	O1D-CGD-CBD	-2.77	119.63	124.60
14	b	4014	BCR	C3-C4-C5	-2.77	109.02	113.78
14	2	4011	BCR	C24-C23-C22	-2.77	122.06	126.21
14	2	4017	BCR	C15-C14-C13	-2.77	123.36	127.31
14	B	4004	BCR	C36-C18-C17	-2.76	119.05	122.92
11	B	1231	CLA	O1D-CGD-CBD	-2.76	119.64	124.60
11	A	1116	CLA	O1D-CGD-CBD	-2.76	119.64	124.60
11	A	1127	CLA	OBD-CAD-C3D	-2.76	122.94	128.03
14	2	4011	BCR	C23-C24-C25	-2.76	119.52	127.25
11	a	1126	CLA	C1-C2-C3	-2.76	120.87	125.96
14	A	4002	BCR	C15-C14-C13	-2.76	123.37	127.31
11	b	1236	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
14	A	4007	BCR	C3-C4-C5	-2.76	109.04	113.78
11	2	1222	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
14	m	4021	BCR	C27-C26-C25	-2.76	118.69	122.74
14	f	4018	BCR	C34-C9-C10	-2.76	119.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1023	CLA	C1-C2-C3	-2.75	120.89	125.96
14	6	4020	BCR	C23-C24-C25	-2.75	119.55	127.25
11	A	1126	CLA	C1-C2-C3	-2.75	120.89	125.96
11	a	1801	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
11	B	1209	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
11	2	1214	CLA	C1-C2-C3	-2.75	120.90	125.96
11	A	1118	CLA	CBC-CAC-C3C	-2.75	104.62	112.41
14	f	4018	BCR	C36-C18-C17	-2.74	119.09	122.92
11	B	1214	CLA	O1D-CGD-CBD	-2.74	119.68	124.60
14	6	4013	BCR	C36-C18-C17	-2.74	119.09	122.92
14	a	4007	BCR	C28-C27-C26	-2.74	109.08	113.78
14	b	4004	BCR	C37-C22-C21	-2.73	119.10	122.92
11	1	1127	CLA	C1-C2-C3	-2.73	120.94	125.96
11	1	1116	CLA	O1D-CGD-CBD	-2.73	119.71	124.60
11	l	1502	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
14	B	4005	BCR	C15-C14-C13	-2.71	123.44	127.31
11	1	1012	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
11	b	1227	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
14	1	4007	BCR	C37-C22-C21	-2.71	119.13	122.92
14	1	4002	BCR	C31-C1-C6	-2.71	105.91	110.31
11	1	1011	CLA	CAA-C2A-C3A	-2.71	105.39	112.81
14	B	4011	BCR	C36-C18-C17	-2.71	119.13	122.92
14	a	4001	BCR	C30-C25-C26	-2.70	118.79	122.59
11	a	1123	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
11	a	1125	CLA	C1-C2-C3	-2.70	120.98	125.96
14	8	4022	BCR	C27-C26-C25	-2.70	118.78	122.74
14	2	4005	BCR	C38-C26-C25	-2.70	121.48	124.51
14	m	4021	BCR	C15-C14-C13	-2.70	123.46	127.31
14	b	4006	BCR	C15-C14-C13	-2.70	123.46	127.31
14	b	4010	BCR	C23-C24-C25	-2.69	119.71	127.25
14	a	4008	BCR	C36-C18-C17	-2.69	119.15	122.92
14	a	4007	BCR	C36-C18-C17	-2.69	119.15	122.92
11	2	1224	CLA	O2D-CGD-O1D	-2.69	118.40	123.82
14	7	4021	BCR	C34-C9-C10	-2.69	119.15	122.92
11	2	1215	CLA	C4-C3-C2	-2.69	116.51	123.69
14	a	4003	BCR	C34-C9-C10	-2.69	119.15	122.92
11	1	1125	CLA	O2D-CGD-O1D	-2.69	118.41	123.82
14	a	4008	BCR	C30-C25-C26	-2.69	118.82	122.59
14	B	4014	BCR	C27-C26-C25	-2.68	118.80	122.74
14	f	4020	BCR	C3-C4-C5	-2.68	109.17	113.78
14	1	4001	BCR	C34-C9-C10	-2.68	119.17	122.92
14	B	4017	BCR	C36-C18-C17	-2.68	119.17	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1131	CLA	O1D-CGD-CBD	-2.68	119.79	124.60
11	A	1107	CLA	C4-C3-C2	-2.67	116.56	123.69
11	a	1116	CLA	O1D-CGD-CBD	-2.67	119.80	124.60
11	1	1012	CLA	OBD-CAD-C3D	-2.67	123.10	128.03
14	2	4006	BCR	C24-C23-C22	-2.67	122.20	126.21
11	1	1120	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
11	b	1215	CLA	C4-C3-C2	-2.67	116.57	123.69
11	1	1112	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
11	b	1211	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
11	A	1103	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
14	1	4008	BCR	C3-C4-C5	-2.67	109.20	113.78
11	2	1204	CLA	C1-C2-C3	-2.66	121.05	125.96
11	B	1205	CLA	C1-C2-C3	-2.66	121.06	125.96
14	B	4005	BCR	C3-C4-C5	-2.66	109.21	113.78
14	l	4019	BCR	C7-C8-C9	-2.66	122.22	126.21
11	A	1137	CLA	OBD-CAD-C3D	-2.66	123.13	128.03
14	B	4017	BCR	C4-C5-C6	-2.65	118.84	122.74
14	m	4021	BCR	C34-C9-C10	-2.65	119.21	122.92
14	2	4009	BCR	C23-C24-C25	-2.65	119.84	127.25
11	l	1501	CLA	O2D-CGD-O1D	-2.65	118.50	123.82
11	A	1118	CLA	O2D-CGD-O1D	-2.65	118.50	123.82
11	A	1107	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
11	A	1128	CLA	C1-C2-C3	-2.64	121.09	125.96
14	L	4019	BCR	C36-C18-C17	-2.64	119.22	122.92
11	b	1222	CLA	C4-C3-C2	-2.64	116.65	123.69
11	2	1214	CLA	CAA-CBA-CGA	-2.64	105.40	113.35
11	1	1120	CLA	O1D-CGD-CBD	-2.64	119.86	124.60
11	b	1230	CLA	O2D-CGD-O1D	-2.64	118.52	123.82
11	A	1012	CLA	O1D-CGD-CBD	-2.64	119.87	124.60
14	6	4020	BCR	C36-C18-C17	-2.63	119.23	122.92
11	B	1013	CLA	O2D-CGD-O1D	-2.63	118.52	123.82
11	B	1223	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
11	2	1238	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
14	A	4007	BCR	C15-C14-C13	-2.63	123.56	127.31
14	A	4007	BCR	C36-C18-C17	-2.63	119.25	122.92
11	1	1134	CLA	O2D-CGD-O1D	-2.62	118.54	123.82
14	6	4018	BCR	C36-C18-C17	-2.62	119.25	122.92
11	b	1215	CLA	O2D-CGD-O1D	-2.62	118.54	123.82
14	A	4001	BCR	C27-C26-C25	-2.62	118.89	122.74
11	2	1223	CLA	C1-C2-C3	-2.62	121.13	125.96
11	a	1133	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
14	B	4017	BCR	C30-C25-C26	-2.62	118.91	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4005	BCR	C37-C22-C21	-2.62	119.26	122.92
11	a	1136	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
11	B	1204	CLA	O1D-CGD-CBD	-2.62	119.90	124.60
11	a	1132	CLA	C1-C2-C3	-2.62	121.14	125.96
11	b	1226	CLA	O2D-CGD-O1D	-2.62	118.56	123.82
14	6	4018	BCR	C30-C25-C26	-2.61	118.92	122.59
11	A	1801	CLA	C1-C2-C3	-2.61	121.14	125.96
11	b	1209	CLA	O2D-CGD-O1D	-2.61	118.56	123.82
11	2	1204	CLA	O1D-CGD-CBD	-2.61	119.91	124.60
11	2	1210	CLA	O1D-CGD-CBD	-2.61	119.91	124.60
14	1	4007	BCR	C28-C27-C26	-2.61	109.29	113.78
14	1	4003	BCR	C34-C9-C10	-2.61	119.27	122.92
11	A	1109	CLA	C1C-NC-C4C	-2.61	105.56	107.06
11	b	1226	CLA	O1D-CGD-CBD	-2.61	119.92	124.60
14	8	4019	BCR	C34-C9-C10	-2.61	119.27	122.92
11	A	1122	CLA	O2D-CGD-O1D	-2.60	118.58	123.82
14	1	4002	BCR	C34-C9-C10	-2.60	119.28	122.92
11	B	1224	CLA	C1-C2-C3	-2.60	121.17	125.96
11	a	1138	CLA	O1D-CGD-CBD	-2.60	119.93	124.60
11	b	1213	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
11	2	1216	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
14	a	4008	BCR	C27-C26-C25	-2.60	118.93	122.74
11	2	1223	CLA	OBD-CAD-C3D	-2.60	123.24	128.03
14	f	4020	BCR	C34-C9-C10	-2.60	119.29	122.92
11	b	1224	CLA	O2D-CGD-O1D	-2.59	118.60	123.82
11	B	1202	CLA	O2D-CGD-O1D	-2.59	118.60	123.82
11	a	1137	CLA	O1D-CGD-CBD	-2.59	119.94	124.60
11	B	1229	CLA	C1-C2-C3	-2.59	121.18	125.96
14	2	4011	BCR	C36-C18-C17	-2.59	119.29	122.92
11	1	1115	CLA	O2D-CGD-O1D	-2.59	118.61	123.82
11	A	1125	CLA	O1D-CGD-CBD	-2.59	119.95	124.60
14	B	4006	BCR	C33-C5-C6	-2.59	121.61	124.51
14	1	4007	BCR	C34-C9-C10	-2.59	119.30	122.92
11	B	1228	CLA	O2D-CGD-O1D	-2.59	118.62	123.82
11	b	1213	CLA	C4-C3-C2	-2.58	116.79	123.69
11	2	1221	CLA	O2D-CGD-O1D	-2.58	118.62	123.82
11	2	1227	CLA	O2D-CGD-O1D	-2.58	118.62	123.82
11	1	1129	CLA	O1D-CGD-CBD	-2.58	119.96	124.60
11	B	1219	CLA	C1-C2-C3	-2.58	121.20	125.96
15	b	5004	LHG	C5-O7-C7	-2.58	111.78	117.88
11	B	1206	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
11	1	1022	CLA	O1D-CGD-CBD	-2.58	119.97	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1101	CLA	C1-C2-C3	-2.58	121.20	125.96
11	b	1205	CLA	C1-C2-C3	-2.58	121.21	125.96
14	f	4018	BCR	C37-C22-C21	-2.58	119.31	122.92
14	a	4007	BCR	C3-C4-C5	-2.58	109.35	113.78
11	b	1232	CLA	O2D-CGD-O1D	-2.58	118.63	123.82
11	A	1137	CLA	O2D-CGD-O1D	-2.58	118.63	123.82
11	a	1140	CLA	O2D-CGD-O1D	-2.58	118.64	123.82
11	B	1210	CLA	C1-C2-C3	-2.57	121.22	125.96
11	l	1503	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
14	6	4020	BCR	C3-C4-C5	-2.57	109.36	113.78
11	a	1120	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
11	2	1230	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
11	k	1401	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
11	2	1231	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
11	0	1401	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
11	2	1209	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
11	a	1110	CLA	O2D-CGD-O1D	-2.56	118.66	123.82
14	b	4005	BCR	C3-C4-C5	-2.56	109.37	113.78
14	b	4004	BCR	C27-C26-C25	-2.56	118.98	122.74
14	2	4010	BCR	C3-C4-C5	-2.56	109.38	113.78
11	A	1104	CLA	O1D-CGD-CBD	-2.56	120.00	124.60
11	a	1124	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
14	B	4004	BCR	C34-C9-C10	-2.56	119.34	122.92
11	L	1502	CLA	O1D-CGD-CBD	-2.56	120.00	124.60
14	B	4010	BCR	C3-C4-C5	-2.56	109.38	113.78
11	K	1401	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
14	f	4020	BCR	C28-C27-C26	-2.56	109.38	113.78
11	A	1104	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
15	a	5003	LHG	C5-O7-C7	-2.56	111.83	117.88
11	2	1213	CLA	O2D-CGD-O1D	-2.56	118.68	123.82
11	B	1235	CLA	O2D-CGD-O1D	-2.56	118.68	123.82
14	b	4011	BCR	C23-C24-C25	-2.55	120.10	127.25
11	2	1225	CLA	CMD-C2D-C3D	-2.55	120.16	124.89
11	1	1126	CLA	C1-C2-C3	-2.55	121.25	125.96
11	B	1223	CLA	O1D-CGD-CBD	-2.55	120.02	124.60
11	1	1101	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
11	a	1112	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
14	B	4017	BCR	C33-C5-C6	-2.55	121.66	124.51
11	a	1119	CLA	C1-C2-C3	-2.55	121.26	125.96
14	B	4017	BCR	C23-C24-C25	-2.55	120.12	127.25
11	B	1212	CLA	O2D-CGD-O1D	-2.55	118.70	123.82
11	1	1132	CLA	O2D-CGD-O1D	-2.54	118.70	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1101	CLA	C4-C3-C2	-2.54	116.90	123.69
11	B	1228	CLA	C1-C2-C3	-2.54	122.66	126.68
11	2	1215	CLA	O2D-CGD-O1D	-2.54	118.70	123.82
14	A	4007	BCR	C37-C22-C21	-2.54	119.36	122.92
11	b	1230	CLA	O1D-CGD-CBD	-2.54	120.04	124.60
14	1	4002	BCR	C30-C25-C26	-2.54	119.02	122.59
11	l	1502	CLA	O1D-CGD-CBD	-2.54	120.05	124.60
14	a	4001	BCR	C27-C26-C25	-2.54	119.02	122.74
11	2	1218	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
11	A	1106	CLA	O1D-CGD-CBD	-2.53	120.05	124.60
11	A	1117	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
11	a	1136	CLA	O1D-CGD-CBD	-2.53	120.05	124.60
14	b	4017	BCR	C33-C5-C6	-2.53	121.67	124.51
14	M	4021	BCR	C23-C24-C25	-2.53	120.17	127.25
11	2	1201	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
11	2	1023	CLA	OBD-CAD-C3D	-2.53	123.37	128.03
11	a	1126	CLA	O1D-CGD-CBD	-2.53	120.06	124.60
11	A	1112	CLA	O1D-CGD-CBD	-2.53	120.06	124.60
14	b	4011	BCR	C27-C26-C25	-2.53	119.03	122.74
11	a	1135	CLA	O2D-CGD-O1D	-2.53	118.74	123.82
11	A	1131	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
11	b	1228	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
11	A	1106	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
11	b	1239	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
11	b	1214	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
11	2	1214	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
11	1	1801	CLA	O2D-CGD-O1D	-2.52	118.76	123.82
11	L	1503	CLA	O1D-CGD-CBD	-2.52	120.08	124.60
11	A	1111	CLA	O2D-CGD-O1D	-2.51	118.76	123.82
14	f	4018	BCR	C32-C1-C6	-2.51	106.23	110.31
14	l	4022	BCR	C3-C4-C5	-2.51	109.46	113.78
14	a	4003	BCR	C4-C5-C6	-2.51	119.06	122.74
14	f	4018	BCR	C4-C5-C6	-2.51	119.06	122.74
11	a	1105	CLA	O2D-CGD-O1D	-2.51	118.77	123.82
14	L	4019	BCR	C7-C6-C5	-2.51	115.56	121.54
11	a	1131	CLA	C1-C2-C3	-2.51	121.33	125.96
11	1	1130	CLA	O2D-CGD-O1D	-2.51	118.78	123.82
11	2	1215	CLA	O1D-CGD-CBD	-2.50	120.10	124.60
11	b	1216	CLA	C1-C2-C3	-2.50	121.35	125.96
11	1	1107	CLA	C4-C3-C2	-2.50	117.02	123.69
11	B	1234	CLA	C1-C2-C3	-2.50	121.35	125.96
14	1	4001	BCR	C30-C25-C26	-2.50	119.08	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4002	BCR	C30-C25-C26	-2.50	119.08	122.59
14	b	4011	BCR	C15-C14-C13	-2.50	123.75	127.31
11	B	1204	CLA	CBC-CAC-C3C	-2.50	105.33	112.41
11	2	1222	CLA	O1D-CGD-CBD	-2.50	120.12	124.60
14	b	4005	BCR	C8-C7-C6	-2.50	120.27	127.25
11	A	1112	CLA	O2D-CGD-O1D	-2.50	118.80	123.82
14	B	4011	BCR	C23-C24-C25	-2.49	120.27	127.25
11	a	1122	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
11	b	1235	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
11	B	1238	CLA	O2D-CGD-O1D	-2.49	118.81	123.82
14	b	4009	BCR	C3-C4-C5	-2.49	109.50	113.78
14	A	4001	BCR	C38-C26-C25	-2.49	121.72	124.51
11	2	1225	CLA	O1D-CGD-CBD	-2.49	120.13	124.60
14	1	4008	BCR	C1-C6-C5	-2.49	119.09	122.59
14	8	4022	BCR	C7-C8-C9	-2.49	122.47	126.21
11	b	1214	CLA	C1-C2-C3	-2.49	121.37	125.96
14	F	4018	BCR	C37-C22-C21	-2.49	119.44	122.92
11	a	1127	CLA	OBD-CAD-C3D	-2.49	123.44	128.03
14	f	4020	BCR	C23-C24-C25	-2.49	120.29	127.25
11	1	1118	CLA	O2D-CGD-O1D	-2.49	118.82	123.82
11	A	1102	CLA	O2D-CGD-O1D	-2.49	118.82	123.82
11	2	1218	CLA	O1D-CGD-CBD	-2.49	120.14	124.60
11	A	1102	CLA	O1D-CGD-CBD	-2.49	120.14	124.60
11	2	1231	CLA	O1D-CGD-CBD	-2.49	120.14	124.60
11	A	1133	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
11	b	1208	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
11	b	1203	CLA	O2D-CGD-O1D	-2.48	118.83	123.82
11	A	1101	CLA	C6-C5-C3	-2.48	107.04	112.66
11	1	1114	CLA	O2D-CGD-O1D	-2.48	118.83	123.82
14	B	4010	BCR	C23-C24-C25	-2.48	120.32	127.25
11	b	1201	CLA	C1-C2-C3	-2.48	121.39	125.96
11	a	1125	CLA	C6-C5-C3	-2.48	110.18	114.55
11	2	1221	CLA	O1D-CGD-CBD	-2.47	120.16	124.60
14	B	4005	BCR	C34-C9-C10	-2.47	119.46	122.92
11	b	1223	CLA	C1-C2-C3	-2.47	121.40	125.96
14	l	4022	BCR	C29-C30-C25	-2.47	106.61	110.48
11	b	1021	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
11	a	1133	CLA	O1D-CGD-CBD	-2.47	120.16	124.60
15	1	5003	LHG	C5-O7-C7	-2.47	112.04	117.88
11	B	1218	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
14	l	4022	BCR	C36-C18-C17	-2.47	119.46	122.92
11	l	1501	CLA	O1D-CGD-CBD	-2.47	120.17	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	4018	BCR	C32-C1-C6	-2.47	106.31	110.31
11	1	1101	CLA	O1D-CGD-CBD	-2.47	120.17	124.60
14	B	4004	BCR	C3-C4-C5	-2.47	109.54	113.78
11	1	1107	CLA	O2D-CGD-O1D	-2.47	118.86	123.82
14	b	4010	BCR	C34-C9-C10	-2.47	119.47	122.92
11	a	1124	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
11	a	1103	CLA	C1-C2-C3	-2.46	121.42	125.96
11	b	1204	CLA	O2D-CGD-O1D	-2.46	118.86	123.82
11	B	1021	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
11	2	1207	CLA	OBD-CAD-C3D	-2.46	123.49	128.03
11	1	1111	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
11	A	1136	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
14	A	4001	BCR	C3-C4-C5	-2.46	109.55	113.78
11	a	1116	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
11	B	1239	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
11	1	1125	CLA	O1D-CGD-CBD	-2.46	120.19	124.60
14	6	4018	BCR	C8-C7-C6	-2.46	120.38	127.25
11	B	1223	CLA	O2D-CGD-O1D	-2.46	118.88	123.82
11	2	1021	CLA	O2D-CGD-O1D	-2.46	118.88	123.82
11	1	1801	CLA	O1D-CGD-CBD	-2.45	120.19	124.60
15	a	5001	LHG	C5-O7-C7	-2.45	112.08	117.88
11	1	1135	CLA	O2D-CGD-O1D	-2.45	118.88	123.82
11	1	1136	CLA	O2D-CGD-O1D	-2.45	118.88	123.82
11	B	1236	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
11	b	1021	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
11	B	1213	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
11	1	1111	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
11	a	1101	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
14	2	4006	BCR	C37-C22-C21	-2.45	119.49	122.92
11	B	1207	CLA	O1D-CGD-CBD	-2.45	120.20	124.60
11	2	1023	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
14	8	4022	BCR	C36-C18-C17	-2.45	119.50	122.92
11	2	1235	CLA	O2D-CGD-O1D	-2.45	118.90	123.82
11	1	1131	CLA	O1D-CGD-CBD	-2.44	120.21	124.60
14	b	4010	BCR	C3-C4-C5	-2.44	109.58	113.78
11	A	1123	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
11	2	1207	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
14	b	4011	BCR	C1-C6-C5	-2.44	119.16	122.59
14	a	4008	BCR	C8-C7-C6	-2.44	120.41	127.25
14	A	4008	BCR	C23-C24-C25	-2.44	120.42	127.25
11	1	1104	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
14	1	4007	BCR	C3-C4-C5	-2.44	109.58	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1230	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
14	a	4007	BCR	C15-C14-C13	-2.44	123.83	127.31
11	B	1231	CLA	O2D-CGD-O1D	-2.44	118.92	123.82
11	2	1203	CLA	CBC-CAC-C3C	-2.44	105.49	112.41
11	1	1117	CLA	C1-C2-C3	-2.44	121.47	125.96
11	1	1140	CLA	O2D-CGD-O1D	-2.44	118.92	123.82
11	2	1227	CLA	O1D-CGD-CBD	-2.43	120.23	124.60
11	2	1229	CLA	O2D-CGD-O1D	-2.43	118.92	123.82
14	6	4018	BCR	C28-C27-C26	-2.43	109.60	113.78
14	B	4004	BCR	C27-C26-C25	-2.43	119.17	122.74
14	2	4017	BCR	C23-C24-C25	-2.43	120.45	127.25
11	b	1240	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
11	a	1104	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
11	a	1132	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
11	a	1130	CLA	O1D-CGD-CBD	-2.43	120.25	124.60
11	a	1118	CLA	O2D-CGD-O1D	-2.42	118.94	123.82
14	B	4011	BCR	C32-C1-C6	-2.42	106.38	110.31
11	a	1103	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
11	L	1503	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
11	b	1205	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
11	1	1117	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
14	a	4008	BCR	C37-C22-C21	-2.42	119.53	122.92
11	a	1130	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
11	b	1212	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
11	2	1225	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
11	2	1224	CLA	O1D-CGD-CBD	-2.42	120.26	124.60
11	2	1210	CLA	O2D-CGD-O1D	-2.41	118.96	123.82
11	a	1119	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
11	a	1131	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
14	l	4019	BCR	C28-C27-C26	-2.41	109.64	113.78
14	8	4019	BCR	C35-C13-C14	-2.41	119.55	122.92
11	1	1112	CLA	O1D-CGD-CBD	-2.41	120.27	124.60
11	a	1140	CLA	C1-C2-C3	-2.41	121.52	125.96
11	2	1204	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
11	A	1110	CLA	C1-C2-C3	-2.41	121.52	125.96
11	a	1115	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
11	a	1117	CLA	C1-C2-C3	-2.40	121.53	125.96
11	A	1130	CLA	O2D-CGD-O1D	-2.40	118.98	123.82
14	B	4017	BCR	C3-C4-C5	-2.40	109.65	113.78
14	1	4007	BCR	C36-C18-C17	-2.40	119.56	122.92
11	2	1223	CLA	O1D-CGD-CBD	-2.40	120.28	124.60
11	1	1110	CLA	C1-C2-C3	-2.40	121.53	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1105	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
11	B	1208	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
11	a	1123	CLA	C1-C2-C3	-2.40	121.54	125.96
11	A	1140	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
11	a	1107	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
11	A	1120	CLA	OBD-CAD-C3D	-2.40	123.61	128.03
11	a	1110	CLA	O1D-CGD-CBD	-2.39	120.30	124.60
11	A	1801	CLA	O2D-CGD-O1D	-2.39	119.00	123.82
11	A	1125	CLA	C6-C5-C3	-2.39	110.33	114.55
14	2	4011	BCR	C32-C1-C6	-2.39	106.43	110.31
14	2	4017	BCR	C30-C25-C26	-2.39	119.23	122.59
14	1	4003	BCR	C8-C7-C6	-2.39	120.56	127.25
11	1	1131	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
11	a	1132	CLA	O1D-CGD-CBD	-2.39	120.31	124.60
11	A	1132	CLA	C1-C2-C3	-2.39	121.56	125.96
14	B	4017	BCR	C37-C22-C21	-2.39	119.58	122.92
11	2	1239	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
11	b	1205	CLA	O1D-CGD-CBD	-2.39	120.31	124.60
14	b	4014	BCR	C27-C26-C25	-2.38	119.24	122.74
11	1	1128	CLA	O2D-CGD-O1D	-2.38	119.02	123.82
14	2	4005	BCR	C37-C22-C21	-2.38	119.59	122.92
11	a	1111	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
11	1	1135	CLA	O1D-CGD-CBD	-2.38	120.33	124.60
11	b	1218	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
14	F	4018	BCR	C32-C1-C6	-2.38	106.45	110.31
11	A	1124	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
11	8	1502	CLA	O1D-CGD-CBD	-2.38	120.33	124.60
11	A	1115	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
11	B	1023	CLA	OBD-CAD-C3D	-2.38	123.65	128.03
11	B	1215	CLA	O2D-CGD-O1D	-2.38	119.04	123.82
11	1	1119	CLA	O1D-CGD-CBD	-2.38	120.33	124.60
11	8	1503	CLA	O2D-CGD-O1D	-2.38	119.04	123.82
14	a	4007	BCR	C23-C24-C25	-2.38	120.60	127.25
14	2	4017	BCR	C4-C5-C6	-2.37	119.25	122.74
11	B	1204	CLA	O2D-CGD-O1D	-2.37	119.04	123.82
11	b	1204	CLA	C1-C2-C3	-2.37	121.58	125.96
11	b	1225	CLA	O2D-CGD-O1D	-2.37	119.04	123.82
11	A	1121	CLA	CMD-C2D-C3D	-2.37	120.49	124.89
11	1	1134	CLA	O1D-CGD-CBD	-2.37	120.34	124.60
11	2	1206	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
14	2	4004	BCR	C15-C14-C13	-2.37	123.93	127.31
11	b	1201	CLA	O2D-CGD-O1D	-2.37	119.05	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1224	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
11	A	1126	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
14	f	4020	BCR	C37-C22-C21	-2.37	119.61	122.92
14	1	4007	BCR	C35-C13-C14	-2.37	119.61	122.92
11	a	1120	CLA	O1D-CGD-CBD	-2.37	120.35	124.60
11	B	1230	CLA	O1D-CGD-CBD	-2.37	120.35	124.60
11	8	1501	CLA	O1D-CGD-CBD	-2.36	120.36	124.60
11	1	1125	CLA	C1-C2-C3	-2.36	121.61	125.96
11	1	1118	CLA	OBD-CAD-C3D	-2.36	123.68	128.03
11	a	1104	CLA	O1D-CGD-CBD	-2.36	120.36	124.60
11	b	1214	CLA	O1D-CGD-CBD	-2.36	120.37	124.60
14	A	4001	BCR	C34-C9-C10	-2.36	119.62	122.92
11	1	1012	CLA	O1D-CGD-CBD	-2.36	120.37	124.60
14	2	4010	BCR	C30-C25-C26	-2.36	119.28	122.59
11	b	1201	CLA	O1D-CGD-CBD	-2.35	120.37	124.60
11	1	1133	CLA	O2D-CGD-O1D	-2.35	119.08	123.82
11	b	1239	CLA	O1D-CGD-CBD	-2.35	120.37	124.60
11	A	1118	CLA	C1-C2-C3	-2.35	121.62	125.96
11	B	1232	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
11	1	1118	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
11	b	1211	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
14	B	4005	BCR	C30-C25-C26	-2.35	119.29	122.59
11	1	1109	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
11	2	1228	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
11	b	1216	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
11	A	1128	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
11	a	1118	CLA	OBD-CAD-C3D	-2.35	123.70	128.03
14	a	4007	BCR	C37-C22-C21	-2.35	119.63	122.92
11	1	1139	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
11	a	1128	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
11	2	1217	CLA	OBD-CAD-C3D	-2.35	123.70	128.03
11	a	1110	CLA	C1-C2-C3	-2.34	121.64	125.96
14	b	4009	BCR	C1-C6-C5	-2.34	119.30	122.59
14	8	4022	BCR	C23-C24-C25	-2.34	120.69	127.25
11	b	1218	CLA	O1D-CGD-CBD	-2.34	120.39	124.60
11	1	1122	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
14	2	4014	BCR	C34-C9-C10	-2.34	119.64	122.92
14	B	4005	BCR	C38-C26-C25	-2.34	121.89	124.51
14	f	4018	BCR	C8-C7-C6	-2.34	120.70	127.25
14	B	4014	BCR	C35-C13-C14	-2.34	119.64	122.92
11	1	1105	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
11	B	1215	CLA	O1D-CGD-CBD	-2.34	120.40	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1224	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
11	A	1140	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
11	a	1135	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
14	2	4009	BCR	C35-C13-C14	-2.34	119.65	122.92
11	1	1130	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
14	A	4002	BCR	C3-C4-C5	-2.34	109.77	113.78
11	1	1101	CLA	C4-C3-C2	-2.34	117.46	123.69
11	1	1126	CLA	O2D-CGD-O1D	-2.34	119.12	123.82
14	b	4010	BCR	C36-C18-C17	-2.33	119.65	122.92
11	A	1131	CLA	C1-C2-C3	-2.33	121.66	125.96
11	1	1125	CLA	C6-C5-C3	-2.33	110.44	114.55
11	a	1118	CLA	O1D-CGD-CBD	-2.33	120.42	124.60
11	l	1503	CLA	O1D-CGD-CBD	-2.33	120.42	124.60
11	b	1013	CLA	O2D-CGD-O1D	-2.32	119.14	123.82
11	2	1230	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
11	A	1105	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
11	b	1235	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
11	2	1013	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
14	b	4005	BCR	C27-C26-C25	-2.32	119.33	122.74
11	2	1236	CLA	O1D-CGD-CBD	-2.32	120.44	124.60
11	B	1021	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
14	b	4004	BCR	C28-C27-C26	-2.32	109.79	113.78
11	2	1208	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
11	B	1226	CLA	C1-C2-C3	-2.32	121.69	125.96
11	1	1116	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
11	b	1207	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
11	a	1121	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
11	B	1216	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
15	A	5003	LHG	O7-C7-O9	-2.31	117.90	123.68
14	L	4022	BCR	C36-C18-C17	-2.31	119.68	122.92
14	B	4010	BCR	C24-C23-C22	-2.31	122.73	126.21
11	b	1234	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
11	B	1210	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
11	b	1021	CLA	C11-C10-C8	-2.31	108.14	115.73
11	A	1109	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
11	2	1216	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
14	a	4003	BCR	C29-C30-C25	-2.31	106.86	110.48
11	B	1235	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
11	a	1127	CLA	C6-C5-C3	-2.31	107.42	112.66
11	a	1011	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
11	a	1139	CLA	C1-C2-C3	-2.31	123.03	126.68
11	b	1220	CLA	O2D-CGD-O1D	-2.31	119.18	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1238	CLA	O2D-CGD-O1D	-2.30	119.18	123.82
14	8	4022	BCR	C28-C27-C26	-2.30	109.82	113.78
11	1	1237	CLA	CBC-CAC-C3C	-2.30	105.88	112.41
11	A	1136	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
14	2	4005	BCR	C27-C26-C25	-2.30	119.37	122.74
11	a	1138	CLA	CMD-C2D-C3D	-2.30	120.63	124.89
11	a	1113	CLA	O2D-CGD-O1D	-2.30	119.20	123.82
14	A	4002	BCR	C35-C13-C14	-2.30	119.71	122.92
11	a	1131	CLA	O1D-CGD-CBD	-2.30	120.48	124.60
11	a	1111	CLA	C1-C2-C3	-2.30	121.73	125.96
11	a	1139	CLA	O2D-CGD-O1D	-2.29	119.20	123.82
11	b	1206	CLA	OBD-CAD-C3D	-2.29	123.80	128.03
11	1	1104	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
14	a	4003	BCR	C8-C7-C6	-2.29	120.84	127.25
11	k	1402	CLA	O2D-CGD-O1D	-2.29	119.21	123.82
11	b	1204	CLA	O1D-CGD-CBD	-2.29	120.49	124.60
14	1	4001	BCR	C3-C4-C5	-2.29	109.85	113.78
14	F	4020	BCR	C31-C1-C6	-2.29	106.60	110.31
14	A	4002	BCR	C36-C18-C17	-2.29	119.72	122.92
14	F	4013	BCR	C40-C30-C25	-2.28	106.60	110.31
14	2	4009	BCR	C7-C8-C9	-2.28	122.78	126.21
14	L	4019	BCR	C3-C4-C5	-2.28	109.86	113.78
14	a	4008	BCR	C35-C13-C14	-2.28	119.72	122.92
14	a	4001	BCR	C35-C13-C14	-2.28	119.72	122.92
11	a	1106	CLA	C4-C3-C2	-2.28	117.60	123.69
11	2	1219	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
11	b	1216	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
11	A	1138	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
11	1	1109	CLA	C1-C2-C3	-2.28	121.76	125.96
11	a	1127	CLA	O2D-CGD-O1D	-2.28	119.23	123.82
11	2	1013	CLA	C1-C2-C3	-2.28	121.76	125.96
11	A	1012	CLA	C5-C3-C2	-2.28	116.44	121.10
11	1	1132	CLA	C1-C2-C3	-2.27	121.77	125.96
11	a	1102	CLA	O2D-CGD-O1D	-2.27	119.24	123.82
14	B	4017	BCR	C38-C26-C25	-2.27	121.96	124.51
14	F	4018	BCR	C36-C18-C17	-2.27	119.74	122.92
11	2	1223	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
11	1	1139	CLA	OBD-CAD-C3D	-2.27	123.84	128.03
11	B	1211	CLA	O1D-CGD-CBD	-2.27	120.52	124.60
11	b	1210	CLA	O1D-CGD-CBD	-2.27	120.52	124.60
11	b	1217	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
14	2	4004	BCR	C27-C26-C25	-2.27	119.41	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1236	CLA	OBD-CAD-C3D	-2.27	123.85	128.03
14	a	4002	BCR	C15-C14-C13	-2.27	124.08	127.31
11	A	1133	CLA	O1D-CGD-CBD	-2.26	120.54	124.60
14	2	4004	BCR	C28-C27-C26	-2.26	109.90	113.78
16	B	5002	LMG	C8-O7-C10	-2.26	112.54	117.88
14	m	4021	BCR	C23-C24-C25	-2.26	120.94	127.25
11	b	1215	CLA	O1D-CGD-CBD	-2.25	120.55	124.60
11	A	1138	CLA	CBC-CAC-C3C	-2.25	106.01	112.41
11	B	1217	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
15	2	5004	LHG	C5-O7-C7	-2.25	112.55	117.88
11	2	1212	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
14	7	4021	BCR	C23-C24-C25	-2.25	120.95	127.25
14	8	4019	BCR	C37-C22-C21	-2.25	119.77	122.92
14	2	4010	BCR	C35-C13-C14	-2.25	119.77	122.92
11	b	1213	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
11	B	1211	CLA	CMD-C2D-C3D	-2.25	120.72	124.89
11	1	1115	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
11	a	1114	CLA	O2D-CGD-O1D	-2.25	119.30	123.82
11	A	1116	CLA	O2D-CGD-O1D	-2.25	119.30	123.82
11	b	1210	CLA	O2D-CGD-O1D	-2.25	119.30	123.82
14	6	4013	BCR	C30-C25-C26	-2.24	119.44	122.59
14	B	4017	BCR	C28-C27-C26	-2.24	109.92	113.78
11	A	1127	CLA	C1-C2-C3	-2.24	121.82	125.96
12	b	2002	PQN	C11-C12-C13	-2.24	122.96	126.71
11	1	1136	CLA	O1D-CGD-CBD	-2.24	120.57	124.60
11	8	1502	CLA	OBD-CAD-C3D	-2.24	123.89	128.03
11	A	1137	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
11	B	1021	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
11	A	1104	CLA	C6-C5-C3	-2.24	107.58	112.66
11	A	1011	CLA	CHA-C1A-NA	-2.24	120.98	126.18
14	l	4022	BCR	C30-C25-C26	-2.24	119.44	122.59
11	B	1211	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
11	A	1120	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
11	A	1111	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
11	1	1138	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
11	2	1229	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
11	a	1127	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
11	b	1224	CLA	C1-C2-C3	-2.23	121.84	125.96
11	A	1135	CLA	CMA-C3A-C4A	-2.23	105.77	111.77
11	b	1223	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
11	2	1213	CLA	C4-C3-C2	-2.23	117.73	123.69
11	2	1219	CLA	C1-C2-C3	-2.23	121.84	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1131	CLA	OBD-CAD-C3D	-2.23	123.92	128.03
11	1	1127	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
11	a	1112	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
11	8	1503	CLA	O1D-CGD-CBD	-2.23	120.59	124.60
14	B	4010	BCR	C34-C9-C10	-2.23	119.80	122.92
11	b	1208	CLA	O1D-CGD-CBD	-2.23	120.60	124.60
14	B	4005	BCR	C23-C24-C25	-2.23	121.02	127.25
11	1	1119	CLA	O2D-CGD-O1D	-2.23	119.34	123.82
11	b	1203	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
11	A	1134	CLA	O2D-CGD-O1D	-2.22	119.34	123.82
11	a	1011	CLA	C1-C2-C3	-2.22	121.86	125.96
14	B	4009	BCR	C36-C18-C17	-2.22	119.81	122.92
14	l	4019	BCR	C37-C22-C21	-2.22	119.81	122.92
11	1	1108	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
16	B	5002	LMG	O7-C10-O9	-2.22	118.13	123.68
11	b	1219	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
14	B	4009	BCR	C3-C4-C5	-2.22	109.96	113.78
14	2	4009	BCR	C8-C7-C6	-2.22	121.03	127.25
11	a	1117	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
11	a	1126	CLA	C4-C3-C2	-2.22	117.77	123.69
14	a	4001	BCR	C34-C9-C10	-2.22	119.82	122.92
11	A	1123	CLA	OBD-CAD-C3D	-2.22	123.94	128.03
11	b	1238	CLA	O1D-CGD-CBD	-2.22	120.62	124.60
14	B	4011	BCR	C1-C6-C5	-2.22	119.48	122.59
11	1	1801	CLA	C1-C2-C3	-2.22	121.88	125.96
14	b	4017	BCR	C23-C24-C25	-2.21	121.05	127.25
14	L	4019	BCR	C35-C13-C14	-2.21	119.82	122.92
11	A	1127	CLA	O2D-CGD-O1D	-2.21	119.37	123.82
11	B	1239	CLA	O1D-CGD-CBD	-2.21	120.63	124.60
11	a	1129	CLA	O1D-CGD-CBD	-2.21	120.63	124.60
11	A	1130	CLA	O1D-CGD-CBD	-2.20	120.64	124.60
14	l	4019	BCR	C8-C7-C6	-2.20	121.08	127.25
11	B	1218	CLA	O1D-CGD-CBD	-2.20	120.64	124.60
11	a	1117	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
11	A	1129	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
11	1	1107	CLA	O1D-CGD-CBD	-2.20	120.65	124.60
11	A	1122	CLA	O1D-CGD-CBD	-2.20	120.65	124.60
14	f	4013	BCR	C3-C4-C5	-2.20	110.00	113.78
11	1	1121	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
11	2	1023	CLA	C11-C10-C8	-2.20	108.51	115.73
11	B	1214	CLA	OBD-CAD-C3D	-2.20	123.97	128.03
14	A	4008	BCR	C28-C27-C26	-2.20	110.00	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1109	CLA	C1-C2-C3	-2.20	121.91	125.96
11	1	1135	CLA	C1-C2-C3	-2.20	121.91	125.96
11	b	1209	CLA	O1D-CGD-CBD	-2.20	120.66	124.60
14	b	4017	BCR	C37-C22-C21	-2.20	119.85	122.92
11	a	1109	CLA	O2D-CGD-O1D	-2.19	119.40	123.82
14	a	4008	BCR	C3-C4-C5	-2.19	110.01	113.78
11	a	1012	CLA	O1D-CGD-CBD	-2.19	120.66	124.60
14	b	4010	BCR	C35-C13-C14	-2.19	119.85	122.92
11	b	1235	CLA	C11-C10-C8	-2.19	108.54	115.73
11	B	1234	CLA	C6-C7-C8	-2.19	108.54	115.73
14	B	4004	BCR	C28-C27-C26	-2.19	110.01	113.78
11	B	1228	CLA	O1D-CGD-CBD	-2.19	120.67	124.60
11	A	1138	CLA	CMD-C2D-C3D	-2.19	120.83	124.89
11	A	1115	CLA	O1D-CGD-CBD	-2.19	120.67	124.60
14	b	4017	BCR	C3-C4-C5	-2.19	110.02	113.78
14	1	4002	BCR	C37-C22-C21	-2.19	119.86	122.92
14	a	4002	BCR	C36-C18-C17	-2.19	119.86	122.92
11	B	1204	CLA	C1-C2-C3	-2.19	121.93	125.96
11	b	1023	CLA	O2D-CGD-O1D	-2.19	119.42	123.82
16	2	5002	LMG	O7-C10-O9	-2.19	118.22	123.68
11	A	1022	CLA	O2D-CGD-O1D	-2.18	119.42	123.82
16	b	5002	LMG	O7-C10-O9	-2.18	118.23	123.68
11	b	1216	CLA	C6-C7-C8	-2.18	108.56	115.73
11	A	1119	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
11	B	1213	CLA	O1D-CGD-CBD	-2.18	120.68	124.60
14	F	4018	BCR	C8-C7-C6	-2.18	121.14	127.25
14	1	4008	BCR	C36-C18-C17	-2.18	119.87	122.92
11	L	1501	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
11	a	1121	CLA	CMD-C2D-C3D	-2.18	120.85	124.89
14	b	4006	BCR	C8-C7-C6	-2.18	121.15	127.25
11	B	1209	CLA	O1D-CGD-CBD	-2.18	120.69	124.60
14	l	4022	BCR	C1-C6-C5	-2.18	119.53	122.59
14	f	4013	BCR	C40-C30-C25	-2.18	106.78	110.31
14	2	4005	BCR	C30-C25-C26	-2.18	119.53	122.59
11	2	1021	CLA	CHA-C1A-NA	-2.18	121.13	126.18
11	A	1101	CLA	O2D-CGD-O1D	-2.17	119.44	123.82
16	b	5002	LMG	C8-O7-C10	-2.17	112.74	117.88
14	1	4003	BCR	C27-C26-C25	-2.17	119.55	122.74
11	b	1206	CLA	O2D-CGD-O1D	-2.17	119.45	123.82
11	0	1402	CLA	O2D-CGD-O1D	-2.17	119.45	123.82
11	B	1229	CLA	O1D-CGD-CBD	-2.17	120.70	124.60
11	b	1219	CLA	C1-C2-C3	-2.17	121.96	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1122	CLA	C1-C2-C3	-2.17	121.96	125.96
11	2	1214	CLA	O1D-CGD-CBD	-2.17	120.70	124.60
11	B	1215	CLA	C11-C10-C8	-2.17	108.61	115.73
14	a	4007	BCR	C31-C1-C6	-2.17	106.79	110.31
11	1	1113	CLA	O2D-CGD-O1D	-2.17	119.46	123.82
11	2	1202	CLA	CMD-C2D-C3D	-2.17	120.87	124.89
12	B	2002	PQN	C11-C12-C13	-2.17	123.09	126.71
14	2	4011	BCR	C1-C6-C5	-2.17	119.55	122.59
14	8	4022	BCR	C35-C13-C14	-2.17	119.89	122.92
11	b	1021	CLA	C5-C3-C2	-2.16	116.67	121.10
11	B	1229	CLA	O2D-CGD-O1D	-2.16	119.47	123.82
14	a	4008	BCR	C23-C24-C25	-2.16	121.19	127.25
14	B	4006	BCR	C35-C13-C14	-2.16	119.89	122.92
11	B	1219	CLA	O2D-CGD-O1D	-2.16	119.47	123.82
11	b	1228	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
11	B	1232	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
14	2	4004	BCR	C1-C6-C5	-2.16	119.55	122.59
11	a	1128	CLA	C1-C2-C3	-2.16	121.97	125.96
11	b	1212	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
11	B	1212	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
11	2	1222	CLA	C4-C3-C2	-2.16	117.93	123.69
14	1	4008	BCR	C28-C27-C26	-2.16	110.07	113.78
11	2	1240	CLA	O2D-CGD-O1D	-2.16	119.48	123.82
11	1	1128	CLA	C11-C12-C13	-2.16	108.65	115.73
14	A	4001	BCR	C35-C13-C14	-2.16	119.90	122.92
11	2	1239	CLA	O1D-CGD-CBD	-2.16	120.73	124.60
11	b	1225	CLA	O1D-CGD-CBD	-2.15	120.73	124.60
11	2	1210	CLA	C11-C10-C8	-2.15	108.66	115.73
11	A	1123	CLA	CMD-C2D-C3D	-2.15	120.90	124.89
11	a	1105	CLA	O1D-CGD-CBD	-2.15	120.73	124.60
11	B	1210	CLA	C4C-C3C-C2C	-2.15	103.61	106.91
11	1	1118	CLA	CBC-CAC-C3C	-2.15	106.31	112.41
11	A	1119	CLA	C4C-C3C-C2C	-2.15	103.61	106.91
14	8	4022	BCR	C4-C5-C6	-2.15	119.58	122.74
14	a	4001	BCR	C3-C4-C5	-2.15	110.09	113.78
14	1	4001	BCR	C27-C26-C25	-2.15	119.59	122.74
14	2	4017	BCR	C38-C26-C25	-2.15	122.10	124.51
11	a	1128	CLA	C11-C10-C8	-2.15	108.68	115.73
11	2	1212	CLA	O1D-CGD-CBD	-2.15	120.75	124.60
11	a	1125	CLA	O2D-CGD-O1D	-2.15	119.50	123.82
11	A	1117	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
11	K	1402	CLA	C1-C2-C3	-2.14	123.30	126.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4017	BCR	C37-C22-C21	-2.14	119.92	122.92
11	a	1801	CLA	OBD-CAD-C3D	-2.14	124.08	128.03
11	A	1134	CLA	CHC-C1C-C2C	-2.14	120.81	126.65
11	2	1231	CLA	CMD-C2D-C3D	-2.14	120.92	124.89
11	1	1114	CLA	O1D-CGD-CBD	-2.14	120.76	124.60
11	1	1106	CLA	C1-C2-C3	-2.14	122.02	125.96
11	b	1226	CLA	C1-C2-C3	-2.14	122.02	125.96
11	A	1120	CLA	O1D-CGD-CBD	-2.14	120.77	124.60
11	b	1217	CLA	O1D-CGD-CBD	-2.13	120.77	124.60
11	B	1238	CLA	O1D-CGD-CBD	-2.13	120.77	124.60
11	l	1501	CLA	OBD-CAD-C3D	-2.13	124.09	128.03
11	1	1133	CLA	O1D-CGD-CBD	-2.13	120.77	124.60
11	A	1011	CLA	OBD-CAD-C3D	-2.13	124.09	128.03
11	B	1223	CLA	C1-C2-C3	-2.13	122.03	125.96
11	a	1108	CLA	O2D-CGD-O1D	-2.13	119.53	123.82
11	a	1128	CLA	O1D-CGD-CBD	-2.13	120.77	124.60
14	1	4008	BCR	C35-C13-C14	-2.13	119.94	122.92
11	B	1227	CLA	CHC-C1C-C2C	-2.13	120.84	126.65
14	1	4001	BCR	C8-C7-C6	-2.13	121.30	127.25
11	a	1011	CLA	CHA-C1A-NA	-2.13	121.24	126.18
11	b	1240	CLA	O1D-CGD-CBD	-2.13	120.78	124.60
11	A	1108	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
14	l	4019	BCR	C34-C9-C10	-2.12	119.95	122.92
11	b	1206	CLA	CHC-C1C-C2C	-2.12	120.86	126.65
14	L	4022	BCR	C29-C30-C25	-2.12	107.16	110.48
11	B	1236	CLA	O1D-CGD-CBD	-2.12	120.79	124.60
11	K	1402	CLA	O1D-CGD-CBD	-2.12	120.79	124.60
14	B	4017	BCR	C35-C13-C14	-2.12	119.95	122.92
11	A	1113	CLA	O2D-CGD-O1D	-2.12	119.56	123.82
14	6	4018	BCR	C29-C30-C25	-2.12	107.16	110.48
11	A	1120	CLA	CMD-C2D-C3D	-2.12	120.97	124.89
11	2	1202	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
11	1	1128	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
11	1	1104	CLA	C1-C2-C3	-2.11	122.07	125.96
14	2	4005	BCR	C3-C4-C5	-2.11	110.15	113.78
14	A	4008	BCR	C37-C22-C21	-2.11	119.97	122.92
11	1	1012	CLA	C5-C3-C2	-2.11	116.79	121.10
11	1	1124	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
11	a	1101	CLA	O1D-CGD-CBD	-2.11	120.82	124.60
14	F	4020	BCR	C3-C4-C5	-2.10	110.16	113.78
11	A	1121	CLA	O1D-CGD-CBD	-2.10	120.82	124.60
11	1	1140	CLA	C4-C3-C2	-2.10	118.08	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1128	CLA	C1-C2-C3	-2.10	122.08	125.96
11	A	1140	CLA	OBD-CAD-C3D	-2.10	124.15	128.03
11	a	1118	CLA	C1-C2-C3	-2.10	122.09	125.96
11	A	1103	CLA	CMD-C2D-C3D	-2.10	121.00	124.89
11	a	1801	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
11	B	1206	CLA	CHC-C1C-C2C	-2.10	120.93	126.65
14	2	4010	BCR	C1-C6-C5	-2.10	119.65	122.59
11	A	1119	CLA	C1-C2-C3	-2.09	122.10	125.96
14	A	4008	BCR	C1-C6-C5	-2.09	119.65	122.59
11	2	1235	CLA	O1D-CGD-CBD	-2.09	120.84	124.60
11	A	1113	CLA	OBD-CAD-C3D	-2.09	124.17	128.03
11	A	1121	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
14	A	4007	BCR	C34-C9-C10	-2.09	120.00	122.92
11	B	1225	CLA	C6-C5-C3	-2.09	107.92	112.66
14	6	4013	BCR	C24-C25-C26	-2.09	116.56	121.54
11	b	1220	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
11	A	1139	CLA	OBD-CAD-C3D	-2.09	124.18	128.03
11	a	1119	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
11	a	1022	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
11	A	1128	CLA	O1D-CGD-CBD	-2.09	120.85	124.60
11	b	1236	CLA	CMD-C2D-C3D	-2.09	121.02	124.89
14	1	4003	BCR	C35-C13-C14	-2.09	120.00	122.92
15	A	5001	LHG	O7-C7-O9	-2.08	118.48	123.68
11	A	1118	CLA	OBD-CAD-C3D	-2.08	124.19	128.03
14	1	4007	BCR	C23-C24-C25	-2.08	121.42	127.25
11	2	1209	CLA	OBD-CAD-C3D	-2.08	124.19	128.03
11	a	1111	CLA	C11-C10-C8	-2.08	108.90	115.73
11	2	1211	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
11	1	1011	CLA	CHC-C1C-C2C	-2.08	120.98	126.65
11	A	1118	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
14	b	4010	BCR	C37-C22-C21	-2.08	120.01	122.92
11	A	1137	CLA	CAA-CBA-CGA	-2.08	107.09	113.35
11	1	1022	CLA	C11-C10-C8	-2.08	108.91	115.73
14	B	4014	BCR	C31-C1-C6	-2.08	106.94	110.31
14	2	4009	BCR	C4-C5-C6	-2.08	119.69	122.74
14	2	4017	BCR	C35-C13-C14	-2.08	120.02	122.92
11	A	1123	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
11	b	1234	CLA	CHC-C1C-C2C	-2.07	121.00	126.65
11	b	1239	CLA	CHC-C1C-C2C	-2.07	121.00	126.65
14	b	4006	BCR	C28-C27-C26	-2.07	110.22	113.78
11	A	1138	CLA	O1D-CGD-CBD	-2.07	120.88	124.60
14	A	4007	BCR	C8-C7-C6	-2.07	121.46	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1133	CLA	CHC-C1C-C2C	-2.07	121.01	126.65
11	1	1137	CLA	OBD-CAD-C3D	-2.07	124.22	128.03
14	b	4009	BCR	C35-C13-C14	-2.07	120.03	122.92
11	b	1202	CLA	C1-C2-C3	-2.07	122.15	125.96
14	1	4007	BCR	C31-C1-C6	-2.07	106.96	110.31
11	b	1021	CLA	O1D-CGD-CBD	-2.06	120.89	124.60
11	1	1106	CLA	O1D-CGD-CBD	-2.06	120.90	124.60
11	B	1231	CLA	CHC-C1C-C2C	-2.06	121.03	126.65
11	b	1229	CLA	O2D-CGD-O1D	-2.06	119.68	123.82
14	b	4005	BCR	C28-C27-C26	-2.06	110.25	113.78
11	2	1206	CLA	O1D-CGD-CBD	-2.06	120.91	124.60
11	b	1231	CLA	O1D-CGD-CBD	-2.05	120.91	124.60
14	B	4004	BCR	C23-C24-C25	-2.05	121.50	127.25
11	B	1232	CLA	CHC-C1C-C2C	-2.05	121.05	126.65
14	8	4022	BCR	C30-C25-C26	-2.05	119.71	122.59
14	L	4022	BCR	C23-C24-C25	-2.05	121.52	127.25
11	A	1801	CLA	C4C-C3C-C2C	-2.05	103.77	106.91
11	B	1021	CLA	CHA-C1A-NA	-2.05	121.42	126.18
12	a	2001	PQN	C2M-C2-C3	-2.05	120.05	124.20
14	1	4003	BCR	C24-C25-C26	-2.05	116.66	121.54
11	a	1140	CLA	O1D-CGD-CBD	-2.05	120.93	124.60
15	B	5004	LHG	O7-C7-O9	-2.04	118.58	123.68
14	b	4005	BCR	C7-C8-C9	-2.04	123.14	126.21
12	b	2002	PQN	C2M-C2-C3	-2.04	120.06	124.20
11	1	1139	CLA	O1D-CGD-CBD	-2.04	120.93	124.60
11	1	1133	CLA	CHC-C1C-C2C	-2.04	121.08	126.65
14	b	4010	BCR	C1-C6-C5	-2.04	119.72	122.59
11	B	1231	CLA	OBD-CAD-C3D	-2.04	124.27	128.03
11	A	1105	CLA	O1D-CGD-CBD	-2.04	120.94	124.60
14	b	4011	BCR	C32-C1-C6	-2.04	107.00	110.31
12	2	2002	PQN	C11-C12-C13	-2.04	123.30	126.71
11	A	1114	CLA	O2D-CGD-O1D	-2.04	119.72	123.82
11	2	1226	CLA	C1-C2-C3	-2.04	122.20	125.96
14	B	4009	BCR	C23-C24-C25	-2.04	121.55	127.25
11	A	1124	CLA	O1D-CGD-CBD	-2.04	120.94	124.60
11	B	1021	CLA	CHC-C1C-C2C	-2.04	121.09	126.65
14	a	4007	BCR	C34-C9-C10	-2.04	120.07	122.92
14	b	4014	BCR	C8-C7-C6	-2.04	121.55	127.25
11	B	1222	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
11	2	1202	CLA	O2D-CGD-O1D	-2.04	119.72	123.82
11	1	1103	CLA	CMD-C2D-C3D	-2.03	121.12	124.89
12	a	2001	PQN	C11-C12-C13	-2.03	123.31	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1232	CLA	O2D-CGD-O1D	-2.03	119.73	123.82
12	A	2001	PQN	C2M-C2-C3	-2.03	120.08	124.20
11	b	1231	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
11	A	1119	CLA	O1D-CGD-CBD	-2.03	120.95	124.60
14	A	4001	BCR	C8-C7-C6	-2.03	121.57	127.25
11	1	1117	CLA	O1D-CGD-CBD	-2.03	120.95	124.60
14	F	4013	BCR	C1-C6-C5	-2.03	119.74	122.59
11	b	1221	CLA	C4-C3-C2	-2.03	118.28	123.69
14	a	4002	BCR	C27-C26-C25	-2.03	119.76	122.74
14	b	4005	BCR	C23-C24-C25	-2.03	121.57	127.25
11	B	1201	CLA	C1-C2-C3	-2.03	122.22	125.96
14	F	4018	BCR	C40-C30-C25	-2.03	107.02	110.31
11	B	1209	CLA	CHC-C1C-C2C	-2.03	121.12	126.65
14	f	4013	BCR	C36-C18-C17	-2.03	120.08	122.92
11	A	1139	CLA	O2D-CGD-O1D	-2.03	119.74	123.82
14	B	4010	BCR	C27-C26-C25	-2.03	119.77	122.74
11	2	1219	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
11	a	1134	CLA	O2D-CGD-O1D	-2.03	119.74	123.82
11	B	1216	CLA	O1D-CGD-CBD	-2.03	120.96	124.60
11	a	1122	CLA	O1D-CGD-CBD	-2.03	120.96	124.60
11	B	1234	CLA	CHC-C1C-C2C	-2.03	121.13	126.65
11	L	1501	CLA	O1D-CGD-CBD	-2.02	120.97	124.60
11	a	1104	CLA	C1-C2-C3	-2.02	122.23	125.96
11	A	1119	CLA	OBD-CAD-C3D	-2.02	124.30	128.03
11	a	1134	CLA	OBD-CAD-C3D	-2.02	124.30	128.03
11	A	1022	CLA	O1D-CGD-CBD	-2.02	120.97	124.60
11	B	1202	CLA	O1D-CGD-CBD	-2.02	120.97	124.60
16	b	5002	LMG	C7-O1-C1	-2.02	109.62	113.76
11	1	1119	CLA	C7-C6-C5	-2.02	107.50	113.11
11	a	1119	CLA	CHC-C1C-C2C	-2.02	121.14	126.65
14	2	4014	BCR	C8-C7-C6	-2.02	121.60	127.25
11	a	1123	CLA	O1D-CGD-CBD	-2.02	120.98	124.60
14	l	4019	BCR	C35-C13-C14	-2.01	120.10	122.92
11	A	1113	CLA	O1D-CGD-CBD	-2.01	120.99	124.60
11	2	1235	CLA	C6-C5-C3	-2.01	108.09	112.66
11	B	1013	CLA	OBD-CAD-C3D	-2.01	124.32	128.03
11	A	1124	CLA	C6-C5-C3	-2.01	108.10	112.66
14	6	4013	BCR	C35-C13-C14	-2.01	120.11	122.92
11	1	1237	CLA	CHC-C1C-C2C	-2.01	121.17	126.65
11	B	1207	CLA	OBD-CAD-C3D	-2.01	124.32	128.03
14	A	4007	BCR	C7-C8-C9	-2.01	123.19	126.21
11	l	1501	CLA	C4-C3-C2	-2.01	118.33	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1223	CLA	CHC-C1C-C2C	-2.01	121.17	126.65
11	2	1234	CLA	O2D-CGD-O1D	-2.01	119.78	123.82
14	8	4022	BCR	C1-C6-C5	-2.01	119.77	122.59
11	1	1126	CLA	C4-C3-C2	-2.00	118.34	123.69
14	2	4009	BCR	C37-C22-C21	-2.00	120.11	122.92
11	1	1138	CLA	O1D-CGD-CBD	-2.00	121.00	124.60
14	2	4010	BCR	C8-C7-C6	-2.00	121.65	127.25
14	f	4013	BCR	C24-C25-C26	-2.00	116.77	121.54
11	2	1230	CLA	C4C-C3C-C2C	-2.00	103.84	106.91
11	B	1216	CLA	CMD-C2D-C3D	-2.00	121.18	124.89
11	A	1113	CLA	CAC-C3C-C4C	2.00	127.65	124.83
11	1	1127	CLA	CED-O2D-CGD	2.00	120.66	115.97
11	b	1206	CLA	C4-C3-C5	2.00	118.76	115.29
11	A	1122	CLA	C9-C8-C7	2.00	118.66	111.36
11	a	1237	CLA	CED-O2D-CGD	2.00	120.66	115.97
11	1	1101	CLA	CMB-C2B-C3B	2.00	128.61	124.89
11	B	1215	CLA	C9-C8-C7	2.00	118.66	111.36
11	B	1227	CLA	CHB-C4A-NA	2.00	127.28	124.51
11	a	1101	CLA	C4-C3-C5	2.00	118.76	115.29
11	b	1215	CLA	C4A-NA-C1A	2.01	108.94	106.45
11	B	1216	CLA	C1-O2A-CGA	2.01	121.59	116.77
11	a	1123	CLA	C9-C8-C7	2.01	118.68	111.36
11	B	1240	CLA	CHB-C4A-NA	2.01	127.29	124.51
11	b	1231	CLA	CAC-C3C-C4C	2.01	127.66	124.83
11	A	1011	CLA	CED-O2D-CGD	2.01	120.68	115.97
11	2	1220	CLA	CED-O2D-CGD	2.01	120.68	115.97
11	1	1118	CLA	CHB-C4A-NA	2.01	127.29	124.51
11	8	1503	CLA	C1-O2A-CGA	2.01	121.59	116.77
11	2	1202	CLA	CED-O2D-CGD	2.01	120.68	115.97
11	a	1135	CLA	CMC-C2C-C1C	2.01	128.07	125.02
11	b	1219	CLA	CAC-C3C-C4C	2.01	127.67	124.83
14	A	4008	BCR	C34-C9-C8	2.01	121.30	118.10
11	B	1230	CLA	CED-O2D-CGD	2.01	120.69	115.97
14	8	4019	BCR	C8-C9-C10	2.01	122.03	118.94
11	2	1232	CLA	C4A-NA-C1A	2.01	108.95	106.45
11	2	1202	CLA	C4A-NA-C1A	2.01	108.95	106.45
11	1	1102	CLA	C1-O2A-CGA	2.01	121.60	116.77
11	A	1113	CLA	CHB-C4A-NA	2.01	127.30	124.51
11	a	1113	CLA	CHB-C4A-NA	2.01	127.30	124.51
11	K	1402	CLA	CHB-C4A-NA	2.02	127.30	124.51
11	2	1222	CLA	CHB-C4A-NA	2.02	127.30	124.51
11	A	1115	CLA	CAC-C3C-C4C	2.02	127.67	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4007	BCR	C35-C13-C12	2.02	121.31	118.10
11	B	1228	CLA	CAC-C3C-C4C	2.02	127.67	124.83
11	2	1021	CLA	CAC-C3C-C4C	2.02	127.67	124.83
11	B	1226	CLA	C1-O2A-CGA	2.02	121.61	116.77
11	a	1131	CLA	C1-O2A-CGA	2.02	121.61	116.77
11	b	1215	CLA	CAC-C3C-C4C	2.02	127.68	124.83
11	2	1230	CLA	CED-O2D-CGD	2.02	120.70	115.97
11	b	1238	CLA	C1-O2A-CGA	2.02	121.62	116.77
14	B	4009	BCR	C23-C22-C21	2.02	122.04	118.94
14	b	4014	BCR	C19-C18-C17	2.02	122.04	118.94
11	b	1201	CLA	CED-O2D-CGD	2.02	120.71	115.97
11	1	1139	CLA	C4A-NA-C1A	2.02	108.96	106.45
11	2	1215	CLA	C9-C8-C10	2.03	118.75	111.36
11	2	1235	CLA	CED-O2D-CGD	2.03	120.72	115.97
11	A	1127	CLA	C4A-NA-C1A	2.03	108.97	106.45
11	1	1121	CLA	CHB-C4A-NA	2.03	127.31	124.51
11	A	1102	CLA	CAC-C3C-C4C	2.03	127.69	124.83
11	2	1228	CLA	C5-C3-C4	2.03	119.33	114.60
11	A	1138	CLA	CED-O2D-CGD	2.03	120.72	115.97
11	A	1118	CLA	C1-O2A-CGA	2.03	121.64	116.77
11	1	1120	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	k	1402	CLA	CAC-C3C-C4C	2.03	127.69	124.83
11	B	1226	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	1	1112	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	b	1219	CLA	CED-O2D-CGD	2.03	120.73	115.97
11	2	1013	CLA	CMC-C2C-C1C	2.03	128.10	125.02
11	2	1239	CLA	CED-O2D-CGD	2.03	120.73	115.97
14	b	4004	BCR	C23-C22-C21	2.03	122.06	118.94
11	B	1208	CLA	CED-O2D-CGD	2.03	120.73	115.97
11	2	1230	CLA	CMC-C2C-C1C	2.03	128.10	125.02
11	B	1223	CLA	C9-C8-C7	2.03	118.77	111.36
11	A	1104	CLA	CHB-C4A-NA	2.03	127.32	124.51
11	2	1212	CLA	CAC-C3C-C4C	2.03	127.70	124.83
11	A	1125	CLA	C4-C3-C5	2.03	118.81	115.29
11	A	1114	CLA	CMB-C2B-C3B	2.03	128.67	124.89
11	a	1022	CLA	C4A-NA-C1A	2.04	108.98	106.45
14	B	4006	BCR	C1-C6-C7	2.04	121.46	115.73
11	1	1124	CLA	CHB-C4A-NA	2.04	127.33	124.51
11	a	1116	CLA	C4A-NA-C1A	2.04	108.98	106.45
14	2	4011	BCR	C19-C18-C17	2.04	122.07	118.94
11	b	1023	CLA	C9-C8-C10	2.04	118.80	111.36
11	B	1219	CLA	CHB-C4A-NA	2.04	127.33	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	4002	BCR	C8-C9-C10	2.04	122.07	118.94
11	k	1402	CLA	C4A-NA-C1A	2.04	108.98	106.45
11	2	1218	CLA	CHB-C4A-NA	2.04	127.33	124.51
11	A	1123	CLA	C1-O2A-CGA	2.04	121.67	116.77
11	1	1113	CLA	CHB-C4A-NA	2.04	127.34	124.51
11	B	1225	CLA	CBA-CAA-C2A	2.04	119.91	113.80
11	1	1106	CLA	CED-O2D-CGD	2.04	120.76	115.97
11	1	1121	CLA	CMB-C2B-C3B	2.04	128.69	124.89
11	B	1202	CLA	C4A-NA-C1A	2.04	108.99	106.45
11	A	1123	CLA	C9-C8-C7	2.05	118.83	111.36
11	2	1218	CLA	CMB-C2B-C3B	2.05	128.69	124.89
11	1	1103	CLA	CED-O2D-CGD	2.05	120.77	115.97
11	b	1206	CLA	CHB-C4A-NA	2.05	127.34	124.51
11	a	1118	CLA	C1-O2A-CGA	2.05	121.69	116.77
11	1	1106	CLA	CAC-C3C-C4C	2.05	127.72	124.83
11	2	1206	CLA	CAC-C3C-C4C	2.05	127.72	124.83
11	A	1128	CLA	C9-C8-C10	2.05	118.83	111.36
14	a	4008	BCR	C1-C6-C7	2.05	121.49	115.73
11	B	1213	CLA	C4-C3-C5	2.05	118.84	115.29
11	b	1223	CLA	C4A-NA-C1A	2.05	109.00	106.45
11	B	1225	CLA	C4-C3-C5	2.05	118.85	115.29
11	b	1225	CLA	C4A-NA-C1A	2.05	109.00	106.45
11	1	1116	CLA	CAC-C3C-C4C	2.05	127.73	124.83
11	b	1216	CLA	CED-O2D-CGD	2.06	120.79	115.97
11	A	1801	CLA	CMB-C2B-C3B	2.06	128.71	124.89
11	A	1110	CLA	CAC-C3C-C4C	2.06	127.73	124.83
14	b	4009	BCR	C38-C26-C27	2.06	117.36	113.45
11	B	1226	CLA	C4-C3-C5	2.06	118.86	115.29
11	1	1110	CLA	C4A-NA-C1A	2.06	109.01	106.45
14	1	4007	BCR	C23-C22-C21	2.06	122.10	118.94
11	2	1224	CLA	C1-O2A-CGA	2.06	121.71	116.77
14	2	4004	BCR	C1-C6-C7	2.06	121.52	115.73
11	B	1219	CLA	CED-O2D-CGD	2.06	120.80	115.97
11	b	1209	CLA	CMC-C2C-C1C	2.06	128.15	125.02
11	1	1115	CLA	C4A-NA-C1A	2.06	109.01	106.45
12	2	2002	PQN	C14-C13-C15	2.06	118.86	115.29
11	b	1239	CLA	CAC-C3C-C4C	2.06	127.74	124.83
11	A	1022	CLA	CHB-C4A-NA	2.06	127.36	124.51
11	a	1124	CLA	C10-C8-C9	2.06	120.26	110.50
11	1	1133	CLA	C4A-NA-C1A	2.07	109.02	106.45
11	A	1120	CLA	CAC-C3C-C4C	2.07	127.75	124.83
11	A	1107	CLA	C1-O2A-CGA	2.07	121.73	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1022	CLA	C4-C3-C5	2.07	118.88	115.29
11	b	1226	CLA	C4A-NA-C1A	2.07	109.02	106.45
11	2	1230	CLA	CAC-C3C-C4C	2.07	127.75	124.83
11	a	1119	CLA	CMC-C2C-C1C	2.07	128.16	125.02
14	2	4006	BCR	C35-C13-C12	2.07	121.40	118.10
11	1	1012	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	1	1136	CLA	CAC-C3C-C4C	2.07	127.75	124.83
11	A	1119	CLA	C9-C8-C7	2.07	118.91	111.36
11	1	1126	CLA	C4A-NA-C1A	2.07	109.02	106.45
11	8	1502	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	b	1214	CLA	C4A-NA-C1A	2.07	109.02	106.45
11	A	1127	CLA	CED-O2D-CGD	2.07	120.83	115.97
14	A	4007	BCR	C38-C26-C27	2.07	117.39	113.45
11	a	1112	CLA	CMB-C2B-C3B	2.07	128.74	124.89
11	a	1123	CLA	C4A-NA-C1A	2.07	109.03	106.45
11	a	1135	CLA	CAC-C3C-C4C	2.07	127.75	124.83
11	a	1138	CLA	CHB-C4A-NA	2.07	127.38	124.51
11	1	1131	CLA	C9-C8-C7	2.07	118.92	111.36
11	1	1131	CLA	CAC-C3C-C4C	2.07	127.76	124.83
14	F	4020	BCR	C34-C9-C8	2.08	121.41	118.10
11	1	1135	CLA	C1-O2A-CGA	2.08	121.75	116.77
11	b	1216	CLA	C1-O2A-CGA	2.08	121.75	116.77
14	6	4013	BCR	C35-C13-C12	2.08	121.41	118.10
11	1	1125	CLA	C4A-NA-C1A	2.08	109.03	106.45
11	1	1103	CLA	C1-O2A-CGA	2.08	121.76	116.77
11	2	1201	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	a	1104	CLA	CHB-C4A-NA	2.08	127.39	124.51
14	1	4008	BCR	C8-C9-C10	2.08	122.13	118.94
11	1	1112	CLA	CED-O2D-CGD	2.08	120.85	115.97
11	2	1223	CLA	C4A-NA-C1A	2.08	109.03	106.45
11	1	1111	CLA	C4-C3-C5	2.08	118.90	115.29
11	b	1216	CLA	CAC-C3C-C4C	2.08	127.77	124.83
11	2	1225	CLA	C4A-NA-C1A	2.08	109.04	106.45
14	b	4006	BCR	C8-C9-C10	2.08	122.14	118.94
11	B	1212	CLA	C4A-NA-C1A	2.08	109.04	106.45
11	2	1210	CLA	CHB-C4A-NA	2.08	127.39	124.51
11	a	1109	CLA	C4A-NA-C1A	2.09	109.04	106.45
11	b	1023	CLA	CMC-C2C-C1C	2.09	128.19	125.02
11	2	1204	CLA	C4A-NA-C1A	2.09	109.05	106.45
11	B	1210	CLA	CHB-C4A-NA	2.09	127.40	124.51
11	A	1237	CLA	C1-O2A-CGA	2.09	121.79	116.77
11	b	1223	CLA	C1-O2A-CGA	2.09	121.79	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1112	CLA	CAC-C3C-C4C	2.09	127.78	124.83
11	2	1206	CLA	CMB-C2B-C3B	2.09	128.78	124.89
11	1	1137	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	B	1229	CLA	C4A-NA-C1A	2.09	109.05	106.45
11	A	1126	CLA	C9-C8-C7	2.09	119.00	111.36
11	B	1226	CLA	CMB-C2B-C3B	2.09	128.78	124.89
11	1	1140	CLA	C9-C8-C10	2.09	119.00	111.36
11	8	1501	CLA	CAC-C3C-C4C	2.09	127.78	124.83
11	a	1112	CLA	C4A-NA-C1A	2.09	109.05	106.45
11	A	1131	CLA	C4-C3-C5	2.09	118.92	115.29
11	b	1205	CLA	CMB-C2B-C3B	2.09	128.78	124.89
11	A	1118	CLA	CHB-C4A-NA	2.09	127.41	124.51
11	b	1230	CLA	CHB-C4A-NA	2.10	127.41	124.51
11	b	1232	CLA	C4A-NA-C1A	2.10	109.06	106.45
11	1	1105	CLA	CAC-C3C-C4C	2.10	127.79	124.83
11	2	1203	CLA	CMB-C2B-C3B	2.10	128.78	124.89
11	1	1126	CLA	CAC-C3C-C4C	2.10	127.79	124.83
14	7	4021	BCR	C35-C13-C12	2.10	121.44	118.10
11	a	1112	CLA	CHB-C4A-NA	2.10	127.42	124.51
11	b	1240	CLA	C4A-NA-C1A	2.10	109.06	106.45
11	B	1220	CLA	C4A-NA-C1A	2.10	109.06	106.45
11	A	1138	CLA	C3C-C4C-NC	2.10	112.34	110.21
11	A	1140	CLA	CMB-C2B-C3B	2.10	128.79	124.89
11	2	1223	CLA	C4-C3-C5	2.10	118.94	115.29
11	B	1219	CLA	CAC-C3C-C4C	2.10	127.80	124.83
11	2	1230	CLA	CHB-C4A-NA	2.10	127.42	124.51
11	B	1205	CLA	C4-C3-C5	2.10	118.94	115.29
11	A	1101	CLA	C9-C8-C10	2.10	119.03	111.36
11	a	1130	CLA	CAC-C3C-C4C	2.10	127.80	124.83
11	a	1110	CLA	C4A-NA-C1A	2.11	109.06	106.45
14	8	4022	BCR	C35-C13-C12	2.11	121.45	118.10
11	A	1129	CLA	CMB-C2B-C3B	2.11	128.80	124.89
11	B	1215	CLA	C9-C8-C10	2.11	119.05	111.36
14	b	4009	BCR	C1-C6-C7	2.11	121.66	115.73
11	2	1229	CLA	C9-C8-C10	2.11	119.05	111.36
11	a	1128	CLA	C1-O2A-CGA	2.11	121.83	116.77
11	b	1239	CLA	CMC-C2C-C1C	2.11	128.22	125.02
11	a	1011	CLA	C4-C3-C5	2.11	118.95	115.29
11	a	1116	CLA	CAC-C3C-C4C	2.11	127.81	124.83
11	B	1222	CLA	C1-O2A-CGA	2.11	121.83	116.77
11	2	1216	CLA	C9-C8-C7	2.11	119.06	111.36
11	2	1224	CLA	CHB-C4A-NA	2.11	127.43	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1217	CLA	CHB-C4A-NA	2.11	127.43	124.51
11	2	1021	CLA	CED-O2D-CGD	2.11	120.92	115.97
11	2	1222	CLA	C1-O2A-CGA	2.11	121.84	116.77
14	L	4022	BCR	C34-C9-C8	2.11	121.46	118.10
11	b	1207	CLA	CED-O2D-CGD	2.11	120.92	115.97
11	2	1208	CLA	CMB-C2B-C3B	2.11	128.81	124.89
11	a	1120	CLA	CMB-C2B-C3B	2.11	128.81	124.89
11	b	1224	CLA	CAC-C3C-C4C	2.11	127.81	124.83
11	B	1230	CLA	CAC-C3C-C4C	2.11	127.81	124.83
14	F	4013	BCR	C30-C25-C24	2.11	121.67	115.73
11	b	1239	CLA	CMB-C2B-C3B	2.11	128.81	124.89
11	B	1203	CLA	CHB-C4A-NA	2.11	127.44	124.51
14	f	4013	BCR	C35-C13-C12	2.11	121.47	118.10
11	a	1119	CLA	C4A-NA-C1A	2.11	109.08	106.45
14	b	4011	BCR	C1-C6-C7	2.12	121.67	115.73
11	b	1201	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	b	1235	CLA	C4-C3-C5	2.12	118.96	115.29
11	a	1134	CLA	C4A-NA-C1A	2.12	109.08	106.45
11	a	1122	CLA	CAC-C3C-C4C	2.12	127.81	124.83
11	B	1235	CLA	C4A-NA-C1A	2.12	109.08	106.45
11	a	1801	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	a	1107	CLA	C1-O2A-CGA	2.12	121.85	116.77
14	B	4017	BCR	C35-C13-C12	2.12	121.47	118.10
11	B	1225	CLA	CHB-C4A-NA	2.12	127.44	124.51
11	B	1225	CLA	C4A-NA-C1A	2.12	109.08	106.45
11	A	1124	CLA	C4A-NA-C1A	2.12	109.08	106.45
11	2	1213	CLA	C4A-NA-C1A	2.12	109.08	106.45
12	B	2002	PQN	C2M-C2-C1	2.12	119.79	116.23
11	b	1210	CLA	CHB-C4A-NA	2.12	127.45	124.51
11	B	1215	CLA	C4A-NA-C1A	2.12	109.09	106.45
11	2	1215	CLA	C4A-NA-C1A	2.12	109.09	106.45
11	a	1131	CLA	CAC-C3C-C4C	2.12	127.82	124.83
11	2	1212	CLA	CED-O2D-CGD	2.12	120.95	115.97
11	a	1121	CLA	C4A-NA-C1A	2.12	109.09	106.45
12	A	2001	PQN	C2M-C2-C1	2.12	119.79	116.23
11	A	1135	CLA	C4A-NA-C1A	2.13	109.09	106.45
11	B	1206	CLA	C1-O2A-CGA	2.13	121.87	116.77
11	b	1013	CLA	C4A-NA-C1A	2.13	109.09	106.45
11	B	1221	CLA	CMB-C2B-C3B	2.13	128.84	124.89
11	a	1106	CLA	C1-O2A-CGA	2.13	121.87	116.77
11	A	1103	CLA	C9-C8-C10	2.13	119.12	111.36
11	2	1209	CLA	CHB-C4A-NA	2.13	127.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1111	CLA	CAC-C3C-C4C	2.13	127.83	124.83
11	b	1013	CLA	C4-C3-C5	2.13	118.98	115.29
11	B	1234	CLA	C9-C8-C7	2.13	119.12	111.36
11	1	1117	CLA	C9-C8-C10	2.13	119.12	111.36
11	b	1208	CLA	C4A-NA-C1A	2.13	109.09	106.45
11	b	1221	CLA	CAC-C3C-C4C	2.13	127.83	124.83
11	2	1229	CLA	C4-C3-C5	2.13	118.98	115.29
11	2	1205	CLA	C4-C3-C5	2.13	118.98	115.29
11	b	1229	CLA	C4A-NA-C1A	2.13	109.09	106.45
11	2	1223	CLA	CMB-C2B-C3B	2.13	128.84	124.89
11	B	1223	CLA	C4A-NA-C1A	2.13	109.10	106.45
11	2	1212	CLA	C4A-NA-C1A	2.13	109.10	106.45
11	2	1209	CLA	C4A-NA-C1A	2.13	109.10	106.45
11	B	1211	CLA	C4A-NA-C1A	2.13	109.10	106.45
11	B	1023	CLA	C4-C3-C5	2.13	118.99	115.29
11	A	1105	CLA	CED-O2D-CGD	2.13	120.97	115.97
11	1	1114	CLA	C4A-NA-C1A	2.13	109.10	106.45
11	a	1129	CLA	CMB-C2B-C3B	2.13	128.85	124.89
11	1	1128	CLA	CMC-C2C-C1C	2.13	128.26	125.02
11	1	1134	CLA	CAC-C3C-C4C	2.13	127.84	124.83
11	2	1207	CLA	CAA-C2A-C1A	2.13	118.97	111.97
11	1	1124	CLA	C4-C3-C5	2.14	118.99	115.29
14	1	4008	BCR	C1-C6-C7	2.14	121.73	115.73
14	8	4022	BCR	C23-C22-C21	2.14	122.22	118.94
11	8	1503	CLA	C4A-NA-C1A	2.14	109.10	106.45
11	b	1218	CLA	C4A-NA-C1A	2.14	109.11	106.45
11	A	1801	CLA	C4A-NA-C1A	2.14	109.11	106.45
11	a	1127	CLA	C4A-NA-C1A	2.14	109.11	106.45
11	1	1116	CLA	C4-C3-C5	2.14	119.00	115.29
11	a	1119	CLA	C4-C3-C5	2.14	119.00	115.29
11	0	1401	CLA	CAC-C3C-C4C	2.14	127.85	124.83
11	a	1140	CLA	CMB-C2B-C3B	2.14	128.87	124.89
11	2	1238	CLA	C4A-NA-C1A	2.14	109.11	106.45
11	b	1226	CLA	C1-O2A-CGA	2.14	121.91	116.77
11	b	1234	CLA	CMC-C2C-C1C	2.14	128.27	125.02
11	B	1222	CLA	CHB-C4A-NA	2.14	127.47	124.51
11	B	1206	CLA	CED-O2D-CGD	2.14	120.99	115.97
11	A	1139	CLA	CED-O2D-CGD	2.14	120.99	115.97
11	A	1112	CLA	CAC-C3C-C4C	2.14	127.85	124.83
11	2	1215	CLA	CMB-C2B-C3B	2.14	128.87	124.89
11	b	1227	CLA	CAC-C3C-C4C	2.14	127.85	124.83
14	B	4011	BCR	C23-C22-C21	2.14	122.23	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1111	CLA	C9-C8-C10	2.15	119.19	111.36
11	B	1223	CLA	C4-C3-C5	2.15	119.01	115.29
14	8	4022	BCR	C30-C25-C24	2.15	121.77	115.73
11	B	1229	CLA	CAC-C3C-C4C	2.15	127.86	124.83
11	A	1124	CLA	CHB-C4A-NA	2.15	127.48	124.51
11	1	1119	CLA	C4A-NA-C1A	2.15	109.12	106.45
11	a	1101	CLA	C4A-NA-C1A	2.15	109.12	106.45
11	A	1131	CLA	CMB-C2B-C3B	2.15	128.88	124.89
11	B	1236	CLA	C1-O2A-CGA	2.15	123.03	116.72
11	b	1203	CLA	CHB-C4A-NA	2.15	127.49	124.51
11	1	1117	CLA	C1-O2A-CGA	2.15	121.93	116.77
11	b	1218	CLA	CMB-C2B-C3B	2.15	128.88	124.89
11	B	1201	CLA	CMC-C2C-C1C	2.15	128.29	125.02
11	a	1113	CLA	CAC-C3C-C4C	2.15	127.87	124.83
11	A	1108	CLA	C4A-NA-C1A	2.15	109.13	106.45
11	2	1205	CLA	C1-O2A-CGA	2.15	121.94	116.77
11	b	1210	CLA	C9-C8-C7	2.16	119.22	111.36
11	1	1122	CLA	C4A-NA-C1A	2.16	109.13	106.45
11	a	1119	CLA	CAC-C3C-C4C	2.16	127.87	124.83
11	B	1222	CLA	C6-C5-C3	2.16	117.55	112.66
11	K	1401	CLA	CAC-C3C-C4C	2.16	127.87	124.83
11	1	1107	CLA	CMB-C2B-C3B	2.16	128.90	124.89
11	1	1127	CLA	C4-C3-C5	2.16	119.03	115.29
11	b	1229	CLA	CMB-C2B-C3B	2.16	128.90	124.89
11	1	1114	CLA	CAC-C3C-C4C	2.16	127.88	124.83
11	L	1503	CLA	CMB-C2B-C3B	2.16	128.90	124.89
11	a	1101	CLA	C9-C8-C10	2.16	119.24	111.36
11	b	1238	CLA	C4A-NA-C1A	2.16	109.14	106.45
11	2	1201	CLA	CMB-C2B-C3B	2.16	128.90	124.89
11	2	1235	CLA	CHB-C4A-NA	2.16	127.50	124.51
11	a	1131	CLA	CHB-C4A-NA	2.16	127.50	124.51
11	A	1101	CLA	C4A-NA-C1A	2.16	109.14	106.45
11	2	1222	CLA	C4A-NA-C1A	2.16	109.14	106.45
11	1	1103	CLA	CMB-C2B-C3B	2.16	128.91	124.89
11	a	1125	CLA	C4A-NA-C1A	2.16	109.14	106.45
11	B	1223	CLA	C1-O2A-CGA	2.16	121.96	116.77
11	1	1101	CLA	CAC-C3C-C4C	2.16	127.88	124.83
11	a	1115	CLA	C4A-NA-C1A	2.17	109.14	106.45
14	B	4004	BCR	C23-C22-C21	2.17	122.27	118.94
11	1	1101	CLA	C4A-NA-C1A	2.17	109.14	106.45
11	2	1227	CLA	CAC-C3C-C4C	2.17	127.89	124.83
11	B	1207	CLA	CHB-C4A-NA	2.17	127.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1104	CLA	C4A-NA-C1A	2.17	109.14	106.45
11	b	1211	CLA	C4A-NA-C1A	2.17	109.14	106.45
11	1	1128	CLA	C4A-NA-C1A	2.17	109.14	106.45
11	A	1109	CLA	C9-C8-C10	2.17	119.27	111.36
11	1	1123	CLA	CMB-C2B-C3B	2.17	128.92	124.89
11	2	1240	CLA	CAC-C3C-C4C	2.17	127.89	124.83
11	a	1140	CLA	C4-C3-C5	2.17	119.06	115.29
11	A	1114	CLA	C4A-NA-C1A	2.17	109.15	106.45
11	1	1114	CLA	CMB-C2B-C3B	2.17	128.92	124.89
11	B	1234	CLA	CAC-C3C-C4C	2.17	127.89	124.83
11	1	1106	CLA	CMB-C2B-C3B	2.17	128.92	124.89
14	f	4013	BCR	C30-C25-C24	2.17	121.84	115.73
11	2	1225	CLA	C4-C3-C5	2.17	119.06	115.29
11	b	1204	CLA	CMB-C2B-C3B	2.18	128.93	124.89
11	A	1131	CLA	CAC-C3C-C4C	2.18	127.90	124.83
11	k	1401	CLA	CAC-C3C-C4C	2.18	127.90	124.83
11	2	1215	CLA	C9-C8-C7	2.18	119.30	111.36
11	B	1208	CLA	C4A-NA-C1A	2.18	109.16	106.45
11	2	1201	CLA	CAC-C3C-C4C	2.18	127.90	124.83
11	b	1230	CLA	C4A-NA-C1A	2.18	109.16	106.45
11	A	1115	CLA	C4A-NA-C1A	2.18	109.16	106.45
14	A	4002	BCR	C34-C9-C8	2.18	121.57	118.10
14	2	4004	BCR	C34-C9-C8	2.18	121.57	118.10
11	1	1133	CLA	CMB-C2B-C3B	2.18	128.94	124.89
11	1	1122	CLA	CED-O2D-CGD	2.18	121.08	115.97
11	B	1209	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	a	1104	CLA	C9-C8-C7	2.18	119.31	111.36
14	M	4021	BCR	C33-C5-C4	2.18	117.59	113.45
11	2	1203	CLA	C1-O2A-CGA	2.18	122.01	116.77
11	a	1237	CLA	CAC-C3C-C4C	2.18	127.91	124.83
11	1	1116	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	B	1205	CLA	CHB-C4A-NA	2.18	127.53	124.51
11	A	1130	CLA	C4A-NA-C1A	2.18	109.16	106.45
11	A	1139	CLA	C4A-NA-C1A	2.18	109.16	106.45
11	B	1228	CLA	C4A-NA-C1A	2.18	109.16	106.45
14	6	4018	BCR	C35-C13-C12	2.18	121.58	118.10
11	b	1236	CLA	C4A-NA-C1A	2.18	109.16	106.45
11	B	1206	CLA	C4-C3-C5	2.18	119.08	115.29
11	b	1210	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	A	1116	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	2	1217	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	A	1801	CLA	CAC-C3C-C2C	2.19	131.29	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1122	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	1	1127	CLA	CAC-C3C-C4C	2.19	127.92	124.83
11	a	1132	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	A	1129	CLA	CAC-C3C-C4C	2.19	127.92	124.83
11	b	1207	CLA	CHB-C4A-NA	2.19	127.54	124.51
11	2	1236	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	B	1213	CLA	CMB-C2B-C3B	2.19	128.96	124.89
11	1	1140	CLA	CMB-C2B-C3B	2.19	128.96	124.89
14	B	4005	BCR	C19-C18-C17	2.19	122.31	118.94
11	B	1209	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	a	1131	CLA	C4A-NA-C1A	2.19	109.17	106.45
11	B	1013	CLA	CMC-C2C-C1C	2.19	128.35	125.02
12	b	2002	PQN	C2M-C2-C1	2.20	119.91	116.23
11	a	1137	CLA	C9-C8-C10	2.20	119.37	111.36
11	L	1501	CLA	CHB-C4A-NA	2.20	127.55	124.51
11	l	1503	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	1	1101	CLA	C4-C3-C5	2.20	119.10	115.29
11	1	1128	CLA	C4-C3-C5	2.20	119.10	115.29
11	b	1217	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	b	1235	CLA	C9-C8-C10	2.20	119.38	111.36
11	b	1227	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	1	1131	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	B	1219	CLA	C4-C3-C5	2.20	119.10	115.29
11	1	1237	CLA	CMB-C2B-C3B	2.20	128.97	124.89
11	b	1226	CLA	CMB-C2B-C3B	2.20	128.97	124.89
11	A	1109	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	2	1230	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	a	1107	CLA	C9-C8-C10	2.20	119.39	111.36
11	A	1106	CLA	C4A-NA-C1A	2.20	109.18	106.45
11	2	1207	CLA	CMB-C2B-C3B	2.20	128.98	124.89
11	2	1235	CLA	C9-C8-C10	2.20	119.39	111.36
11	a	1122	CLA	C9-C8-C7	2.20	119.40	111.36
11	b	1214	CLA	CAC-C3C-C4C	2.20	127.94	124.83
11	1	1237	CLA	CHB-C4A-NA	2.20	127.56	124.51
14	1	4008	BCR	C30-C25-C24	2.21	121.93	115.73
11	a	1133	CLA	CAC-C3C-C4C	2.21	127.94	124.83
11	B	1222	CLA	C9-C8-C7	2.21	119.41	111.36
11	B	1230	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	1	1011	CLA	CMB-C2B-C3B	2.21	128.99	124.89
11	2	1219	CLA	CHB-C4A-NA	2.21	127.57	124.51
14	a	4008	BCR	C34-C9-C8	2.21	121.62	118.10
11	a	1139	CLA	C1-O2A-CGA	2.21	122.08	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1217	CLA	CMB-C2B-C3B	2.21	129.00	124.89
11	2	1203	CLA	CHB-C4A-NA	2.21	127.57	124.51
11	A	1129	CLA	C4A-NA-C1A	2.21	109.20	106.45
14	f	4013	BCR	C38-C26-C27	2.21	117.65	113.45
11	b	1021	CLA	C4A-NA-C1A	2.21	109.20	106.45
12	2	2002	PQN	C25-C23-C22	2.21	122.75	112.10
14	a	4001	BCR	C35-C13-C12	2.22	121.63	118.10
11	0	1402	CLA	C4A-NA-C1A	2.22	109.20	106.45
11	A	1102	CLA	C9-C8-C10	2.22	119.44	111.36
11	b	1223	CLA	CMB-C2B-C3B	2.22	129.00	124.89
11	a	1108	CLA	C4A-NA-C1A	2.22	109.20	106.45
11	b	1209	CLA	C4A-NA-C1A	2.22	109.20	106.45
11	A	1136	CLA	CAC-C3C-C4C	2.22	127.96	124.83
11	b	1220	CLA	C4A-NA-C1A	2.22	109.20	106.45
11	1	1132	CLA	CMB-C2B-C3B	2.22	129.01	124.89
11	a	1134	CLA	CHB-C4A-NA	2.22	127.58	124.51
11	1	1112	CLA	C4A-NA-C1A	2.22	109.21	106.45
11	1	1129	CLA	CMB-C2B-C3B	2.22	129.01	124.89
11	A	1105	CLA	CMB-C2B-C3B	2.22	129.01	124.89
11	2	1214	CLA	CAC-C3C-C4C	2.22	127.96	124.83
11	a	1128	CLA	C4A-NA-C1A	2.22	109.21	106.45
11	A	1122	CLA	C4A-NA-C1A	2.22	109.21	106.45
11	1	1237	CLA	CMC-C2C-C1C	2.22	128.39	125.02
11	a	1108	CLA	CED-O2D-CGD	2.22	121.18	115.97
11	1	1109	CLA	C4A-NA-C1A	2.22	109.21	106.45
11	a	1139	CLA	C4A-NA-C1A	2.22	109.21	106.45
11	b	1219	CLA	C4-C3-C5	2.22	119.14	115.29
11	b	1234	CLA	CMB-C2B-C3B	2.22	129.02	124.89
11	2	1231	CLA	C4A-NA-C1A	2.22	109.21	106.45
11	a	1107	CLA	CMB-C2B-C3B	2.22	129.02	124.89
11	1	1139	CLA	C5-C3-C4	2.22	119.79	114.60
11	a	1131	CLA	C9-C8-C10	2.22	119.47	111.36
11	a	1118	CLA	CMB-C2B-C3B	2.22	129.02	124.89
11	B	1230	CLA	CMC-C2C-C1C	2.22	128.39	125.02
11	A	1104	CLA	CMB-C2B-C3B	2.23	129.02	124.89
14	2	4010	BCR	C30-C25-C24	2.23	121.99	115.73
11	B	1216	CLA	CAC-C3C-C4C	2.23	127.97	124.83
11	b	1228	CLA	C1-O2A-CGA	2.23	122.11	116.77
11	A	1108	CLA	CED-O2D-CGD	2.23	121.19	115.97
11	2	1235	CLA	C4A-NA-C1A	2.23	109.22	106.45
11	B	1219	CLA	C4A-NA-C1A	2.23	109.22	106.45
11	1	1105	CLA	C4A-NA-C1A	2.23	109.22	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1117	CLA	C4A-NA-C1A	2.23	109.22	106.45
11	a	1138	CLA	CED-O2D-CGD	2.23	121.19	115.97
11	A	1109	CLA	C9-C8-C7	2.23	119.49	111.36
11	a	1109	CLA	CAC-C3C-C4C	2.23	127.97	124.83
14	b	4009	BCR	C8-C9-C10	2.23	122.36	118.94
11	b	1215	CLA	C1-O2A-CGA	2.23	122.12	116.77
11	B	1228	CLA	C1-O2A-CGA	2.23	122.12	116.77
11	A	1131	CLA	C1-O2A-CGA	2.23	122.12	116.77
11	1	1138	CLA	CMB-C2B-C3B	2.23	129.03	124.89
11	b	1224	CLA	C4-C3-C5	2.23	119.16	115.29
11	1	1102	CLA	C4A-NA-C1A	2.23	109.22	106.45
14	7	4021	BCR	C19-C18-C17	2.23	122.37	118.94
11	B	1214	CLA	C9-C8-C10	2.23	119.50	111.36
14	l	4022	BCR	C30-C25-C24	2.23	122.01	115.73
11	2	1210	CLA	C1-O2A-CGA	2.23	122.13	116.77
11	a	1131	CLA	C9-C8-C7	2.24	119.51	111.36
11	A	1133	CLA	CMB-C2B-C3B	2.24	129.04	124.89
11	a	1137	CLA	C4A-NA-C1A	2.24	109.23	106.45
11	2	1211	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	a	1114	CLA	CMB-C2B-C3B	2.24	129.04	124.89
11	b	1013	CLA	CMC-C2C-C1C	2.24	128.41	125.02
11	b	1204	CLA	C4A-NA-C1A	2.24	109.23	106.45
11	b	1210	CLA	C4-C3-C5	2.24	119.17	115.29
11	1	1101	CLA	C9-C8-C10	2.24	119.53	111.36
11	A	1113	CLA	C4A-NA-C1A	2.24	109.23	106.45
11	a	1113	CLA	C4A-NA-C1A	2.24	109.23	106.45
11	B	1236	CLA	C4A-NA-C1A	2.24	109.23	106.45
11	1	1134	CLA	C4A-NA-C1A	2.24	109.23	106.45
14	A	4003	BCR	C19-C18-C17	2.24	122.38	118.94
11	1	1133	CLA	CMC-C2C-C1C	2.24	128.42	125.02
11	1	1116	CLA	C4A-NA-C1A	2.24	109.23	106.45
11	a	1129	CLA	CHB-C4A-NA	2.24	127.61	124.51
11	A	1135	CLA	CAC-C3C-C4C	2.24	127.99	124.83
11	a	1117	CLA	C1-O2A-CGA	2.24	122.15	116.77
12	2	2002	PQN	C2M-C2-C1	2.24	119.99	116.23
11	A	1022	CLA	C1-O2A-CGA	2.24	122.16	116.77
11	A	1133	CLA	CAC-C3C-C4C	2.24	128.00	124.83
11	a	1105	CLA	C4A-NA-C1A	2.25	109.24	106.45
11	a	1101	CLA	C9-C8-C7	2.25	119.55	111.36
11	1	1237	CLA	CAC-C3C-C4C	2.25	128.00	124.83
11	2	1234	CLA	C4A-NA-C1A	2.25	109.24	106.45
11	b	1228	CLA	C4A-NA-C1A	2.25	109.25	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1203	CLA	C4A-NA-C1A	2.25	109.25	106.45
11	A	1108	CLA	CHB-C4A-NA	2.25	127.62	124.51
11	1	1129	CLA	C4A-NA-C1A	2.25	109.25	106.45
11	A	1136	CLA	C4A-NA-C1A	2.25	109.25	106.45
11	b	1222	CLA	CHB-C4A-NA	2.25	127.62	124.51
11	1	1125	CLA	CMB-C2B-C3B	2.25	129.07	124.89
14	2	4006	BCR	C29-C28-C27	2.25	116.71	111.34
11	1	1123	CLA	C4A-NA-C1A	2.25	109.25	106.45
11	2	1224	CLA	CMB-C2B-C3B	2.25	129.07	124.89
11	a	1124	CLA	C4-C3-C5	2.25	119.20	115.29
11	a	1133	CLA	CMC-C2C-C1C	2.26	128.44	125.02
11	B	1201	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	1	1124	CLA	C4A-NA-C1A	2.26	109.25	106.45
11	B	1021	CLA	C9-C8-C10	2.26	119.59	111.36
11	A	1114	CLA	CAC-C3C-C4C	2.26	128.01	124.83
11	b	1231	CLA	CHB-C4A-NA	2.26	127.63	124.51
11	a	1022	CLA	C1-O2A-CGA	2.26	122.19	116.77
11	b	1023	CLA	C4-C3-C5	2.26	119.21	115.29
11	2	1214	CLA	CMB-C2B-C3B	2.26	129.08	124.89
11	B	1206	CLA	CMC-C2C-C1C	2.26	128.45	125.02
11	b	1211	CLA	CMB-C2B-C3B	2.26	129.09	124.89
11	a	1106	CLA	C4A-NA-C1A	2.26	109.26	106.45
11	B	1238	CLA	C1-O2A-CGA	2.26	122.19	116.77
11	a	1111	CLA	CHB-C4A-NA	2.26	127.64	124.51
11	2	1021	CLA	C4A-NA-C1A	2.26	109.26	106.45
14	2	4004	BCR	C30-C25-C24	2.26	122.08	115.73
14	1	4007	BCR	C34-C9-C8	2.26	121.70	118.10
11	a	1140	CLA	C4A-NA-C1A	2.26	109.26	106.45
11	2	1210	CLA	C4A-NA-C1A	2.26	109.26	106.45
11	b	1209	CLA	CMB-C2B-C3B	2.26	129.09	124.89
11	a	1134	CLA	CMB-C2B-C3B	2.26	129.09	124.89
11	a	1133	CLA	C4A-NA-C1A	2.26	109.26	106.45
11	b	1229	CLA	C4-C3-C5	2.26	119.22	115.29
11	B	1013	CLA	C4A-NA-C1A	2.27	109.26	106.45
11	b	1235	CLA	CHB-C4A-NA	2.27	127.64	124.51
11	a	1237	CLA	C1-O2A-CGA	2.27	122.21	116.77
11	2	1202	CLA	C1-O2A-CGA	2.27	122.21	116.77
14	A	4008	BCR	C1-C6-C7	2.27	122.10	115.73
11	1	1122	CLA	C1-O2A-CGA	2.27	122.21	116.77
11	1	1120	CLA	C4A-NA-C1A	2.27	109.27	106.45
11	B	1208	CLA	CMB-C2B-C3B	2.27	129.10	124.89
11	a	1012	CLA	C4A-NA-C1A	2.27	109.27	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	4021	BCR	C38-C26-C27	2.27	117.76	113.45
11	b	1013	CLA	CED-O2D-CGD	2.27	121.29	115.97
11	a	1135	CLA	C4A-NA-C1A	2.27	109.27	106.45
11	a	1106	CLA	CMB-C2B-C3B	2.27	129.10	124.89
11	2	1229	CLA	C4A-NA-C1A	2.27	109.27	106.45
11	2	1023	CLA	C4A-NA-C1A	2.27	109.27	106.45
11	1	1132	CLA	C4A-NA-C1A	2.27	109.27	106.45
11	B	1217	CLA	C4A-NA-C1A	2.27	109.27	106.45
11	b	1229	CLA	C9-C8-C10	2.27	119.65	111.36
11	b	1206	CLA	CMB-C2B-C3B	2.27	129.11	124.89
11	A	1122	CLA	CMB-C2B-C3B	2.28	129.11	124.89
11	a	1105	CLA	CAC-C3C-C4C	2.28	128.04	124.83
11	a	1114	CLA	C4A-NA-C1A	2.28	109.28	106.45
11	A	1134	CLA	C4A-NA-C1A	2.28	109.28	106.45
11	b	1227	CLA	CMB-C2B-C3B	2.28	129.12	124.89
11	b	1232	CLA	CAC-C3C-C4C	2.28	128.04	124.83
11	2	1228	CLA	C4A-NA-C1A	2.28	109.28	106.45
11	b	1207	CLA	CMC-C2C-C1C	2.28	128.47	125.02
11	a	1135	CLA	CMB-C2B-C3B	2.28	129.12	124.89
14	b	4004	BCR	C30-C25-C24	2.28	122.14	115.73
12	A	2001	PQN	C24-C23-C25	2.28	119.67	111.36
11	B	1222	CLA	C4A-NA-C1A	2.28	109.28	106.45
11	2	1214	CLA	C4-C3-C5	2.28	119.24	115.29
11	2	1217	CLA	C4A-NA-C1A	2.28	109.28	106.45
11	b	1202	CLA	C4-C3-C5	2.28	119.25	115.29
11	A	1105	CLA	C4A-NA-C1A	2.28	109.28	106.45
11	2	1209	CLA	CMC-C2C-C1C	2.28	128.48	125.02
11	a	1128	CLA	CMC-C2C-C1C	2.28	128.48	125.02
11	a	1109	CLA	CMB-C2B-C3B	2.28	129.13	124.89
11	A	1102	CLA	C1-O2A-CGA	2.28	122.25	116.77
11	a	1108	CLA	CMB-C2B-C3B	2.28	129.13	124.89
11	A	1116	CLA	C1-O2A-CGA	2.28	122.25	116.77
11	B	1232	CLA	C4A-NA-C1A	2.29	109.29	106.45
11	b	1202	CLA	C4A-NA-C1A	2.29	109.29	106.45
11	B	1227	CLA	CMC-C2C-C1C	2.29	128.49	125.02
11	a	1114	CLA	CAC-C3C-C4C	2.29	128.06	124.83
11	B	1223	CLA	CMB-C2B-C3B	2.29	129.14	124.89
11	2	1224	CLA	C4-C3-C5	2.29	119.26	115.29
11	b	1215	CLA	C9-C8-C7	2.29	119.71	111.36
11	A	1116	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	1	1237	CLA	CBA-CAA-C2A	2.29	120.65	113.80
12	2	2002	PQN	C24-C23-C25	2.29	119.72	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1023	CLA	CAC-C3C-C4C	2.29	128.06	124.83
11	b	1229	CLA	C9-C8-C7	2.29	119.72	111.36
11	A	1135	CLA	CHB-C4A-NA	2.29	127.68	124.51
11	A	1137	CLA	C4A-NA-C1A	2.29	109.30	106.45
11	2	1221	CLA	CMB-C2B-C3B	2.29	129.15	124.89
11	A	1138	CLA	CMB-C2B-C3B	2.29	129.15	124.89
11	2	1239	CLA	CMB-C2B-C3B	2.29	129.15	124.89
11	A	1112	CLA	C4A-NA-C1A	2.30	109.30	106.45
11	a	1102	CLA	CHB-C4A-NA	2.30	127.69	124.51
11	1	1116	CLA	CMB-C2B-C3B	2.30	129.15	124.89
11	a	1101	CLA	CED-O2D-CGD	2.30	121.35	115.97
11	L	1502	CLA	C4A-NA-C1A	2.30	109.30	106.45
11	a	1126	CLA	C4A-NA-C1A	2.30	109.30	106.45
11	b	1215	CLA	CMB-C2B-C3B	2.30	129.16	124.89
11	A	1123	CLA	C9-C8-C10	2.30	119.74	111.36
11	2	1240	CLA	C4A-NA-C1A	2.30	109.30	106.45
11	a	1117	CLA	C4-C3-C5	2.30	119.28	115.29
11	b	1021	CLA	CHB-C4A-NA	2.30	127.69	124.51
11	a	1012	CLA	C1-O2A-CGA	2.30	122.29	116.77
11	2	1232	CLA	CAC-C3C-C4C	2.30	128.07	124.83
11	2	1225	CLA	CAC-C3C-C4C	2.30	128.07	124.83
11	B	1215	CLA	C6-C5-C3	2.30	117.87	112.66
11	1	1022	CLA	CMB-C2B-C3B	2.30	129.16	124.89
11	B	1229	CLA	C4-C3-C5	2.30	119.28	115.29
11	2	1220	CLA	C4A-NA-C1A	2.30	109.31	106.45
11	b	1211	CLA	CAC-C3C-C4C	2.30	128.08	124.83
11	B	1207	CLA	CMC-C2C-C1C	2.30	128.51	125.02
11	2	1228	CLA	CED-O2D-CGD	2.30	121.37	115.97
11	A	1140	CLA	CAC-C3C-C4C	2.30	128.08	124.83
11	a	1127	CLA	CMB-C2B-C3B	2.30	129.17	124.89
11	B	1203	CLA	CMB-C2B-C3B	2.31	129.17	124.89
11	2	1239	CLA	C4A-NA-C1A	2.31	109.31	106.45
11	1	1118	CLA	C4-C3-C5	2.31	119.29	115.29
11	B	1229	CLA	C9-C8-C7	2.31	119.77	111.36
11	A	1237	CLA	CED-O2D-CGD	2.31	121.38	115.97
11	B	1239	CLA	CMB-C2B-C3B	2.31	129.17	124.89
11	a	1125	CLA	CMB-C2B-C3B	2.31	129.17	124.89
11	A	1117	CLA	C4-C3-C5	2.31	119.29	115.29
11	1	1139	CLA	CMB-C2B-C3B	2.31	129.18	124.89
11	a	1127	CLA	C10-C8-C7	2.31	123.19	112.10
11	L	1501	CLA	C4-C3-C5	2.31	119.29	115.29
11	b	1234	CLA	C4-C3-C5	2.31	119.30	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1133	CLA	CMC-C2C-C1C	2.31	128.52	125.02
14	2	4011	BCR	C35-C13-C12	2.31	121.78	118.10
11	1	1801	CLA	CHB-C4A-NA	2.31	127.71	124.51
11	1	1123	CLA	C9-C8-C10	2.31	119.80	111.36
11	b	1224	CLA	C4A-NA-C1A	2.31	109.33	106.45
11	a	1106	CLA	CHB-C4A-NA	2.31	127.71	124.51
11	A	1133	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	2	1013	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	B	1203	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	2	1216	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	1	1103	CLA	CAC-C3C-C4C	2.32	128.10	124.83
11	1	1107	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	l	1501	CLA	CMB-C2B-C3B	2.32	129.19	124.89
11	1	1104	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	B	1231	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	b	1023	CLA	C4A-NA-C1A	2.32	109.33	106.45
14	8	4019	BCR	C1-C6-C7	2.32	122.25	115.73
11	b	1228	CLA	CMC-C2C-C1C	2.32	128.54	125.02
11	b	1224	CLA	CMB-C2B-C3B	2.32	129.20	124.89
11	A	1117	CLA	C9-C8-C10	2.32	119.83	111.36
11	A	1131	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	1	1137	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	B	1226	CLA	C4A-NA-C1A	2.32	109.33	106.45
11	A	1107	CLA	CHB-C4A-NA	2.32	127.72	124.51
11	2	1207	CLA	CHB-C4A-NA	2.32	127.73	124.51
11	1	1121	CLA	C4A-NA-C1A	2.33	109.34	106.45
14	a	4007	BCR	C34-C9-C8	2.33	121.81	118.10
11	1	1135	CLA	C4A-NA-C1A	2.33	109.34	106.45
11	b	1222	CLA	CMB-C2B-C3B	2.33	129.21	124.89
16	B	5002	LMG	O8-C28-C29	2.33	118.68	111.90
11	b	1213	CLA	C4A-NA-C1A	2.33	109.34	106.45
11	A	1123	CLA	C4A-NA-C1A	2.33	109.34	106.45
11	B	1214	CLA	CAC-C3C-C4C	2.33	128.12	124.83
11	a	1136	CLA	C4A-NA-C1A	2.33	109.34	106.45
11	2	1221	CLA	CHB-C4A-NA	2.33	127.74	124.51
11	A	1118	CLA	C4-C3-C5	2.33	119.33	115.29
11	A	1123	CLA	C4-C3-C5	2.33	119.34	115.29
11	B	1214	CLA	C4A-NA-C1A	2.33	109.35	106.45
11	B	1218	CLA	C4A-NA-C1A	2.33	109.35	106.45
11	1	1108	CLA	C4A-NA-C1A	2.33	109.35	106.45
11	b	1205	CLA	C4-C3-C5	2.33	119.34	115.29
14	1	4002	BCR	C35-C13-C12	2.34	121.82	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1234	CLA	C9-C8-C10	2.34	119.89	111.36
11	A	1125	CLA	C1-O2A-CGA	2.34	122.38	116.77
11	B	1021	CLA	CMC-C2C-C1C	2.34	128.57	125.02
14	2	4005	BCR	C33-C5-C4	2.34	117.89	113.45
11	B	1229	CLA	C9-C8-C10	2.34	119.89	111.36
11	B	1220	CLA	CMB-C2B-C3B	2.34	129.24	124.89
11	A	1134	CLA	CMC-C2C-C1C	2.34	128.57	125.02
11	a	1012	CLA	CMB-C2B-C3B	2.34	129.24	124.89
11	b	1222	CLA	C4A-NA-C1A	2.34	109.36	106.45
11	1	1801	CLA	CMB-C2B-C3B	2.34	129.24	124.89
11	A	1117	CLA	CMC-C2C-C1C	2.34	128.57	125.02
11	2	1234	CLA	C9-C8-C7	2.35	119.91	111.36
11	B	1213	CLA	C4A-NA-C1A	2.35	109.36	106.45
11	b	1235	CLA	C4A-NA-C1A	2.35	109.36	106.45
11	B	1210	CLA	CMC-C2C-C1C	2.35	128.58	125.02
11	B	1214	CLA	CHB-C4A-NA	2.35	127.76	124.51
11	A	1111	CLA	CMB-C2B-C3B	2.35	129.25	124.89
11	1	1104	CLA	CMB-C2B-C3B	2.35	129.25	124.89
11	A	1118	CLA	C3C-C4C-NC	2.35	112.59	110.21
11	A	1022	CLA	C4-C3-C5	2.35	119.36	115.29
11	2	1216	CLA	CAC-C3C-C4C	2.35	128.14	124.83
11	1	1118	CLA	CMB-C2B-C3B	2.35	129.25	124.89
16	b	5002	LMG	O8-C28-C29	2.35	118.73	111.90
11	b	1229	CLA	C1-O2A-CGA	2.35	122.41	116.77
11	B	1023	CLA	C4A-NA-C1A	2.35	109.37	106.45
11	1	1119	CLA	C9-C8-C7	2.35	119.93	111.36
11	A	1133	CLA	CHB-C4A-NA	2.35	127.76	124.51
14	1	4003	BCR	C19-C18-C17	2.35	122.55	118.94
11	B	1236	CLA	CMB-C2B-C3B	2.35	129.25	124.89
11	K	1402	CLA	C4A-NA-C1A	2.35	109.37	106.45
11	a	1117	CLA	C4A-NA-C1A	2.35	109.37	106.45
11	A	1124	CLA	CMB-C2B-C3B	2.35	129.26	124.89
12	a	2001	PQN	C2M-C2-C1	2.35	120.17	116.23
11	A	1126	CLA	C4A-NA-C1A	2.35	109.37	106.45
11	B	1216	CLA	C4-C3-C5	2.35	119.37	115.29
11	2	1223	CLA	C9-C8-C7	2.35	119.94	111.36
11	1	1118	CLA	C4A-NA-C1A	2.35	109.37	106.45
11	A	1106	CLA	CHB-C4A-NA	2.36	127.77	124.51
11	B	1215	CLA	CMB-C2B-C3B	2.36	129.27	124.89
11	a	1101	CLA	CMB-C2B-C3B	2.36	129.27	124.89
11	b	1240	CLA	CMB-C2B-C3B	2.36	129.27	124.89
11	2	1201	CLA	CMC-C2C-C1C	2.36	128.60	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1801	CLA	C4A-NA-C1A	2.36	109.38	106.45
11	a	1134	CLA	CAC-C3C-C4C	2.36	128.16	124.83
11	B	1218	CLA	CMB-C2B-C3B	2.36	129.27	124.89
11	A	1128	CLA	C4A-NA-C1A	2.36	109.38	106.45
14	L	4022	BCR	C23-C22-C21	2.36	122.56	118.94
11	A	1103	CLA	C4A-NA-C1A	2.36	109.39	106.45
11	k	1401	CLA	CBA-CAA-C2A	2.36	120.87	113.80
11	b	1209	CLA	CHB-C4A-NA	2.36	127.78	124.51
11	1	1109	CLA	CMB-C2B-C3B	2.36	129.28	124.89
11	A	1110	CLA	C4A-NA-C1A	2.36	109.39	106.45
11	1	1101	CLA	C9-C8-C7	2.36	119.98	111.36
11	A	1012	CLA	C4A-NA-C1A	2.36	109.39	106.45
11	B	1221	CLA	CHB-C4A-NA	2.36	127.78	124.51
14	b	4006	BCR	C23-C22-C21	2.36	122.57	118.94
11	A	1111	CLA	C4A-NA-C1A	2.37	109.39	106.45
11	2	1222	CLA	CMB-C2B-C3B	2.37	129.28	124.89
11	b	1225	CLA	C1-O2A-CGA	2.37	122.45	116.77
11	2	1238	CLA	C1-O2A-CGA	2.37	122.45	116.77
11	B	1225	CLA	CMB-C2B-C3B	2.37	129.28	124.89
11	a	1138	CLA	CMB-C2B-C3B	2.37	129.28	124.89
11	A	1109	CLA	C3C-C4C-NC	2.37	112.61	110.21
11	A	1109	CLA	CMB-C2B-C3B	2.37	129.29	124.89
11	2	1206	CLA	C4A-NA-C1A	2.37	109.39	106.45
11	b	1219	CLA	C4A-NA-C1A	2.37	109.39	106.45
11	l	1502	CLA	C4A-NA-C1A	2.37	109.39	106.45
11	A	1128	CLA	CMC-C2C-C1C	2.37	128.61	125.02
11	a	1102	CLA	C4A-NA-C1A	2.37	109.39	106.45
14	b	4006	BCR	C1-C6-C7	2.37	122.39	115.73
11	A	1237	CLA	CHB-C4A-NA	2.37	127.79	124.51
11	2	1021	CLA	C9-C8-C10	2.37	120.01	111.36
11	K	1401	CLA	CBA-CAA-C2A	2.37	120.89	113.80
11	2	1240	CLA	CMC-C2C-C1C	2.37	128.62	125.02
11	b	1232	CLA	CMB-C2B-C3B	2.37	129.29	124.89
11	K	1401	CLA	C1-O2A-CGA	2.37	122.47	116.77
11	0	1401	CLA	C1-O2A-CGA	2.37	122.47	116.77
14	2	4006	BCR	C23-C22-C21	2.37	122.58	118.94
11	1	1139	CLA	CAC-C3C-C4C	2.37	128.18	124.83
11	1	1136	CLA	C4A-NA-C1A	2.37	109.40	106.45
11	2	1203	CLA	CED-O2D-CGD	2.37	121.54	115.97
11	a	1105	CLA	CMB-C2B-C3B	2.37	129.30	124.89
11	B	1230	CLA	C4A-NA-C1A	2.38	109.40	106.45
11	B	1206	CLA	CAC-C3C-C4C	2.38	128.18	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1111	CLA	CMB-C2B-C3B	2.38	129.30	124.89
11	1	1120	CLA	CMB-C2B-C3B	2.38	129.30	124.89
11	1	1119	CLA	CMB-C2B-C3B	2.38	129.30	124.89
14	2	4011	BCR	C23-C22-C21	2.38	122.59	118.94
11	A	1022	CLA	CMC-C2C-C1C	2.38	128.62	125.02
11	k	1401	CLA	C1-O2A-CGA	2.38	122.48	116.77
11	8	1501	CLA	CHB-C4A-NA	2.38	127.80	124.51
11	A	1801	CLA	C1-O2A-CGA	2.38	122.48	116.77
11	a	1121	CLA	CMB-C2B-C3B	2.38	129.31	124.89
11	a	1107	CLA	CMC-C2C-C1C	2.38	128.63	125.02
11	0	1401	CLA	CBA-CAA-C2A	2.38	120.92	113.80
11	2	1208	CLA	C4A-NA-C1A	2.38	109.41	106.45
11	B	1234	CLA	C4A-NA-C1A	2.38	109.41	106.45
11	L	1501	CLA	CMB-C2B-C3B	2.38	129.31	124.89
11	a	1108	CLA	CAC-C3C-C4C	2.38	128.19	124.83
11	8	1502	CLA	C4A-NA-C1A	2.38	109.41	106.45
11	b	1221	CLA	C4A-NA-C1A	2.38	109.41	106.45
11	A	1101	CLA	CMB-C2B-C3B	2.39	129.32	124.89
11	b	1206	CLA	CMC-C2C-C1C	2.39	128.64	125.02
11	b	1231	CLA	C4A-NA-C1A	2.39	109.41	106.45
11	1	1011	CLA	CAA-C2A-C1A	2.39	119.80	111.97
11	A	1107	CLA	C4A-NA-C1A	2.39	109.42	106.45
11	A	1128	CLA	C4-C3-C5	2.39	119.43	115.29
11	B	1229	CLA	C1-O2A-CGA	2.39	122.50	116.77
11	B	1210	CLA	C4-C3-C5	2.39	119.43	115.29
11	a	1125	CLA	C4-C3-C5	2.39	119.43	115.29
11	b	1216	CLA	C9-C8-C7	2.39	120.08	111.36
11	2	1226	CLA	CMC-C2C-C1C	2.39	128.65	125.02
11	b	1221	CLA	CMB-C2B-C3B	2.39	129.33	124.89
11	A	1110	CLA	CMB-C2B-C3B	2.39	129.33	124.89
11	B	1238	CLA	C4A-NA-C1A	2.39	109.42	106.45
11	2	1217	CLA	CMC-C2C-C1C	2.39	128.65	125.02
11	1	1135	CLA	CMB-C2B-C3B	2.39	129.33	124.89
11	A	1012	CLA	CMC-C2C-C1C	2.39	128.65	125.02
11	b	1225	CLA	C9-C8-C7	2.39	120.09	111.36
11	1	1140	CLA	C4A-NA-C1A	2.39	109.42	106.45
11	B	1238	CLA	CMB-C2B-C3B	2.39	129.33	124.89
11	1	1108	CLA	CMB-C2B-C3B	2.39	129.34	124.89
11	K	1401	CLA	C4A-NA-C1A	2.39	109.42	106.45
11	b	1222	CLA	C9-C8-C7	2.40	120.10	111.36
11	0	1401	CLA	C4A-NA-C1A	2.40	109.43	106.45
11	B	1240	CLA	C4A-NA-C1A	2.40	109.43	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	1401	CLA	C4A-NA-C1A	2.40	109.43	106.45
11	b	1206	CLA	CAC-C3C-C4C	2.40	128.21	124.83
14	L	4022	BCR	C35-C13-C12	2.40	121.92	118.10
11	a	1103	CLA	CED-O2D-CGD	2.40	121.60	115.97
11	B	1216	CLA	CMC-C2C-C1C	2.40	128.66	125.02
11	A	1107	CLA	CMC-C2C-C1C	2.40	128.66	125.02
11	1	1127	CLA	CMB-C2B-C3B	2.40	129.35	124.89
11	a	1136	CLA	CMC-C2C-C1C	2.40	128.66	125.02
11	1	1137	CLA	C9-C8-C7	2.40	120.13	111.36
11	a	1110	CLA	C4-C3-C5	2.40	119.46	115.29
11	L	1502	CLA	CMB-C2B-C3B	2.41	129.35	124.89
11	b	1013	CLA	CHB-C4A-NA	2.41	127.84	124.51
11	B	1202	CLA	C1-O2A-CGA	2.41	122.54	116.77
11	2	1227	CLA	C4A-NA-C1A	2.41	109.44	106.45
11	L	1503	CLA	C4-C3-C5	2.41	119.46	115.29
11	A	1132	CLA	C4A-NA-C1A	2.41	109.44	106.45
11	A	1131	CLA	C9-C8-C10	2.41	120.14	111.36
11	b	1023	CLA	CMB-C2B-C3B	2.41	129.36	124.89
11	1	1502	CLA	CMB-C2B-C3B	2.41	129.37	124.89
11	a	1119	CLA	C9-C8-C7	2.41	120.15	111.36
11	a	1113	CLA	CMB-C2B-C3B	2.41	129.37	124.89
11	b	1210	CLA	C9-C8-C10	2.41	120.16	111.36
14	B	4009	BCR	C33-C5-C4	2.41	118.03	113.45
11	B	1229	CLA	CMC-C2C-C1C	2.41	128.68	125.02
11	1	1012	CLA	C4A-NA-C1A	2.42	109.45	106.45
11	a	1104	CLA	CMB-C2B-C3B	2.42	129.38	124.89
11	2	1203	CLA	C4A-NA-C1A	2.42	109.45	106.45
11	1	1113	CLA	C4A-NA-C1A	2.42	109.45	106.45
11	a	1138	CLA	C4A-NA-C1A	2.42	109.45	106.45
11	1	1137	CLA	CMC-C2C-C1C	2.42	128.69	125.02
11	B	1213	CLA	C9-C8-C10	2.42	120.18	111.36
11	a	1131	CLA	CMB-C2B-C3B	2.42	129.38	124.89
11	A	1129	CLA	CMC-C2C-C1C	2.42	128.69	125.02
11	2	1215	CLA	CMC-C2C-C1C	2.42	128.69	125.02
11	b	1226	CLA	C4-C3-C5	2.42	119.48	115.29
11	B	1224	CLA	C4A-NA-C1A	2.42	109.45	106.45
14	1	4001	BCR	C35-C13-C12	2.42	121.95	118.10
14	L	4019	BCR	C1-C6-C7	2.42	122.53	115.73
11	2	1211	CLA	C4A-NA-C1A	2.42	109.45	106.45
11	B	1202	CLA	CHB-C4A-NA	2.42	127.86	124.51
11	a	1124	CLA	CMC-C2C-C1C	2.42	128.69	125.02
11	B	1201	CLA	C4-C3-C5	2.42	119.49	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1011	CLA	CMC-C2C-C1C	2.43	128.70	125.02
11	2	1222	CLA	C9-C8-C7	2.43	120.21	111.36
11	A	1102	CLA	C4A-NA-C1A	2.43	109.46	106.45
11	A	1134	CLA	CED-O2D-CGD	2.43	121.66	115.97
11	2	1229	CLA	C9-C8-C7	2.43	120.21	111.36
11	B	1231	CLA	CHB-C4A-NA	2.43	127.87	124.51
11	b	1225	CLA	CAC-C3C-C4C	2.43	128.25	124.83
11	B	1225	CLA	C1-O2A-CGA	2.43	122.60	116.77
11	2	1207	CLA	CAC-C3C-C4C	2.43	128.26	124.83
11	b	1230	CLA	CMC-C2C-C1C	2.43	128.71	125.02
11	a	1022	CLA	CMB-C2B-C3B	2.43	129.40	124.89
11	a	1129	CLA	C4A-NA-C1A	2.43	109.47	106.45
11	a	1104	CLA	C9-C8-C10	2.43	120.23	111.36
11	B	1210	CLA	C4A-NA-C1A	2.43	109.47	106.45
12	A	2001	PQN	C24-C23-C22	2.43	120.23	111.36
11	a	1102	CLA	C1-O2A-CGA	2.43	122.61	116.77
11	B	1209	CLA	CMC-C2C-C1C	2.43	128.71	125.02
11	A	1116	CLA	CAC-C3C-C4C	2.43	128.26	124.83
11	l	1501	CLA	C4A-NA-C1A	2.44	109.48	106.45
11	b	1206	CLA	C4A-NA-C1A	2.44	109.48	106.45
11	a	1137	CLA	C1-O2A-CGA	2.44	122.62	116.77
11	L	1502	CLA	CMC-C2C-C1C	2.44	128.72	125.02
11	B	1214	CLA	CMB-C2B-C3B	2.44	129.41	124.89
14	l	4022	BCR	C35-C13-C12	2.44	121.98	118.10
14	a	4002	BCR	C30-C25-C24	2.44	122.58	115.73
14	A	4007	BCR	C35-C13-C12	2.44	121.98	118.10
11	b	1239	CLA	C4A-NA-C1A	2.44	109.48	106.45
11	b	1234	CLA	C4A-NA-C1A	2.44	109.48	106.45
11	2	1013	CLA	CED-O2D-CGD	2.44	121.69	115.97
12	A	2001	PQN	C14-C13-C15	2.44	119.52	115.29
12	1	2001	PQN	C14-C13-C15	2.44	119.52	115.29
11	b	1203	CLA	CMB-C2B-C3B	2.44	129.42	124.89
11	b	1221	CLA	C1-O2A-CGA	2.44	122.63	116.77
11	2	1204	CLA	CMB-C2B-C3B	2.44	129.43	124.89
11	A	1130	CLA	CMB-C2B-C3B	2.44	129.43	124.89
11	1	1116	CLA	C1-O2A-CGA	2.44	122.63	116.77
11	A	1108	CLA	CMB-C2B-C3B	2.44	129.43	124.89
11	b	1210	CLA	CMB-C2B-C3B	2.44	129.43	124.89
14	2	4005	BCR	C19-C18-C17	2.45	122.69	118.94
11	2	1227	CLA	CMC-C2C-C1C	2.45	128.73	125.02
11	2	1220	CLA	CMB-C2B-C3B	2.45	129.43	124.89
11	B	1203	CLA	C9-C8-C7	2.45	120.29	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1120	CLA	CHB-C4A-NA	2.45	127.90	124.51
11	a	1116	CLA	CMC-C2C-C1C	2.45	128.74	125.02
11	a	1119	CLA	C9-C8-C10	2.45	120.30	111.36
11	B	1217	CLA	CMC-C2C-C1C	2.45	128.74	125.02
11	L	1503	CLA	C4A-NA-C1A	2.45	109.50	106.45
11	2	1209	CLA	CMB-C2B-C3B	2.45	129.45	124.89
11	A	1114	CLA	CMC-C2C-C1C	2.45	128.74	125.02
11	A	1132	CLA	CMC-C2C-C1C	2.45	128.74	125.02
11	b	1216	CLA	C4-C3-C5	2.45	119.55	115.29
11	B	1215	CLA	CMC-C2C-C1C	2.46	128.74	125.02
11	B	1210	CLA	CMB-C2B-C3B	2.46	129.45	124.89
11	a	1110	CLA	CMB-C2B-C3B	2.46	129.45	124.89
11	2	1210	CLA	C4-C3-C5	2.46	119.55	115.29
11	B	1220	CLA	CMC-C2C-C1C	2.46	128.75	125.02
11	b	1215	CLA	C9-C8-C10	2.46	120.32	111.36
11	1	1131	CLA	CMB-C2B-C3B	2.46	129.45	124.89
11	b	1230	CLA	CMB-C2B-C3B	2.46	129.46	124.89
11	1	1110	CLA	CMB-C2B-C3B	2.46	129.46	124.89
11	1	1801	CLA	CMC-C2C-C3C	2.46	132.90	126.09
11	1	1012	CLA	CMB-C2B-C3B	2.46	129.46	124.89
11	B	1230	CLA	CMB-C2B-C3B	2.46	129.46	124.89
11	A	1116	CLA	C4-C3-C5	2.46	119.56	115.29
11	1	1119	CLA	C9-C8-C10	2.46	120.34	111.36
11	a	1120	CLA	CMC-C2C-C1C	2.46	128.75	125.02
11	a	1115	CLA	CMB-C2B-C3B	2.46	129.46	124.89
11	b	1210	CLA	C1-O2A-CGA	2.46	122.68	116.77
11	B	1217	CLA	CMB-C2B-C3B	2.46	129.46	124.89
11	A	1104	CLA	CMC-C2C-C1C	2.46	128.76	125.02
11	B	1234	CLA	C4-C3-C5	2.46	119.56	115.29
11	b	1230	CLA	CAC-C3C-C4C	2.46	128.31	124.83
14	2	4017	BCR	C1-C6-C7	2.47	122.66	115.73
11	B	1205	CLA	CMC-C2C-C1C	2.47	128.76	125.02
14	B	4010	BCR	C30-C25-C24	2.47	122.66	115.73
14	B	4004	BCR	C30-C25-C24	2.47	122.66	115.73
14	B	4006	BCR	C19-C18-C17	2.47	122.73	118.94
11	b	1213	CLA	CMB-C2B-C3B	2.47	129.47	124.89
11	0	1401	CLA	CHB-C4A-NA	2.47	127.93	124.51
11	2	1236	CLA	CMB-C2B-C3B	2.47	129.47	124.89
11	B	1211	CLA	CMC-C2C-C1C	2.47	128.77	125.02
11	1	1107	CLA	CMC-C2C-C1C	2.47	128.77	125.02
11	2	1226	CLA	C4A-NA-C1A	2.47	109.52	106.45
11	K	1401	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	a	2001	PQN	C14-C13-C15	2.47	119.58	115.29
11	A	1115	CLA	CMB-C2B-C3B	2.47	129.48	124.89
11	a	1131	CLA	C4-C3-C5	2.47	119.58	115.29
11	A	1102	CLA	C9-C8-C7	2.47	120.38	111.36
11	A	1111	CLA	CHB-C4A-NA	2.47	127.93	124.51
11	1	1117	CLA	CMC-C2C-C1C	2.48	128.77	125.02
11	B	1023	CLA	CHB-C4A-NA	2.48	127.94	124.51
11	2	1217	CLA	C1-O2A-CGA	2.48	124.00	116.72
11	b	1208	CLA	CAC-C3C-C4C	2.48	128.33	124.83
11	2	1231	CLA	CHB-C4A-NA	2.48	127.94	124.51
11	2	1224	CLA	C4A-NA-C1A	2.48	109.53	106.45
11	L	1501	CLA	C4A-NA-C1A	2.48	109.53	106.45
11	b	1223	CLA	C4-C3-C5	2.48	119.59	115.29
11	b	1220	CLA	CMC-C2C-C1C	2.48	128.78	125.02
11	B	1021	CLA	C9-C8-C7	2.48	120.41	111.36
11	a	1139	CLA	CAC-C3C-C4C	2.48	128.33	124.83
11	1	1103	CLA	C9-C8-C7	2.48	120.42	111.36
11	2	1023	CLA	CAC-C3C-C4C	2.48	128.33	124.83
11	2	1219	CLA	C4A-NA-C1A	2.48	109.54	106.45
11	k	1402	CLA	CMC-C2C-C1C	2.49	128.79	125.02
14	8	4019	BCR	C33-C5-C4	2.49	118.17	113.45
11	a	1123	CLA	CMB-C2B-C3B	2.49	129.51	124.89
11	k	1401	CLA	CHB-C4A-NA	2.49	127.95	124.51
11	B	1223	CLA	CMC-C2C-C1C	2.49	128.79	125.02
11	1	1138	CLA	CMC-C2C-C1C	2.49	128.79	125.02
11	A	1112	CLA	CHB-C4A-NA	2.49	127.95	124.51
14	f	4020	BCR	C19-C18-C17	2.49	122.76	118.94
11	B	1202	CLA	CMC-C2C-C1C	2.49	128.80	125.02
11	a	1103	CLA	CMB-C2B-C3B	2.49	129.52	124.89
14	F	4018	BCR	C8-C9-C10	2.49	122.77	118.94
11	8	1502	CLA	CMC-C2C-C1C	2.49	128.80	125.02
11	B	1224	CLA	CMB-C2B-C3B	2.49	129.52	124.89
11	B	1239	CLA	C4A-NA-C1A	2.49	109.55	106.45
14	B	4004	BCR	C19-C18-C17	2.49	122.77	118.94
11	b	1206	CLA	C1-O2A-CGA	2.50	122.76	116.77
11	b	1202	CLA	CHB-C4A-NA	2.50	127.96	124.51
14	b	4006	BCR	C35-C13-C12	2.50	122.08	118.10
11	A	1119	CLA	CAC-C3C-C4C	2.50	128.35	124.83
11	A	1139	CLA	CMB-C2B-C3B	2.50	129.53	124.89
11	A	1119	CLA	C9-C8-C10	2.50	120.47	111.36
11	A	1104	CLA	C9-C8-C10	2.50	120.47	111.36
11	A	1103	CLA	CHB-C4A-NA	2.50	127.97	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1124	CLA	CAC-C3C-C4C	2.50	128.35	124.83
11	a	1138	CLA	CMC-C2C-C1C	2.50	128.81	125.02
11	k	1402	CLA	C1-O2A-CGA	2.50	122.77	116.77
14	b	4005	BCR	C33-C5-C4	2.50	118.19	113.45
11	B	1234	CLA	C9-C8-C10	2.50	120.47	111.36
14	l	4019	BCR	C19-C18-C17	2.50	122.78	118.94
11	2	1213	CLA	CMC-C2C-C3C	2.50	133.02	126.09
11	A	1012	CLA	CMB-C2B-C3B	2.51	129.54	124.89
11	A	1128	CLA	C9-C8-C7	2.51	120.50	111.36
11	a	1117	CLA	CMB-C2B-C3B	2.51	129.54	124.89
11	1	1104	CLA	C9-C8-C10	2.51	120.50	111.36
11	A	1237	CLA	CMC-C2C-C1C	2.51	128.82	125.02
11	0	1401	CLA	CAA-C2A-C3A	2.51	119.69	112.81
11	a	1107	CLA	C9-C8-C7	2.51	120.51	111.36
11	K	1401	CLA	CAA-C2A-C3A	2.51	119.69	112.81
11	A	1237	CLA	C4A-NA-C1A	2.51	109.57	106.45
11	b	1212	CLA	C4A-NA-C1A	2.51	109.57	106.45
11	2	1226	CLA	C9-C8-C7	2.51	120.52	111.36
11	1	1138	CLA	C4A-NA-C1A	2.51	109.57	106.45
11	A	1140	CLA	C4A-NA-C1A	2.51	109.57	106.45
11	a	1124	CLA	CED-O2D-CGD	2.51	121.86	115.97
14	l	4022	BCR	C19-C18-C17	2.51	122.80	118.94
12	1	2001	PQN	C24-C23-C25	2.51	120.53	111.36
11	2	1211	CLA	CMB-C2B-C3B	2.51	129.56	124.89
14	7	4021	BCR	C33-C5-C4	2.51	118.22	113.45
14	a	4003	BCR	C38-C26-C27	2.51	118.22	113.45
11	1	1110	CLA	CAC-C3C-C4C	2.51	128.38	124.83
11	2	1021	CLA	CMC-C2C-C1C	2.51	128.83	125.02
11	a	1116	CLA	C1-O2A-CGA	2.51	122.81	116.77
11	B	1224	CLA	C1-O2A-CGA	2.51	122.81	116.77
11	B	1228	CLA	CMB-C2B-C3B	2.52	129.56	124.89
11	A	1124	CLA	CMC-C2C-C1C	2.52	128.84	125.02
11	A	1138	CLA	C4A-NA-C1A	2.52	109.58	106.45
11	B	1204	CLA	C4A-NA-C1A	2.52	109.58	106.45
11	A	1101	CLA	C9-C8-C7	2.52	120.55	111.36
11	2	1228	CLA	CMC-C2C-C1C	2.52	128.84	125.02
11	A	1121	CLA	CMB-C2B-C3B	2.52	129.57	124.89
11	2	1218	CLA	C4A-NA-C1A	2.52	109.58	106.45
11	a	1123	CLA	C9-C8-C10	2.52	120.56	111.36
11	A	1125	CLA	CMB-C2B-C3B	2.52	129.57	124.89
14	b	4005	BCR	C19-C18-C17	2.52	122.81	118.94
11	A	1125	CLA	CMC-C2C-C1C	2.52	128.85	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4005	BCR	C35-C13-C12	2.52	122.12	118.10
11	A	1110	CLA	C4-C3-C5	2.53	119.67	115.29
11	b	1203	CLA	C4-C3-C5	2.53	119.67	115.29
11	1	1117	CLA	C4-C3-C5	2.53	119.67	115.29
11	k	1401	CLA	CAA-C2A-C3A	2.53	119.74	112.81
11	2	1212	CLA	CMB-C2B-C3B	2.53	129.59	124.89
11	b	1201	CLA	C4-C3-C5	2.53	119.68	115.29
11	A	1109	CLA	CED-O2D-CGD	2.53	121.91	115.97
11	B	1227	CLA	C4A-NA-C1A	2.53	109.60	106.45
11	a	1111	CLA	C4A-NA-C1A	2.53	109.60	106.45
11	2	1234	CLA	C4-C3-C5	2.53	119.69	115.29
11	2	1240	CLA	CMB-C2B-C3B	2.54	129.60	124.89
11	8	1501	CLA	C4A-NA-C1A	2.54	109.60	106.45
11	B	1023	CLA	CMC-C2C-C1C	2.54	128.87	125.02
11	B	1013	CLA	CMB-C2B-C3B	2.54	129.60	124.89
11	0	1402	CLA	CMC-C2C-C1C	2.54	128.87	125.02
11	1	1134	CLA	CMB-C2B-C3B	2.54	129.61	124.89
11	1	1117	CLA	C9-C8-C7	2.54	120.63	111.36
11	A	1140	CLA	C1-O2A-CGA	2.54	122.87	116.77
11	8	1503	CLA	C4-C3-C5	2.54	119.70	115.29
11	A	1237	CLA	CMB-C2B-C3B	2.54	129.61	124.89
11	b	1214	CLA	CMB-C2B-C3B	2.54	129.61	124.89
11	2	1201	CLA	C4A-NA-C1A	2.54	109.61	106.45
11	b	1205	CLA	C4A-NA-C1A	2.54	109.61	106.45
14	F	4018	BCR	C38-C26-C27	2.54	118.28	113.45
11	b	1240	CLA	CMC-C2C-C1C	2.54	128.88	125.02
11	1	1109	CLA	CMC-C2C-C1C	2.54	128.88	125.02
11	1	1117	CLA	CMB-C2B-C3B	2.55	129.62	124.89
11	1	1237	CLA	C4A-NA-C1A	2.55	109.62	106.45
11	2	1223	CLA	C9-C8-C10	2.55	120.66	111.36
11	b	1023	CLA	CHB-C4A-NA	2.55	128.04	124.51
11	A	1012	CLA	CHB-C4A-NA	2.55	128.04	124.51
14	l	4019	BCR	C33-C5-C4	2.55	118.29	113.45
11	2	1203	CLA	C9-C8-C7	2.55	120.67	111.36
14	m	4021	BCR	C33-C5-C4	2.55	118.30	113.45
11	1	1801	CLA	CAC-C3C-C2C	2.55	131.92	127.49
11	1	1122	CLA	CMB-C2B-C3B	2.55	129.63	124.89
11	2	1230	CLA	CMB-C2B-C3B	2.55	129.63	124.89
11	b	1201	CLA	CMC-C2C-C1C	2.55	128.89	125.02
11	1	1136	CLA	CMC-C2C-C1C	2.55	128.89	125.02
11	a	1237	CLA	C4A-NA-C1A	2.55	109.62	106.45
11	A	1104	CLA	C4A-NA-C1A	2.55	109.62	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1109	CLA	C3C-C4C-NC	2.56	112.80	110.21
14	f	4018	BCR	C35-C13-C12	2.56	122.17	118.10
11	2	1202	CLA	C4-C3-C5	2.56	119.72	115.29
11	b	1021	CLA	C9-C8-C10	2.56	120.69	111.36
11	A	1130	CLA	CMC-C2C-C1C	2.56	128.90	125.02
11	B	1206	CLA	C4A-NA-C1A	2.56	109.63	106.45
11	B	1204	CLA	C4-C3-C5	2.56	119.73	115.29
11	8	1501	CLA	CMB-C2B-C3B	2.56	129.65	124.89
11	2	1221	CLA	C4A-NA-C1A	2.56	109.63	106.45
11	2	1211	CLA	O2A-CGA-CBA	2.56	122.90	112.33
11	A	1117	CLA	C1-O2A-CGA	2.56	122.92	116.77
11	A	1104	CLA	C4-C3-C5	2.56	119.73	115.29
11	A	1113	CLA	CMB-C2B-C3B	2.57	129.65	124.89
14	B	4014	BCR	C19-C18-C17	2.57	122.88	118.94
11	1	1133	CLA	CAC-C3C-C4C	2.57	128.45	124.83
14	1	4001	BCR	C19-C18-C17	2.57	122.88	118.94
11	a	1138	CLA	C3C-C4C-NC	2.57	112.81	110.21
11	a	1121	CLA	CAC-C3C-C4C	2.57	128.46	124.83
11	b	1217	CLA	CMC-C2C-C1C	2.57	128.92	125.02
11	A	1118	CLA	C4A-NA-C1A	2.57	109.64	106.45
14	A	4007	BCR	C33-C5-C4	2.57	118.33	113.45
11	B	1224	CLA	C4-C3-C5	2.58	119.76	115.29
14	f	4018	BCR	C38-C26-C27	2.58	118.34	113.45
11	b	1201	CLA	C4A-NA-C1A	2.58	109.65	106.45
11	2	1013	CLA	C4-C3-C5	2.58	119.76	115.29
11	B	1021	CLA	C4A-NA-C1A	2.58	109.66	106.45
11	b	1209	CLA	CAC-C3C-C4C	2.58	128.47	124.83
11	A	1121	CLA	CMC-C2C-C1C	2.58	128.94	125.02
11	a	1109	CLA	C3C-C4C-NC	2.58	112.83	110.21
11	1	1118	CLA	C1-O2A-CGA	2.58	122.97	116.77
11	A	1122	CLA	CMC-C2C-C1C	2.58	128.94	125.02
14	8	4022	BCR	C34-C9-C8	2.58	122.22	118.10
11	2	1239	CLA	CMC-C2C-C1C	2.59	128.94	125.02
11	a	1129	CLA	CMC-C2C-C1C	2.59	128.94	125.02
11	8	1501	CLA	CMC-C2C-C1C	2.59	128.94	125.02
11	b	1021	CLA	CED-O2D-CGD	2.59	122.04	115.97
11	A	1131	CLA	CMC-C2C-C1C	2.59	128.94	125.02
11	b	1224	CLA	CMC-C2C-C1C	2.59	128.94	125.02
11	1	1132	CLA	CMC-C2C-C1C	2.59	128.95	125.02
11	A	1103	CLA	C1-O2A-CGA	2.59	122.99	116.77
11	B	1207	CLA	C4A-NA-C1A	2.59	109.67	106.45
11	2	1225	CLA	C3C-C4C-NC	2.59	112.84	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4010	BCR	C19-C18-C17	2.59	122.92	118.94
11	L	1501	CLA	CMC-C2C-C1C	2.60	128.96	125.02
11	2	1207	CLA	CMC-C2C-C1C	2.60	128.96	125.02
11	A	1104	CLA	C9-C8-C7	2.60	120.84	111.36
11	a	1137	CLA	CMC-C2C-C1C	2.60	128.96	125.02
11	2	1023	CLA	CMB-C2B-C3B	2.60	129.72	124.89
11	a	1119	CLA	CMB-C2B-C3B	2.60	129.72	124.89
11	a	1127	CLA	CMC-C2C-C1C	2.60	128.97	125.02
11	a	1120	CLA	C4A-NA-C1A	2.60	109.68	106.45
11	B	1013	CLA	CED-O2D-CGD	2.61	122.08	115.97
11	2	1210	CLA	CMC-C2C-C1C	2.61	128.97	125.02
11	l	1503	CLA	CMB-C2B-C3B	2.61	129.73	124.89
11	B	1023	CLA	CMB-C2B-C3B	2.61	129.73	124.89
11	1	1114	CLA	CMC-C2C-C1C	2.61	128.98	125.02
11	1	1122	CLA	CMC-C2C-C1C	2.61	128.98	125.02
11	b	1021	CLA	CMB-C2B-C3B	2.61	129.74	124.89
11	A	1011	CLA	CMC-C2C-C1C	2.61	128.98	125.02
11	A	1108	CLA	CMC-C2C-C1C	2.61	128.98	125.02
11	1	1131	CLA	C9-C8-C10	2.61	120.89	111.36
11	b	1021	CLA	C9-C8-C7	2.61	120.89	111.36
11	2	1216	CLA	CMB-C2B-C3B	2.61	129.74	124.89
11	L	1502	CLA	O2A-CGA-CBA	2.61	123.11	112.33
11	B	1221	CLA	CMC-C2C-C1C	2.61	128.98	125.02
11	A	1116	CLA	CMB-C2B-C3B	2.61	129.74	124.89
11	A	1103	CLA	C9-C8-C7	2.62	120.90	111.36
11	A	1111	CLA	C4-C3-C5	2.62	119.83	115.29
11	1	1103	CLA	C4A-NA-C1A	2.62	109.70	106.45
11	B	1221	CLA	C4A-NA-C1A	2.62	109.70	106.45
11	a	1127	CLA	CED-O2D-CGD	2.62	122.11	115.97
14	6	4013	BCR	C38-C26-C27	2.62	118.42	113.45
11	a	1101	CLA	CMC-C2C-C1C	2.62	128.99	125.02
11	a	1115	CLA	CMC-C2C-C1C	2.62	129.00	125.02
11	b	1215	CLA	CMC-C2C-C1C	2.62	129.00	125.02
11	b	1230	CLA	C1-O2A-CGA	2.62	123.07	116.77
11	B	1204	CLA	C1-O2A-CGA	2.62	123.07	116.77
11	B	1023	CLA	C9-C8-C7	2.62	120.93	111.36
11	1	1115	CLA	CMC-C2C-C1C	2.63	129.00	125.02
11	a	1122	CLA	CMB-C2B-C3B	2.63	129.76	124.89
11	a	1129	CLA	O2A-CGA-CBA	2.63	123.16	112.33
11	b	1229	CLA	CMC-C2C-C1C	2.63	129.00	125.02
11	2	1235	CLA	CAC-C3C-C4C	2.63	128.54	124.83
11	a	1127	CLA	C4-C3-C5	2.63	119.85	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1127	CLA	C9-C8-C10	2.63	120.95	111.36
11	2	1224	CLA	CMC-C2C-C1C	2.63	129.01	125.02
11	A	1102	CLA	CMB-C2B-C3B	2.63	129.77	124.89
11	A	1138	CLA	O2A-CGA-CBA	2.63	123.19	112.33
11	2	1205	CLA	C4A-NA-C1A	2.63	109.72	106.45
11	1	1113	CLA	CMC-C2C-C1C	2.63	129.01	125.02
11	1	1110	CLA	C4-C3-C5	2.63	119.86	115.29
11	A	1127	CLA	CMB-C2B-C3B	2.63	129.78	124.89
11	K	1401	CLA	CMC-C2C-C1C	2.63	129.01	125.02
11	1	1120	CLA	CMC-C2C-C1C	2.63	129.01	125.02
11	A	1120	CLA	CMB-C2B-C3B	2.63	129.78	124.89
11	1	1124	CLA	CMB-C2B-C3B	2.63	129.78	124.89
11	l	1501	CLA	C1-O2A-CGA	2.63	123.09	116.77
11	a	1118	CLA	C4A-NA-C1A	2.64	109.72	106.45
11	b	1205	CLA	CMC-C2C-C1C	2.64	129.02	125.02
14	m	4021	BCR	C23-C22-C21	2.64	122.99	118.94
11	0	1401	CLA	CMC-C2C-C1C	2.64	129.02	125.02
11	2	1021	CLA	C9-C8-C7	2.64	120.99	111.36
11	8	1502	CLA	CMB-C2B-C3B	2.64	129.79	124.89
11	1	1104	CLA	C4-C3-C5	2.64	119.87	115.29
11	a	1130	CLA	CMC-C2C-C1C	2.64	129.03	125.02
11	b	1023	CLA	C9-C8-C7	2.64	121.00	111.36
14	l	4019	BCR	C38-C26-C27	2.64	118.47	113.45
11	A	1122	CLA	C9-C8-C10	2.64	121.01	111.36
11	2	1228	CLA	CMB-C2B-C3B	2.65	129.80	124.89
11	B	1013	CLA	CHB-C4A-NA	2.65	128.17	124.51
11	B	1231	CLA	C3C-C4C-NC	2.65	112.89	110.21
11	1	1130	CLA	CMC-C2C-C1C	2.65	129.03	125.02
11	2	1226	CLA	C9-C8-C10	2.65	121.01	111.36
11	2	1231	CLA	CAC-C3C-C4C	2.65	128.56	124.83
11	b	1223	CLA	CMC-C2C-C1C	2.65	129.04	125.02
11	A	1106	CLA	C3C-C4C-NC	2.65	112.90	110.21
11	2	1207	CLA	C4A-NA-C1A	2.65	109.75	106.45
11	1	1109	CLA	C9-C8-C10	2.65	121.04	111.36
11	1	1111	CLA	C4A-NA-C1A	2.65	109.75	106.45
14	B	4006	BCR	C23-C22-C21	2.65	123.02	118.94
11	b	1231	CLA	CMB-C2B-C3B	2.66	129.82	124.89
11	a	1111	CLA	C4-C3-C5	2.66	119.90	115.29
11	b	1023	CLA	C1-O2A-CGA	2.66	123.15	116.77
11	a	1104	CLA	C4-C3-C5	2.66	119.90	115.29
11	B	1201	CLA	C1-O2A-CGA	2.66	123.15	116.77
11	k	1401	CLA	CMC-C2C-C1C	2.66	129.05	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1237	CLA	C4-C3-C5	2.66	119.90	115.29
14	b	4017	BCR	C8-C9-C10	2.66	123.02	118.94
11	a	1102	CLA	CMB-C2B-C3B	2.66	129.83	124.89
11	b	1238	CLA	CMC-C2C-C1C	2.66	129.06	125.02
11	A	1103	CLA	CMB-C2B-C3B	2.66	129.83	124.89
11	A	1117	CLA	C3C-C4C-NC	2.66	112.91	110.21
11	b	1234	CLA	CAC-C3C-C4C	2.66	128.59	124.83
11	B	1227	CLA	C3C-C4C-NC	2.67	112.91	110.21
11	a	1117	CLA	CMC-C2C-C1C	2.67	129.06	125.02
11	A	1123	CLA	CMC-C2C-C1C	2.67	129.06	125.02
11	A	1103	CLA	CMC-C2C-C1C	2.67	129.06	125.02
11	a	1116	CLA	CMB-C2B-C3B	2.67	129.84	124.89
11	B	1213	CLA	C9-C8-C7	2.67	121.09	111.36
11	1	1125	CLA	C4-C3-C5	2.67	119.92	115.29
11	B	1209	CLA	CAC-C3C-C4C	2.67	128.60	124.83
14	B	4005	BCR	C33-C5-C4	2.67	118.52	113.45
11	A	1102	CLA	CHB-C4A-NA	2.67	128.21	124.51
11	2	1219	CLA	CMC-C2C-C1C	2.67	129.07	125.02
11	B	1211	CLA	O2A-CGA-CBA	2.67	123.35	112.33
14	B	4011	BCR	C35-C13-C12	2.67	122.36	118.10
14	B	4017	BCR	C1-C6-C7	2.67	123.24	115.73
11	A	1137	CLA	C9-C8-C7	2.67	121.11	111.36
11	a	1132	CLA	CMC-C2C-C1C	2.67	129.07	125.02
11	1	1106	CLA	C4-C3-C5	2.67	119.93	115.29
11	0	1402	CLA	CMB-C2B-C3B	2.68	129.86	124.89
11	b	1217	CLA	CMB-C2B-C3B	2.68	129.86	124.89
14	M	4021	BCR	C23-C22-C21	2.68	123.05	118.94
11	a	1125	CLA	CMC-C2C-C1C	2.68	129.08	125.02
11	1	1119	CLA	CMC-C2C-C1C	2.68	129.08	125.02
14	a	4007	BCR	C33-C5-C4	2.68	118.53	113.45
11	1	1138	CLA	O2A-CGA-CBA	2.68	123.37	112.33
11	B	1224	CLA	CMC-C2C-C1C	2.68	129.08	125.02
11	1	1124	CLA	CMC-C2C-C1C	2.68	129.08	125.02
14	b	4009	BCR	C33-C5-C4	2.68	118.54	113.45
11	B	1218	CLA	CMC-C2C-C1C	2.68	129.09	125.02
11	2	1206	CLA	CMC-C2C-C1C	2.68	129.09	125.02
11	1	1103	CLA	CMC-C2C-C1C	2.68	129.09	125.02
11	b	1228	CLA	CMB-C2B-C3B	2.68	129.87	124.89
11	1	1140	CLA	CMC-C2C-C1C	2.68	129.09	125.02
11	B	1221	CLA	C1-O2A-CGA	2.69	123.21	116.77
11	B	1221	CLA	C4-C3-C5	2.69	119.95	115.29
11	a	1132	CLA	CMB-C2B-C3B	2.69	129.88	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1220	CLA	CMB-C2B-C3B	2.69	129.88	124.89
14	A	4002	BCR	C33-C5-C4	2.69	118.55	113.45
11	B	1231	CLA	CMC-C2C-C1C	2.69	129.10	125.02
11	1	1115	CLA	CMB-C2B-C3B	2.69	129.88	124.89
11	b	1206	CLA	C3C-C4C-NC	2.69	112.94	110.21
11	a	1140	CLA	C9-C8-C7	2.69	121.17	111.36
11	1	1104	CLA	C9-C8-C7	2.69	121.17	111.36
11	1	1022	CLA	CMC-C2C-C1C	2.69	129.10	125.02
14	L	4019	BCR	C8-C9-C10	2.69	123.07	118.94
11	a	1137	CLA	CMB-C2B-C3B	2.69	129.88	124.89
11	2	1210	CLA	CMB-C2B-C3B	2.69	129.88	124.89
11	1	1103	CLA	C3C-C4C-NC	2.69	112.94	110.21
11	1	1129	CLA	O2A-CGA-CBA	2.69	123.44	112.33
14	A	4002	BCR	C23-C22-C21	2.69	123.08	118.94
11	2	1204	CLA	C1-O2A-CGA	2.70	123.24	116.77
11	B	1204	CLA	C3C-C4C-NC	2.70	112.94	110.21
11	B	1232	CLA	CAC-C3C-C4C	2.70	128.63	124.83
11	a	1134	CLA	CED-O2D-CGD	2.70	122.29	115.97
11	2	1238	CLA	CMB-C2B-C3B	2.70	129.90	124.89
11	2	1231	CLA	C3C-C4C-NC	2.70	112.94	110.21
11	B	1201	CLA	C4A-NA-C1A	2.70	109.80	106.45
11	2	1013	CLA	CHB-C4A-NA	2.70	128.24	124.51
11	A	1136	CLA	O2A-CGA-CBA	2.70	123.46	112.33
11	A	1022	CLA	CMB-C2B-C3B	2.70	129.90	124.89
14	b	4006	BCR	C38-C26-C27	2.70	118.58	113.45
11	a	1801	CLA	CMB-C2B-C3B	2.70	129.91	124.89
11	a	1124	CLA	CMB-C2B-C3B	2.70	129.91	124.89
11	a	1110	CLA	CMC-C2C-C1C	2.70	129.12	125.02
11	b	1216	CLA	CMC-C2C-C1C	2.70	129.12	125.02
11	B	1235	CLA	CMB-C2B-C3B	2.71	129.91	124.89
11	A	1130	CLA	O2A-CGA-CBA	2.71	123.50	112.33
11	b	1021	CLA	CBA-CAA-C2A	2.71	121.90	113.80
11	2	1203	CLA	C4-C3-C5	2.71	119.99	115.29
11	a	1136	CLA	O2A-CGA-CBA	2.71	123.50	112.33
11	b	1013	CLA	CMB-C2B-C3B	2.71	129.92	124.89
11	2	1023	CLA	C9-C8-C7	2.71	121.25	111.36
11	1	1801	CLA	C1-O2A-CGA	2.71	123.28	116.77
11	A	1136	CLA	CMC-C2C-C1C	2.71	129.13	125.02
11	b	1226	CLA	C9-C8-C7	2.71	121.25	111.36
11	b	1214	CLA	C9-C8-C10	2.71	121.26	111.36
11	K	1402	CLA	CMB-C2B-C3B	2.72	129.93	124.89
11	1	1012	CLA	C9-C8-C10	2.72	121.27	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1108	CLA	CMC-C2C-C1C	2.72	129.14	125.02
11	b	1222	CLA	CMC-C2C-C1C	2.72	129.14	125.02
11	2	1218	CLA	CMC-C2C-C1C	2.72	129.14	125.02
11	1	1134	CLA	CMC-C2C-C1C	2.72	129.14	125.02
11	a	1139	CLA	C3C-C4C-NC	2.72	112.97	110.21
11	1	1012	CLA	CMC-C2C-C1C	2.72	129.14	125.02
11	1	1115	CLA	O2A-CGA-CBA	2.72	123.55	112.33
11	B	1219	CLA	CMC-C2C-C1C	2.72	129.15	125.02
11	A	1133	CLA	O2A-CGA-CBA	2.72	123.56	112.33
11	b	1214	CLA	CMC-C2C-C1C	2.72	129.15	125.02
11	2	1213	CLA	CMB-C2B-C3B	2.72	129.95	124.89
11	1	1138	CLA	CED-O2D-CGD	2.72	122.36	115.97
11	1	1138	CLA	C3C-C4C-NC	2.73	112.97	110.21
11	k	1402	CLA	CMB-C2B-C3B	2.73	129.96	124.89
14	8	4022	BCR	C19-C18-C17	2.73	123.13	118.94
15	b	5004	LHG	O8-C23-C24	2.73	119.84	111.90
11	2	1212	CLA	CMC-C2C-C1C	2.73	129.16	125.02
11	B	1232	CLA	CMC-C2C-C1C	2.73	129.16	125.02
11	b	1207	CLA	C4A-NA-C1A	2.73	109.84	106.45
11	B	1214	CLA	CMC-C2C-C1C	2.73	129.16	125.02
11	A	1120	CLA	C3C-C4C-NC	2.73	112.98	110.21
11	B	1238	CLA	C4-C3-C5	2.73	120.03	115.29
11	a	1134	CLA	CMC-C2C-C1C	2.73	129.17	125.02
11	B	1232	CLA	C3C-C4C-NC	2.74	112.98	110.21
11	a	1130	CLA	C3C-C4C-NC	2.74	112.98	110.21
11	B	1238	CLA	CMC-C2C-C1C	2.74	129.17	125.02
11	a	1131	CLA	CMC-C2C-C1C	2.74	129.17	125.02
11	l	1502	CLA	O2A-CGA-CBA	2.74	123.62	112.33
11	1	1130	CLA	CMB-C2B-C3B	2.74	129.97	124.89
11	b	1225	CLA	CMC-C2C-C1C	2.74	129.17	125.02
11	a	1022	CLA	CMC-C2C-C1C	2.74	129.18	125.02
11	A	1135	CLA	CMB-C2B-C3B	2.74	129.98	124.89
11	a	1011	CLA	CMC-C2C-C1C	2.74	129.18	125.02
11	A	1011	CLA	C3C-C4C-NC	2.75	112.99	110.21
11	B	1210	CLA	C9-C8-C7	2.75	121.37	111.36
11	1	1108	CLA	CMC-C2C-C1C	2.75	129.18	125.02
14	L	4019	BCR	C38-C26-C27	2.75	118.66	113.45
11	B	1234	CLA	CMC-C2C-C1C	2.75	129.19	125.02
14	b	4004	BCR	C19-C18-C17	2.75	123.16	118.94
11	B	1216	CLA	C3C-C4C-NC	2.75	113.00	110.21
11	1	1130	CLA	O2A-CGA-CBA	2.75	123.67	112.33
14	B	4006	BCR	C38-C26-C27	2.75	118.67	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1210	CLA	C9-C8-C7	2.75	121.40	111.36
11	2	1202	CLA	C3C-C4C-NC	2.75	113.00	110.21
11	8	1503	CLA	CMC-C2C-C1C	2.75	129.19	125.02
11	1	1114	CLA	C3C-C4C-NC	2.75	113.00	110.21
11	b	1021	CLA	CMC-C2C-C1C	2.76	129.20	125.02
11	1	1111	CLA	C1-O2A-CGA	2.76	123.38	116.77
11	1	1121	CLA	CMC-C2C-C1C	2.76	129.20	125.02
11	2	1231	CLA	CMB-C2B-C3B	2.76	130.01	124.89
11	A	1110	CLA	CMC-C2C-C1C	2.76	129.20	125.02
11	a	1118	CLA	CMC-C2C-C1C	2.76	129.21	125.02
11	A	1011	CLA	C4-C3-C5	2.76	120.08	115.29
11	l	1501	CLA	CMC-C2C-C1C	2.76	129.21	125.02
11	A	1106	CLA	C1-O2A-CGA	2.76	123.39	116.77
11	2	1223	CLA	CMC-C2C-C1C	2.76	129.21	125.02
11	A	1114	CLA	O2A-CGA-CBA	2.76	123.72	112.33
14	l	4022	BCR	C23-C22-C21	2.76	123.18	118.94
11	A	1134	CLA	CAC-C3C-C4C	2.76	128.73	124.83
11	L	1501	CLA	C1-O2A-CGA	2.76	123.40	116.77
11	B	1201	CLA	CMB-C2B-C3B	2.77	130.02	124.89
11	b	1211	CLA	O2A-CGA-CBA	2.77	123.74	112.33
11	b	1202	CLA	CMB-C2B-C3B	2.77	130.03	124.89
11	b	1226	CLA	CMC-C2C-C1C	2.77	129.22	125.02
11	B	1226	CLA	CMC-C2C-C1C	2.77	129.22	125.02
11	B	1212	CLA	CMB-C2B-C3B	2.77	130.03	124.89
11	B	1203	CLA	CMC-C2C-C1C	2.77	129.22	125.02
11	1	1116	CLA	CMC-C2C-C1C	2.77	129.22	125.02
11	a	1011	CLA	CED-O2D-CGD	2.77	122.47	115.97
11	A	1112	CLA	CMC-C2C-C1C	2.78	129.23	125.02
11	1	1126	CLA	CMB-C2B-C3B	2.78	130.04	124.89
11	A	1134	CLA	C3C-C4C-NC	2.78	113.03	110.21
11	a	1107	CLA	CHB-C4A-NA	2.78	128.35	124.51
11	b	1239	CLA	C3C-C4C-NC	2.78	113.03	110.21
11	a	1118	CLA	C3C-C4C-NC	2.78	113.03	110.21
11	1	1114	CLA	O2A-CGA-CBA	2.78	123.80	112.33
11	2	1232	CLA	CMC-C2C-C1C	2.78	129.24	125.02
11	a	1103	CLA	CMC-C2C-C1C	2.78	129.24	125.02
11	1	1136	CLA	O2A-CGA-CBA	2.78	123.81	112.33
11	a	1107	CLA	C4A-NA-C1A	2.78	109.91	106.45
11	a	1138	CLA	O2A-CGA-CBA	2.78	123.82	112.33
11	1	1135	CLA	CMC-C2C-C1C	2.79	129.24	125.02
14	b	4014	BCR	C23-C22-C21	2.79	123.22	118.94
11	a	1111	CLA	CAC-C3C-C4C	2.79	128.76	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1102	CLA	CMB-C2B-C3B	2.79	130.07	124.89
11	2	1209	CLA	CAC-C3C-C4C	2.79	128.77	124.83
11	2	1021	CLA	CMB-C2B-C3B	2.79	130.07	124.89
11	a	1105	CLA	C3C-C4C-NC	2.79	113.04	110.21
11	A	1103	CLA	C3C-C4C-NC	2.79	113.04	110.21
11	1	1117	CLA	C3C-C4C-NC	2.80	113.05	110.21
11	b	1209	CLA	C3C-C4C-NC	2.80	113.05	110.21
11	2	1227	CLA	C3C-C4C-NC	2.80	113.05	110.21
11	B	1226	CLA	C9-C8-C7	2.80	121.57	111.36
11	b	1225	CLA	CMB-C2B-C3B	2.80	130.09	124.89
11	B	1213	CLA	CMC-C2C-C1C	2.80	129.27	125.02
11	1	1133	CLA	O2A-CGA-CBA	2.80	123.89	112.33
11	2	1214	CLA	CMC-C2C-C1C	2.80	129.27	125.02
11	A	1121	CLA	C3C-C4C-NC	2.81	113.05	110.21
11	A	1011	CLA	C4A-NA-C1A	2.81	109.94	106.45
11	b	1235	CLA	CMC-C2C-C1C	2.81	129.28	125.02
11	A	1134	CLA	CMB-C2B-C3B	2.81	130.11	124.89
11	1	1106	CLA	CMC-C2C-C1C	2.81	129.28	125.02
16	2	5002	LMG	O8-C28-C29	2.81	120.08	111.90
11	a	1105	CLA	CMC-C2C-C1C	2.81	129.28	125.02
11	B	1225	CLA	CMC-C2C-C1C	2.81	129.28	125.02
11	2	1225	CLA	CMB-C2B-C3B	2.81	130.11	124.89
11	2	1203	CLA	CMC-C2C-C1C	2.81	129.29	125.02
11	a	1119	CLA	C3C-C4C-NC	2.82	113.06	110.21
11	1	1129	CLA	CMC-C2C-C1C	2.82	129.29	125.02
11	b	1238	CLA	CMB-C2B-C3B	2.82	130.12	124.89
15	B	5004	LHG	O8-C23-C24	2.82	120.10	111.90
11	L	1503	CLA	CMC-C2C-C1C	2.82	129.29	125.02
11	B	1231	CLA	CMB-C2B-C3B	2.82	130.12	124.89
14	L	4022	BCR	C19-C18-C17	2.82	123.27	118.94
14	a	4001	BCR	C33-C5-C4	2.82	118.80	113.45
11	B	1023	CLA	C1-O2A-CGA	2.82	123.54	116.77
11	2	1013	CLA	C9-C8-C10	2.82	121.65	111.36
11	1	1110	CLA	CMC-C2C-C1C	2.82	129.30	125.02
11	1	1134	CLA	O2A-CGA-CBA	2.82	123.98	112.33
11	b	1236	CLA	CMB-C2B-C3B	2.83	130.14	124.89
11	2	1013	CLA	CMB-C2B-C3B	2.83	130.14	124.89
11	a	1011	CLA	C4A-NA-C1A	2.83	109.96	106.45
11	1	1140	CLA	C1-O2A-CGA	2.83	123.56	116.77
11	b	1215	CLA	C3C-C4C-NC	2.83	113.08	110.21
14	B	4010	BCR	C19-C18-C17	2.83	123.29	118.94
11	A	1111	CLA	C3C-C4C-NC	2.83	113.08	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1137	CLA	C9-C8-C10	2.83	121.69	111.36
11	2	1208	CLA	CMC-C2C-C1C	2.83	129.32	125.02
11	2	1215	CLA	C3C-C4C-NC	2.84	113.08	110.21
11	2	1226	CLA	CMB-C2B-C3B	2.84	130.16	124.89
11	b	1231	CLA	CMC-C2C-C1C	2.84	129.32	125.02
11	1	1111	CLA	C9-C8-C7	2.84	121.71	111.36
11	B	1214	CLA	C9-C8-C7	2.84	121.71	111.36
14	A	4008	BCR	C8-C9-C10	2.84	123.30	118.94
11	b	1208	CLA	CMC-C2C-C1C	2.84	129.32	125.02
11	A	1134	CLA	O2A-CGA-CBA	2.84	124.04	112.33
11	a	1109	CLA	C9-C8-C10	2.84	121.72	111.36
11	2	1203	CLA	C3C-C4C-NC	2.84	113.09	110.21
11	1	1104	CLA	CMC-C2C-C1C	2.84	129.33	125.02
11	B	1240	CLA	CMC-C2C-C1C	2.84	129.33	125.02
11	B	1220	CLA	O2A-CGA-CBA	2.84	124.06	112.33
11	b	1227	CLA	CMC-C2C-C1C	2.84	129.33	125.02
11	B	1202	CLA	C3C-C4C-NC	2.84	113.09	110.21
11	B	1021	CLA	C3C-C4C-NC	2.84	113.09	110.21
11	2	1208	CLA	C3C-C4C-NC	2.85	113.09	110.21
11	1	1105	CLA	C3C-C4C-NC	2.85	113.09	110.21
11	a	1134	CLA	O2A-CGA-CBA	2.85	124.07	112.33
11	b	1231	CLA	C3C-C4C-NC	2.85	113.10	110.21
11	2	1221	CLA	CMC-C2C-C1C	2.85	129.34	125.02
14	1	4001	BCR	C33-C5-C4	2.85	118.86	113.45
11	b	1219	CLA	CMC-C2C-C1C	2.85	129.34	125.02
11	1	1127	CLA	C3C-C4C-NC	2.85	113.10	110.21
11	1	1111	CLA	CMC-C2C-C1C	2.85	129.35	125.02
11	b	1223	CLA	CAC-C3C-C4C	2.85	128.86	124.83
11	A	1801	CLA	CMC-C2C-C3C	2.85	134.00	126.09
11	B	1228	CLA	C3C-C4C-NC	2.86	113.11	110.21
14	b	4011	BCR	C33-C5-C4	2.86	118.87	113.45
11	2	1238	CLA	CMC-C2C-C1C	2.86	129.35	125.02
14	B	4017	BCR	C34-C9-C8	2.86	122.65	118.10
11	2	1235	CLA	C9-C8-C7	2.86	121.79	111.36
11	2	1225	CLA	CMC-C2C-C1C	2.86	129.36	125.02
11	B	1231	CLA	CAC-C3C-C4C	2.86	128.86	124.83
11	A	1129	CLA	O2A-CGA-CBA	2.86	124.14	112.33
11	1	1104	CLA	C3C-C4C-NC	2.86	113.11	110.21
14	7	4021	BCR	C38-C26-C27	2.86	118.89	113.45
11	1	1133	CLA	C3C-C4C-NC	2.86	113.11	110.21
11	a	1112	CLA	CMC-C2C-C1C	2.86	129.36	125.02
11	B	1220	CLA	C3C-C4C-NC	2.86	113.11	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1139	CLA	C3C-C4C-NC	2.87	113.11	110.21
11	2	1204	CLA	C3C-C4C-NC	2.87	113.11	110.21
11	B	1208	CLA	CMC-C2C-C1C	2.87	129.37	125.02
11	b	1214	CLA	C1-O2A-CGA	2.87	123.65	116.77
11	1	1106	CLA	C3C-C4C-NC	2.87	113.12	110.21
14	A	4003	BCR	C38-C26-C27	2.87	118.89	113.45
14	a	4007	BCR	C38-C26-C27	2.87	118.89	113.45
11	A	1137	CLA	C9-C8-C10	2.87	121.82	111.36
11	B	1209	CLA	CMB-C2B-C3B	2.87	130.22	124.89
11	A	1135	CLA	CMC-C2C-C1C	2.87	129.37	125.02
11	2	1215	CLA	C6-C5-C3	2.87	119.17	112.66
11	b	1208	CLA	C3C-C4C-NC	2.87	113.12	110.21
11	1	1101	CLA	CMC-C2C-C1C	2.87	129.38	125.02
11	b	1232	CLA	C3C-C4C-NC	2.88	113.12	110.21
11	A	1102	CLA	C3C-C4C-NC	2.88	113.12	110.21
11	A	1127	CLA	CMC-C2C-C1C	2.88	129.38	125.02
11	A	1101	CLA	CMC-C2C-C1C	2.88	129.39	125.02
11	a	1138	CLA	CAC-C3C-C4C	2.88	128.89	124.83
11	B	1235	CLA	CMC-C2C-C1C	2.88	129.39	125.02
11	2	1214	CLA	C3C-C4C-NC	2.88	113.13	110.21
11	1	1140	CLA	C4-C3-C5	2.88	120.29	115.29
11	2	1214	CLA	C1-O2A-CGA	2.88	123.69	116.77
11	2	1220	CLA	CMC-C2C-C1C	2.88	129.39	125.02
11	A	1104	CLA	C3C-C4C-NC	2.89	113.13	110.21
11	b	1220	CLA	O2A-CGA-CBA	2.89	124.23	112.33
14	m	4021	BCR	C19-C18-C17	2.89	123.37	118.94
11	B	1211	CLA	CMB-C2B-C3B	2.89	130.25	124.89
14	2	4006	BCR	C19-C18-C17	2.89	123.37	118.94
14	B	4011	BCR	C8-C9-C10	2.89	123.38	118.94
11	A	1132	CLA	C1-O2A-CGA	2.89	123.71	116.77
11	b	1218	CLA	CMC-C2C-C1C	2.89	129.41	125.02
14	2	4011	BCR	C33-C5-C4	2.89	118.94	113.45
11	a	1134	CLA	C3C-C4C-NC	2.89	113.14	110.21
11	b	1217	CLA	O2A-C1-C2	2.89	119.19	108.40
14	a	4003	BCR	C30-C25-C24	2.89	123.86	115.73
11	a	1106	CLA	CMC-C2C-C1C	2.89	129.41	125.02
11	2	1220	CLA	O2A-CGA-CBA	2.89	124.27	112.33
11	A	1123	CLA	C3C-C4C-NC	2.90	113.14	110.21
11	2	1229	CLA	CMC-C2C-C1C	2.90	129.41	125.02
14	A	4001	BCR	C33-C5-C4	2.90	118.95	113.45
11	2	1235	CLA	C4-C3-C5	2.90	120.31	115.29
11	1	1011	CLA	CHB-C4A-NA	2.90	128.52	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1214	CLA	C4-C3-C5	2.90	120.32	115.29
11	2	1013	CLA	C3C-C4C-NC	2.90	113.15	110.21
11	b	1224	CLA	C1-O2A-CGA	2.90	123.73	116.77
11	A	1111	CLA	CMC-C2C-C1C	2.90	129.42	125.02
11	2	1219	CLA	C4-C3-C5	2.90	120.32	115.29
11	l	1503	CLA	CMC-C2C-C1C	2.90	129.42	125.02
14	1	4002	BCR	C33-C5-C4	2.90	118.96	113.45
11	2	1202	CLA	CMC-C2C-C1C	2.90	129.42	125.02
11	1	1105	CLA	CMC-C2C-C1C	2.91	129.43	125.02
11	a	1126	CLA	CMB-C2B-C3B	2.91	130.28	124.89
11	B	1013	CLA	C9-C8-C10	2.91	121.97	111.36
11	a	1114	CLA	CMC-C2C-C1C	2.91	129.44	125.02
11	a	1122	CLA	C4-C3-C5	2.91	120.34	115.29
11	A	1135	CLA	C3C-C4C-NC	2.91	113.16	110.21
11	B	1222	CLA	CMC-C2C-C1C	2.91	129.44	125.02
11	B	1236	CLA	CMC-C2C-C1C	2.91	129.44	125.02
11	1	1131	CLA	CMC-C2C-C1C	2.91	129.44	125.02
11	1	1132	CLA	C1-O2A-CGA	2.91	123.76	116.77
14	2	4006	BCR	C1-C6-C7	2.91	123.92	115.73
11	B	1208	CLA	C3C-C4C-NC	2.91	113.16	110.21
11	a	1131	CLA	C3C-C4C-NC	2.92	113.17	110.21
11	A	1109	CLA	CMC-C2C-C1C	2.92	129.44	125.02
14	F	4013	BCR	C33-C5-C4	2.92	118.99	113.45
11	2	1238	CLA	C3C-C4C-NC	2.92	113.17	110.21
14	2	4006	BCR	C8-C9-C10	2.92	123.42	118.94
11	a	1128	CLA	C9-C8-C7	2.92	122.00	111.36
11	a	1114	CLA	O2A-CGA-CBA	2.92	124.37	112.33
11	B	1218	CLA	C3C-C4C-NC	2.92	113.17	110.21
11	a	1122	CLA	CMC-C2C-C1C	2.92	129.45	125.02
11	a	1130	CLA	O2A-CGA-CBA	2.92	124.37	112.33
11	b	1210	CLA	CMC-C2C-C1C	2.92	129.45	125.02
11	2	1217	CLA	CAC-C3C-C4C	2.92	128.95	124.83
11	8	1501	CLA	C3C-C4C-NC	2.92	113.17	110.21
11	B	1212	CLA	CMC-C2C-C1C	2.92	129.45	125.02
11	2	1218	CLA	C3C-C4C-NC	2.92	113.17	110.21
11	a	1106	CLA	C4-C3-C5	2.93	120.36	115.29
11	B	1239	CLA	C3C-C4C-NC	2.93	113.18	110.21
11	B	1239	CLA	CMC-C2C-C1C	2.93	129.46	125.02
11	B	1238	CLA	C3C-C4C-NC	2.93	113.18	110.21
11	1	1132	CLA	C3C-C4C-NC	2.93	113.18	110.21
11	2	1204	CLA	CMC-C2C-C1C	2.93	129.46	125.02
11	b	1228	CLA	C3C-C4C-NC	2.93	113.18	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1127	CLA	C3C-C4C-NC	2.93	113.18	110.21
14	8	4019	BCR	C19-C18-C17	2.93	123.44	118.94
11	1	1127	CLA	CMC-C2C-C1C	2.93	129.47	125.02
11	1	1125	CLA	CMC-C2C-C1C	2.93	129.47	125.02
11	a	1137	CLA	C9-C8-C7	2.93	122.06	111.36
11	a	1111	CLA	C9-C8-C7	2.94	122.07	111.36
11	1	1126	CLA	C9-C8-C10	2.94	122.07	111.36
11	a	1104	CLA	CMC-C2C-C1C	2.94	129.48	125.02
11	1	1130	CLA	C3C-C4C-NC	2.94	113.19	110.21
11	2	1201	CLA	C3C-C4C-NC	2.94	113.19	110.21
11	B	1201	CLA	C3C-C4C-NC	2.94	113.19	110.21
11	b	1211	CLA	CMC-C2C-C1C	2.94	129.48	125.02
12	b	2002	PQN	C24-C23-C25	2.94	122.09	111.36
11	0	1402	CLA	C3C-C4C-NC	2.94	113.19	110.21
11	1	1124	CLA	C3C-C4C-NC	2.94	113.19	110.21
11	b	1236	CLA	C3C-C4C-NC	2.94	113.19	110.21
11	a	1102	CLA	CMC-C2C-C1C	2.94	129.48	125.02
11	b	1235	CLA	C1-O2A-CGA	2.94	123.83	116.77
15	a	5003	LHG	O8-C23-C24	2.94	120.46	111.90
14	f	4013	BCR	C33-C5-C4	2.94	119.04	113.45
11	2	1211	CLA	CMC-C2C-C1C	2.94	129.48	125.02
14	6	4013	BCR	C30-C25-C24	2.94	124.00	115.73
14	2	4004	BCR	C19-C18-C17	2.95	123.46	118.94
11	A	1106	CLA	CMC-C2C-C1C	2.95	129.49	125.02
11	a	1127	CLA	CAC-C3C-C4C	2.95	128.99	124.83
11	b	1202	CLA	CMC-C2C-C1C	2.95	129.49	125.02
15	A	5001	LHG	O8-C23-C24	2.95	120.48	111.90
11	1	1122	CLA	C4-C3-C5	2.95	120.41	115.29
11	a	1105	CLA	C1-O2A-CGA	2.95	123.85	116.77
11	2	1234	CLA	CMC-C2C-C1C	2.95	129.50	125.02
11	a	1123	CLA	C3C-C4C-NC	2.95	113.20	110.21
11	2	1216	CLA	CMC-C2C-C1C	2.96	129.50	125.02
11	2	1217	CLA	O2A-C1-C2	2.96	119.42	108.40
11	A	1237	CLA	C4-C3-C5	2.96	120.42	115.29
11	1	1131	CLA	C3C-C4C-NC	2.96	113.21	110.21
11	b	1236	CLA	CMC-C2C-C1C	2.96	129.51	125.02
14	6	4013	BCR	C33-C5-C4	2.96	119.07	113.45
11	B	1207	CLA	C1-O2A-CGA	2.96	123.87	116.77
11	1	1118	CLA	C3C-C4C-NC	2.96	113.21	110.21
14	B	4004	BCR	C33-C5-C4	2.96	119.07	113.45
11	b	1205	CLA	C3C-C4C-NC	2.96	113.21	110.21
11	l	1503	CLA	C4-C3-C5	2.96	120.43	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1103	CLA	C3C-C4C-NC	2.96	113.21	110.21
11	a	1117	CLA	C9-C8-C7	2.96	122.17	111.36
11	B	1204	CLA	CMC-C2C-C1C	2.97	129.52	125.02
11	1	1103	CLA	CHB-C4A-NA	2.97	128.61	124.51
11	b	1238	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	b	1204	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	B	1234	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	1	1012	CLA	C9-C8-C7	2.97	122.19	111.36
11	a	1128	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	a	1123	CLA	CAC-C3C-C4C	2.97	129.02	124.83
11	2	1210	CLA	CAC-C3C-C4C	2.97	129.02	124.83
11	B	1205	CLA	C4A-NA-C1A	2.97	110.14	106.45
11	A	1111	CLA	CAC-C3C-C4C	2.97	129.02	124.83
11	b	1021	CLA	C1-O2A-CGA	2.97	123.90	116.77
11	1	1011	CLA	C4A-NA-C1A	2.97	110.14	106.45
11	B	1215	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	a	1112	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	b	1201	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	a	1133	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	a	1113	CLA	CMC-C2C-C1C	2.97	129.53	125.02
14	2	4004	BCR	C23-C22-C21	2.97	123.51	118.94
11	A	1136	CLA	C3C-C4C-NC	2.97	113.22	110.21
11	1	1123	CLA	CAC-C3C-C4C	2.98	129.03	124.83
11	b	1204	CLA	CMC-C2C-C1C	2.98	129.53	125.02
11	b	1218	CLA	C3C-C4C-NC	2.98	113.23	110.21
11	a	1117	CLA	C3C-C4C-NC	2.98	113.23	110.21
11	b	1013	CLA	C3C-C4C-NC	2.98	113.23	110.21
11	A	1102	CLA	CMC-C2C-C1C	2.98	129.54	125.02
11	1	1119	CLA	C4-C3-C5	2.98	120.46	115.29
11	a	1133	CLA	O2A-CGA-CBA	2.98	124.63	112.33
11	2	1209	CLA	C3C-C4C-NC	2.98	113.23	110.21
11	A	1126	CLA	CMB-C2B-C3B	2.99	130.43	124.89
11	b	1203	CLA	C9-C8-C7	2.99	122.25	111.36
14	8	4019	BCR	C38-C26-C27	2.99	119.12	113.45
11	b	1235	CLA	C3C-C4C-NC	2.99	113.24	110.21
11	k	1402	CLA	C3C-C4C-NC	2.99	113.24	110.21
11	A	1114	CLA	C3C-C4C-NC	2.99	113.24	110.21
11	2	1202	CLA	CMB-C2B-C3B	2.99	130.44	124.89
11	1	1112	CLA	CMC-C2C-C1C	2.99	129.56	125.02
14	2	4014	BCR	C38-C26-C27	2.99	119.13	113.45
11	2	1207	CLA	C3C-C4C-NC	2.99	113.25	110.21
11	1	1116	CLA	C3C-C4C-NC	3.00	113.25	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1137	CLA	CMC-C2C-C1C	3.00	129.56	125.02
14	B	4009	BCR	C38-C26-C27	3.00	119.14	113.45
11	a	1108	CLA	C3C-C4C-NC	3.00	113.25	110.21
11	b	1203	CLA	CMC-C2C-C1C	3.00	129.57	125.02
14	6	4020	BCR	C8-C9-C10	3.00	123.55	118.94
14	2	4005	BCR	C38-C26-C27	3.00	119.14	113.45
11	A	1132	CLA	C3C-C4C-NC	3.00	113.25	110.21
11	A	1133	CLA	C3C-C4C-NC	3.00	113.25	110.21
14	a	4001	BCR	C19-C18-C17	3.00	123.55	118.94
11	l	1503	CLA	C3C-C4C-NC	3.01	113.26	110.21
11	a	1121	CLA	O2A-CGA-CBA	3.01	124.75	112.33
11	a	1140	CLA	CMC-C2C-C1C	3.01	129.59	125.02
11	A	1120	CLA	CMC-C2C-C1C	3.01	129.59	125.02
11	1	1128	CLA	C9-C8-C7	3.01	122.36	111.36
11	A	1105	CLA	C3C-C4C-NC	3.02	113.27	110.21
14	F	4020	BCR	C33-C5-C4	3.02	119.18	113.45
11	B	1217	CLA	O2A-C1-C2	3.02	119.65	108.40
11	B	1220	CLA	CAC-C3C-C4C	3.02	129.09	124.83
11	2	1217	CLA	C3C-C4C-NC	3.02	113.27	110.21
11	b	1225	CLA	C3C-C4C-NC	3.02	113.27	110.21
11	b	1227	CLA	C3C-C4C-NC	3.02	113.27	110.21
11	8	1502	CLA	O2A-CGA-CBA	3.02	124.80	112.33
11	B	1203	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	a	1106	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	A	1105	CLA	O2A-C1-C2	3.03	119.77	109.31
11	1	1128	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	a	1135	CLA	C4-C3-C5	3.03	119.43	115.85
11	8	1503	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	1	1123	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	1	1134	CLA	C3C-C4C-NC	3.03	113.28	110.21
14	1	4003	BCR	C33-C5-C4	3.03	119.20	113.45
11	1	1237	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	a	1132	CLA	C3C-C4C-NC	3.03	113.28	110.21
14	1	4003	BCR	C38-C26-C27	3.03	119.20	113.45
11	B	1206	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	b	1212	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	b	1216	CLA	C9-C8-C10	3.03	122.42	111.36
11	b	1222	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	2	1021	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	B	1013	CLA	C3C-C4C-NC	3.03	113.28	110.21
11	1	1101	CLA	C3C-C4C-NC	3.04	113.29	110.21
14	1	4001	BCR	C38-C26-C27	3.04	119.22	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	0	1401	CLA	C3C-C4C-NC	3.04	113.29	110.21
11	2	1236	CLA	CMC-C2C-C1C	3.04	129.63	125.02
11	b	1212	CLA	CMC-C2C-C1C	3.04	129.63	125.02
11	A	1126	CLA	C9-C8-C10	3.04	122.45	111.36
14	1	4007	BCR	C38-C26-C27	3.04	119.22	113.45
15	1	5001	LHG	O8-C23-C24	3.04	120.75	111.90
11	A	1121	CLA	O2A-CGA-CBA	3.04	124.89	112.33
11	A	1022	CLA	C3C-C4C-NC	3.05	113.30	110.21
11	b	1239	CLA	O2A-CGA-CBA	3.05	124.89	112.33
11	A	1124	CLA	C3C-C4C-NC	3.05	113.30	110.21
14	A	4003	BCR	C33-C5-C4	3.05	119.24	113.45
11	a	1116	CLA	C3C-C4C-NC	3.05	113.30	110.21
11	k	1401	CLA	C3C-C4C-NC	3.05	113.30	110.21
11	a	1135	CLA	C3C-C4C-NC	3.05	113.30	110.21
11	B	1205	CLA	C3C-C4C-NC	3.05	113.30	110.21
11	1	1140	CLA	C9-C8-C7	3.06	122.50	111.36
11	2	1222	CLA	CMC-C2C-C1C	3.06	129.65	125.02
11	A	1115	CLA	C3C-C4C-NC	3.06	113.31	110.21
11	a	1012	CLA	CMC-C2C-C1C	3.06	129.66	125.02
11	B	1209	CLA	C3C-C4C-NC	3.06	113.31	110.21
11	2	1023	CLA	CHB-C4A-NA	3.06	128.74	124.51
11	B	1213	CLA	C3C-C4C-NC	3.06	113.31	110.21
11	2	1201	CLA	C1-O2A-CGA	3.06	124.11	116.77
11	1	1111	CLA	C3C-C4C-NC	3.06	113.31	110.21
11	1	1121	CLA	C3C-C4C-NC	3.06	113.31	110.21
11	A	1107	CLA	CMB-C2B-C3B	3.06	130.58	124.89
11	b	1213	CLA	C3C-C4C-NC	3.07	113.32	110.21
11	1	1110	CLA	C3C-C4C-NC	3.07	113.32	110.21
11	2	1222	CLA	C3C-C4C-NC	3.07	113.32	110.21
14	2	4006	BCR	C38-C26-C27	3.07	119.27	113.45
11	K	1401	CLA	C3C-C4C-NC	3.07	113.32	110.21
11	1	1139	CLA	CMC-C2C-C1C	3.07	129.67	125.02
15	A	5003	LHG	O8-C23-C24	3.07	120.83	111.90
11	A	1126	CLA	CMC-C2C-C1C	3.07	129.68	125.02
11	1	1119	CLA	C3C-C4C-NC	3.07	113.32	110.21
14	A	4007	BCR	C34-C9-C8	3.07	122.99	118.10
11	K	1402	CLA	C3C-C4C-NC	3.07	113.32	110.21
11	a	1140	CLA	C3C-C4C-NC	3.07	113.32	110.21
11	2	1023	CLA	C3C-C4C-NC	3.07	113.32	110.21
11	A	1126	CLA	C3C-C4C-NC	3.07	113.33	110.21
11	1	1136	CLA	C3C-C4C-NC	3.07	113.33	110.21
11	A	1108	CLA	C3C-C4C-NC	3.07	113.33	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1236	CLA	O2A-C1-C2	3.07	119.86	108.40
11	1	1120	CLA	O2A-CGA-CBA	3.08	125.02	112.33
14	f	4020	BCR	C33-C5-C4	3.08	119.29	113.45
11	1	1126	CLA	C3C-C4C-NC	3.08	113.33	110.21
11	b	1232	CLA	CMC-C2C-C1C	3.08	129.69	125.02
15	a	5001	LHG	O8-C23-C24	3.08	120.86	111.90
11	A	1116	CLA	CMC-C2C-C1C	3.08	129.69	125.02
11	2	1023	CLA	C4-C3-C5	3.08	120.63	115.29
11	B	1229	CLA	C3C-C4C-NC	3.08	113.33	110.21
11	L	1503	CLA	C3C-C4C-NC	3.08	113.33	110.21
11	a	1114	CLA	C3C-C4C-NC	3.08	113.33	110.21
11	2	1206	CLA	C3C-C4C-NC	3.08	113.34	110.21
11	2	1234	CLA	C3C-C4C-NC	3.09	113.34	110.21
14	M	4021	BCR	C19-C18-C17	3.09	123.68	118.94
15	1	5003	LHG	O8-C23-C24	3.09	120.89	111.90
11	a	1136	CLA	C3C-C4C-NC	3.09	113.34	110.21
11	a	1137	CLA	C3C-C4C-NC	3.09	113.34	110.21
11	2	1216	CLA	C9-C8-C10	3.09	122.63	111.36
11	a	1110	CLA	C3C-C4C-NC	3.09	113.34	110.21
11	1	1112	CLA	C3C-C4C-NC	3.09	113.34	110.21
11	1	1022	CLA	C3C-C4C-NC	3.09	113.34	110.21
11	a	1124	CLA	C3C-C4C-NC	3.09	113.34	110.21
11	A	1113	CLA	CMC-C2C-C1C	3.10	129.72	125.02
11	1	1111	CLA	CHB-C4A-NA	3.10	128.80	124.51
11	B	1235	CLA	C3C-C4C-NC	3.10	113.35	110.21
14	b	4014	BCR	C33-C5-C4	3.10	119.33	113.45
14	b	4004	BCR	C33-C5-C4	3.10	119.34	113.45
11	b	1021	CLA	C3C-C4C-NC	3.10	113.35	110.21
15	2	5004	LHG	O8-C23-C24	3.10	120.93	111.90
11	b	1229	CLA	C3C-C4C-NC	3.10	113.36	110.21
14	b	4010	BCR	C38-C26-C27	3.10	119.34	113.45
11	2	1232	CLA	C3C-C4C-NC	3.11	113.36	110.21
11	A	1119	CLA	CMB-C2B-C3B	3.11	130.66	124.89
11	B	1239	CLA	O2A-CGA-CBA	3.11	125.14	112.33
11	1	1126	CLA	CMC-C2C-C1C	3.11	129.74	125.02
11	a	1102	CLA	C3C-C4C-NC	3.11	113.36	110.21
11	A	1122	CLA	C1-O2A-CGA	3.11	124.24	116.77
11	1	1122	CLA	C9-C8-C10	3.11	122.71	111.36
11	A	1139	CLA	C3C-C4C-NC	3.11	113.36	110.21
11	2	1220	CLA	C3C-C4C-NC	3.11	113.36	110.21
11	A	1115	CLA	O2A-CGA-CBA	3.12	125.18	112.33
11	A	1130	CLA	C3C-C4C-NC	3.12	113.37	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1119	CLA	C3C-C4C-NC	3.12	113.37	110.21
11	A	1115	CLA	CMC-C2C-C1C	3.12	129.75	125.02
11	a	1104	CLA	C3C-C4C-NC	3.12	113.37	110.21
14	a	4002	BCR	C33-C5-C4	3.12	119.38	113.45
11	a	1103	CLA	C4-C3-C5	3.12	120.71	115.29
11	1	1107	CLA	C4-C3-C5	3.12	120.71	115.29
11	A	1131	CLA	C3C-C4C-NC	3.12	113.38	110.21
14	2	4017	BCR	C34-C9-C8	3.12	123.08	118.10
11	A	1110	CLA	C3C-C4C-NC	3.13	113.38	110.21
14	A	4001	BCR	C38-C26-C27	3.13	119.39	113.45
11	2	1225	CLA	O2A-CGA-CBA	3.13	121.01	111.90
11	b	1213	CLA	CMC-C2C-C1C	3.13	129.77	125.02
14	6	4020	BCR	C33-C5-C4	3.14	119.40	113.45
11	1	1137	CLA	CMB-C2B-C3B	3.14	130.71	124.89
11	b	1203	CLA	C3C-C4C-NC	3.14	113.39	110.21
11	1	1237	CLA	C4-C3-C5	3.14	120.73	115.29
11	2	1239	CLA	C3C-C4C-NC	3.14	113.39	110.21
11	A	1011	CLA	O2D-CGD-CBD	3.14	116.91	111.30
11	2	1205	CLA	C3C-C4C-NC	3.14	113.40	110.21
11	2	1231	CLA	CMC-C2C-C1C	3.14	129.79	125.02
14	1	4007	BCR	C33-C5-C4	3.14	119.42	113.45
14	b	4017	BCR	C34-C9-C8	3.15	123.11	118.10
11	2	1229	CLA	C3C-C4C-NC	3.15	113.40	110.21
11	l	1502	CLA	CMC-C2C-C1C	3.15	129.79	125.02
11	B	1210	CLA	C3C-C4C-NC	3.15	113.40	110.21
11	a	1237	CLA	CMC-C2C-C1C	3.15	129.79	125.02
14	2	4011	BCR	C8-C9-C10	3.15	123.77	118.94
14	f	4020	BCR	C38-C26-C27	3.15	119.43	113.45
11	A	1140	CLA	C3C-C4C-NC	3.15	113.40	110.21
11	a	1111	CLA	C3C-C4C-NC	3.15	113.40	110.21
11	B	1211	CLA	C3C-C4C-NC	3.15	113.41	110.21
14	F	4020	BCR	C38-C26-C27	3.15	119.44	113.45
11	2	1221	CLA	C1-O2A-CGA	3.15	124.34	116.77
12	B	2002	PQN	C24-C23-C25	3.15	122.86	111.36
11	b	1217	CLA	C3C-C4C-NC	3.16	113.41	110.21
11	2	1228	CLA	C3C-C4C-NC	3.16	113.41	110.21
11	a	1113	CLA	C3C-C4C-NC	3.16	113.41	110.21
14	B	4011	BCR	C33-C5-C4	3.16	119.44	113.45
11	a	1121	CLA	C3C-C4C-NC	3.16	113.41	110.21
11	b	1216	CLA	C3C-C4C-NC	3.16	113.41	110.21
11	a	1801	CLA	C3C-C4C-NC	3.16	113.41	110.21
11	1	1118	CLA	CMC-C2C-C1C	3.16	129.81	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1120	CLA	O2A-CGA-CBA	3.17	125.38	112.33
11	b	1211	CLA	C3C-C4C-NC	3.17	113.42	110.21
11	2	1205	CLA	CMC-C2C-C1C	3.17	129.82	125.02
11	A	1138	CLA	CAC-C3C-C4C	3.17	129.30	124.83
11	2	1235	CLA	C3C-C4C-NC	3.17	113.42	110.21
11	1	1102	CLA	C3C-C4C-NC	3.17	113.42	110.21
11	B	1212	CLA	C3C-C4C-NC	3.17	113.42	110.21
11	a	1101	CLA	C3C-C4C-NC	3.18	113.43	110.21
11	2	1213	CLA	CAC-C3C-C2C	3.18	133.01	127.49
14	B	4017	BCR	C33-C5-C4	3.18	119.49	113.45
11	b	1023	CLA	C3C-C4C-NC	3.18	113.44	110.21
11	b	1219	CLA	C3C-C4C-NC	3.19	113.44	110.21
11	2	1239	CLA	O2A-CGA-CBA	3.19	125.48	112.33
11	a	1801	CLA	C1-O2A-CGA	3.19	124.43	116.77
14	F	4020	BCR	C19-C18-C17	3.19	123.84	118.94
11	a	1121	CLA	CMC-C2C-C1C	3.19	129.86	125.02
11	B	1235	CLA	C1-O2A-CGA	3.19	124.43	116.77
11	1	1108	CLA	C3C-C4C-NC	3.20	113.45	110.21
11	2	1212	CLA	C3C-C4C-NC	3.20	113.45	110.21
11	a	1011	CLA	C3C-C4C-NC	3.20	113.45	110.21
11	2	1240	CLA	C3C-C4C-NC	3.20	113.45	110.21
14	2	4017	BCR	C33-C5-C4	3.20	119.52	113.45
11	B	1227	CLA	CAC-C3C-C4C	3.20	129.34	124.83
14	2	4011	BCR	C38-C26-C27	3.20	119.53	113.45
11	A	1012	CLA	C9-C8-C10	3.21	123.06	111.36
11	b	1236	CLA	O2A-C1-C2	3.21	120.36	108.40
11	B	1219	CLA	C3C-C4C-NC	3.21	113.46	110.21
11	2	1236	CLA	C3C-C4C-NC	3.21	113.47	110.21
14	A	4003	BCR	C30-C25-C24	3.21	124.76	115.73
11	A	1125	CLA	C3C-C4C-NC	3.21	113.47	110.21
11	1	1115	CLA	C3C-C4C-NC	3.21	113.47	110.21
11	B	1236	CLA	O2A-C1-C2	3.22	120.41	108.40
14	6	4018	BCR	C38-C26-C27	3.22	119.56	113.45
11	2	1221	CLA	C4-C3-C5	3.22	120.88	115.29
14	B	4014	BCR	C33-C5-C4	3.23	119.57	113.45
14	2	4014	BCR	C33-C5-C4	3.23	119.57	113.45
14	b	4010	BCR	C33-C5-C4	3.23	119.57	113.45
11	b	1210	CLA	C3C-C4C-NC	3.23	113.48	110.21
14	a	4001	BCR	C38-C26-C27	3.23	119.58	113.45
14	1	4022	BCR	C38-C26-C27	3.23	119.58	113.45
11	1	1120	CLA	C3C-C4C-NC	3.23	113.49	110.21
11	2	1210	CLA	C3C-C4C-NC	3.23	113.49	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1140	CLA	C1-O2A-CGA	3.23	124.53	116.77
11	A	1105	CLA	CMC-C2C-C1C	3.24	129.93	125.02
14	F	4018	BCR	C33-C5-C4	3.24	119.59	113.45
11	b	1214	CLA	C3C-C4C-NC	3.24	113.50	110.21
11	B	1217	CLA	C3C-C4C-NC	3.25	113.50	110.21
14	a	4003	BCR	C23-C22-C21	3.25	123.92	118.94
11	A	1128	CLA	C3C-C4C-NC	3.25	113.50	110.21
11	A	1119	CLA	C1-O2A-CGA	3.25	124.57	116.77
11	b	1240	CLA	C3C-C4C-NC	3.25	113.50	110.21
14	1	4003	BCR	C30-C25-C24	3.25	124.86	115.73
11	1	1105	CLA	O2A-C1-C2	3.25	120.55	109.31
11	A	1118	CLA	CMC-C2C-C1C	3.25	129.95	125.02
11	b	1202	CLA	C3C-C4C-NC	3.25	113.51	110.21
11	1	1132	CLA	O2A-CGA-CBA	3.26	121.37	111.90
11	L	1502	CLA	C3C-C4C-NC	3.26	113.51	110.21
11	B	1219	CLA	CMB-C2B-C3B	3.26	130.94	124.89
14	2	4017	BCR	C38-C26-C27	3.26	119.64	113.45
11	a	1237	CLA	C3C-C4C-NC	3.26	113.51	110.21
11	1	1125	CLA	C3C-C4C-NC	3.26	113.51	110.21
14	l	4022	BCR	C33-C5-C4	3.26	119.64	113.45
11	A	1103	CLA	O2A-CGA-CBA	3.26	121.40	111.90
11	a	1130	CLA	CMB-C2B-C3B	3.27	130.96	124.89
11	A	1137	CLA	C4-C3-C5	3.27	120.96	115.29
11	b	1234	CLA	C3C-C4C-NC	3.27	113.52	110.21
11	b	1216	CLA	CMB-C2B-C3B	3.28	130.97	124.89
11	2	1211	CLA	C3C-C4C-NC	3.28	113.53	110.21
11	a	1115	CLA	O2A-CGA-CBA	3.28	125.84	112.33
11	1	1011	CLA	C3C-C4C-NC	3.28	113.53	110.21
11	b	1235	CLA	C9-C8-C7	3.28	123.32	111.36
11	A	1011	CLA	CMB-C2B-C3B	3.28	130.98	124.89
14	a	4002	BCR	C23-C22-C21	3.28	123.98	118.94
14	B	4010	BCR	C38-C26-C27	3.29	119.69	113.45
11	a	1120	CLA	O2A-CGA-CBA	3.29	125.88	112.33
11	a	1022	CLA	C3C-C4C-NC	3.29	113.54	110.21
11	A	1127	CLA	C9-C8-C10	3.29	123.35	111.36
11	1	1129	CLA	C3C-C4C-NC	3.29	113.54	110.21
14	B	4005	BCR	C38-C26-C27	3.29	119.70	113.45
11	B	1236	CLA	C3C-C4C-NC	3.29	113.55	110.21
11	0	1401	CLA	C4-C3-C5	3.29	121.00	115.29
11	a	1129	CLA	C3C-C4C-NC	3.29	113.55	110.21
11	B	1214	CLA	C3C-C4C-NC	3.30	113.55	110.21
11	a	1125	CLA	C3C-C4C-NC	3.30	113.55	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1223	CLA	C3C-C4C-NC	3.30	113.55	110.21
14	a	4001	BCR	C23-C22-C21	3.30	124.00	118.94
11	2	1235	CLA	CMB-C2B-C3B	3.30	131.02	124.89
11	K	1401	CLA	C4-C3-C5	3.30	121.02	115.29
11	1	1140	CLA	C3C-C4C-NC	3.30	113.56	110.21
11	2	1021	CLA	CHB-C4A-NA	3.30	129.08	124.51
11	k	1401	CLA	C4-C3-C5	3.31	121.03	115.29
14	1	4002	BCR	C38-C26-C27	3.31	119.73	113.45
11	A	1011	CLA	CHB-C4A-NA	3.31	129.09	124.51
14	2	4010	BCR	C38-C26-C27	3.31	119.74	113.45
11	2	1235	CLA	CMC-C2C-C1C	3.31	130.05	125.02
14	6	4018	BCR	C33-C5-C4	3.32	119.74	113.45
11	1	1123	CLA	CMC-C2C-C1C	3.32	130.05	125.02
11	A	1135	CLA	C4-C3-C5	3.32	119.78	115.85
11	L	1501	CLA	C3C-C4C-NC	3.32	113.58	110.21
11	B	1207	CLA	C3C-C4C-NC	3.32	113.58	110.21
11	A	1237	CLA	C3C-C4C-NC	3.32	113.58	110.21
11	a	1011	CLA	CHB-C4A-NA	3.32	129.11	124.51
14	2	4010	BCR	C33-C5-C4	3.33	119.77	113.45
11	B	1240	CLA	C3C-C4C-NC	3.33	113.59	110.21
11	a	1109	CLA	CMC-C2C-C1C	3.33	130.07	125.02
11	a	1139	CLA	CMC-C2C-C1C	3.34	130.08	125.02
11	2	1224	CLA	C3C-C4C-NC	3.34	113.59	110.21
11	b	1220	CLA	CAC-C3C-C4C	3.34	129.53	124.83
11	A	1123	CLA	CAC-C3C-C4C	3.34	129.54	124.83
11	B	1225	CLA	C3C-C4C-NC	3.34	113.59	110.21
11	b	1207	CLA	C1-O2A-CGA	3.34	124.79	116.77
11	B	1226	CLA	C3C-C4C-NC	3.34	113.60	110.21
14	2	4014	BCR	C19-C18-C17	3.34	124.07	118.94
14	b	4014	BCR	C38-C26-C27	3.34	119.80	113.45
11	b	1207	CLA	C3C-C4C-NC	3.35	113.60	110.21
11	1	1121	CLA	O2A-CGA-CBA	3.35	126.13	112.33
11	1	1113	CLA	C3C-C4C-NC	3.35	113.61	110.21
11	a	1128	CLA	C4-C3-C5	3.35	121.11	115.29
14	L	4022	BCR	C38-C26-C27	3.36	119.83	113.45
11	B	1216	CLA	CMB-C2B-C3B	3.36	131.13	124.89
11	1	1102	CLA	CMC-C2C-C1C	3.36	130.12	125.02
14	2	4009	BCR	C33-C5-C4	3.36	119.84	113.45
11	A	1112	CLA	C3C-C4C-NC	3.37	113.62	110.21
11	a	1120	CLA	C3C-C4C-NC	3.37	113.62	110.21
11	a	1126	CLA	CMC-C2C-C1C	3.37	130.13	125.02
11	a	1122	CLA	C3C-C4C-NC	3.37	113.63	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4009	BCR	C23-C22-C21	3.38	124.12	118.94
14	b	4011	BCR	C8-C9-C10	3.38	124.13	118.94
11	1	1107	CLA	C3C-C4C-NC	3.38	113.64	110.21
11	b	1226	CLA	C3C-C4C-NC	3.38	113.64	110.21
11	A	1119	CLA	O2A-CGA-CBA	3.39	121.75	111.90
14	A	4008	BCR	C19-C18-C17	3.39	124.14	118.94
11	A	1127	CLA	C3C-C4C-NC	3.39	113.64	110.21
11	a	1123	CLA	CMC-C2C-C1C	3.39	130.16	125.02
14	8	4022	BCR	C33-C5-C4	3.39	119.89	113.45
11	A	1113	CLA	C3C-C4C-NC	3.39	113.65	110.21
11	l	1501	CLA	C3C-C4C-NC	3.40	113.65	110.21
11	B	1023	CLA	C3C-C4C-NC	3.40	113.65	110.21
11	2	1226	CLA	C3C-C4C-NC	3.40	113.65	110.21
11	b	1013	CLA	C1-O2A-CGA	3.41	124.95	116.77
11	a	1011	CLA	O2D-CGD-CBD	3.41	117.40	111.30
14	6	4013	BCR	C23-C22-C21	3.42	124.19	118.94
11	1	1106	CLA	C1-O2A-CGA	3.42	124.97	116.77
11	A	1116	CLA	C3C-C4C-NC	3.42	113.68	110.21
11	B	1230	CLA	C3C-C4C-NC	3.42	113.68	110.21
11	B	1203	CLA	C4-C3-C5	3.42	121.22	115.29
11	A	1107	CLA	C3C-C4C-NC	3.42	113.68	110.21
11	1	1137	CLA	C3C-C4C-NC	3.43	113.68	110.21
11	2	1219	CLA	C3C-C4C-NC	3.43	113.68	110.21
11	b	1224	CLA	C3C-C4C-NC	3.43	113.68	110.21
11	b	1221	CLA	CMC-C2C-C1C	3.43	130.22	125.02
11	1	1237	CLA	O2A-CGA-CBA	3.43	121.89	111.90
11	a	1105	CLA	O2A-C1-C2	3.46	121.25	109.31
11	B	1240	CLA	CMB-C2B-C3B	3.46	131.31	124.89
11	A	1129	CLA	C3C-C4C-NC	3.46	113.72	110.21
11	B	1204	CLA	O2A-CGA-CBA	3.46	121.97	111.90
14	2	4004	BCR	C33-C5-C4	3.46	120.02	113.45
11	B	1223	CLA	C3C-C4C-NC	3.47	113.72	110.21
11	2	1023	CLA	C1-O2A-CGA	3.47	125.10	116.77
11	2	1221	CLA	C3C-C4C-NC	3.47	113.73	110.21
11	A	1140	CLA	C4-C3-C5	3.48	121.32	115.29
11	a	1107	CLA	C3C-C4C-NC	3.48	113.73	110.21
14	B	4014	BCR	C38-C26-C27	3.48	120.05	113.45
11	A	1101	CLA	C3C-C4C-NC	3.48	113.74	110.21
14	b	4017	BCR	C33-C5-C4	3.48	120.06	113.45
11	a	1115	CLA	C3C-C4C-NC	3.48	113.74	110.21
11	2	1204	CLA	O2A-CGA-CBA	3.48	122.04	111.90
11	1	1801	CLA	C3C-C4C-NC	3.48	113.74	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4005	BCR	C38-C26-C27	3.49	120.08	113.45
11	a	1126	CLA	C3C-C4C-NC	3.50	113.75	110.21
11	2	1207	CLA	C1-O2A-CGA	3.50	125.17	116.77
11	A	1107	CLA	C4-C3-C5	3.50	121.36	115.29
11	B	1225	CLA	O2A-CGA-CBA	3.50	122.08	111.90
11	2	1223	CLA	C3C-C4C-NC	3.50	113.76	110.21
14	A	4002	BCR	C38-C26-C27	3.50	120.10	113.45
11	1	1135	CLA	C3C-C4C-NC	3.51	113.76	110.21
11	1	1107	CLA	C1-O2A-CGA	3.51	125.19	116.77
11	b	1220	CLA	C3C-C4C-NC	3.52	113.77	110.21
14	b	4017	BCR	C38-C26-C27	3.52	120.12	113.45
14	A	4001	BCR	C19-C18-C17	3.52	124.34	118.94
11	B	1021	CLA	CHB-C4A-NA	3.52	129.38	124.51
11	b	1210	CLA	CAC-C3C-C4C	3.52	129.80	124.83
11	A	1122	CLA	C3C-C4C-NC	3.52	113.78	110.21
14	2	4004	BCR	C38-C26-C27	3.52	120.14	113.45
11	2	1230	CLA	C3C-C4C-NC	3.53	113.78	110.21
14	b	4017	BCR	C19-C18-C17	3.53	124.36	118.94
11	1	1122	CLA	C3C-C4C-NC	3.53	113.79	110.21
11	A	1012	CLA	C3C-C4C-NC	3.54	113.80	110.21
11	2	1214	CLA	O2A-CGA-CBA	3.54	122.21	111.90
14	A	4008	BCR	C33-C5-C4	3.55	120.18	113.45
14	f	4013	BCR	C23-C22-C21	3.55	124.39	118.94
11	b	1230	CLA	C3C-C4C-NC	3.55	113.81	110.21
11	A	1137	CLA	C3C-C4C-NC	3.55	113.81	110.21
11	2	1216	CLA	C3C-C4C-NC	3.56	113.82	110.21
11	B	1224	CLA	C3C-C4C-NC	3.56	113.82	110.21
11	l	1502	CLA	C3C-C4C-NC	3.56	113.82	110.21
11	a	1137	CLA	C4-C3-C5	3.56	121.47	115.29
11	2	1013	CLA	C1-O2A-CGA	3.57	125.33	116.77
11	A	1801	CLA	C3C-C4C-NC	3.57	113.83	110.21
11	1	1125	CLA	O2A-CGA-CBA	3.57	122.29	111.90
11	a	1012	CLA	C3C-C4C-NC	3.58	113.83	110.21
11	B	1222	CLA	C3C-C4C-NC	3.58	113.84	110.21
14	B	4017	BCR	C38-C26-C27	3.58	120.25	113.45
11	2	1230	CLA	O2A-CGA-CBA	3.60	122.37	111.90
14	F	4013	BCR	C23-C22-C21	3.60	124.47	118.94
11	2	1215	CLA	C1-O2A-CGA	3.60	125.42	116.77
11	A	1139	CLA	CMC-C2C-C1C	3.61	130.49	125.02
14	1	4001	BCR	C23-C22-C21	3.61	124.48	118.94
11	b	1221	CLA	C3C-C4C-NC	3.61	113.87	110.21
11	2	1221	CLA	O2A-CGA-CBA	3.62	122.42	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1238	CLA	O2A-CGA-CBA	3.62	122.44	111.90
11	A	1138	CLA	CMC-C2C-C1C	3.63	130.52	125.02
14	L	4022	BCR	C33-C5-C4	3.64	120.35	113.45
11	A	1237	CLA	O2A-CGA-CBA	3.64	122.48	111.90
11	b	1221	CLA	O2A-CGA-CBA	3.64	122.49	111.90
11	B	1235	CLA	O2A-CGA-CBA	3.64	122.50	111.90
11	B	1201	CLA	O2A-CGA-CBA	3.65	122.52	111.90
11	a	1132	CLA	C1-O2A-CGA	3.65	125.53	116.77
14	B	4010	BCR	C33-C5-C4	3.65	120.38	113.45
11	B	1221	CLA	C3C-C4C-NC	3.65	113.91	110.21
14	a	4003	BCR	C33-C5-C4	3.66	120.39	113.45
14	b	4004	BCR	C38-C26-C27	3.67	120.41	113.45
11	2	1238	CLA	O2A-CGA-CBA	3.67	122.57	111.90
14	2	4014	BCR	C23-C22-C21	3.67	124.57	118.94
11	b	1204	CLA	O2A-CGA-CBA	3.67	122.58	111.90
14	B	4004	BCR	C38-C26-C27	3.67	120.42	113.45
11	a	1125	CLA	O2A-CGA-CBA	3.68	122.62	111.90
14	B	4011	BCR	C38-C26-C27	3.69	120.45	113.45
14	8	4022	BCR	C38-C26-C27	3.70	120.46	113.45
11	a	1126	CLA	O2A-CGA-CBA	3.70	122.66	111.90
11	b	1225	CLA	O2A-CGA-CBA	3.70	122.66	111.90
14	B	4014	BCR	C23-C22-C21	3.70	124.62	118.94
11	A	1131	CLA	O2A-CGA-CBA	3.70	122.68	111.90
11	B	1230	CLA	C4-C3-C5	3.71	121.72	115.29
14	L	4019	BCR	C23-C22-C21	3.71	124.64	118.94
11	a	1122	CLA	C1-O2A-CGA	3.71	125.68	116.77
14	m	4021	BCR	C38-C26-C27	3.72	120.52	113.45
14	a	4002	BCR	C38-C26-C27	3.73	120.52	113.45
11	a	1107	CLA	O2A-CGA-CBA	3.73	122.75	111.90
14	b	4011	BCR	C38-C26-C27	3.73	120.53	113.45
14	B	4006	BCR	C33-C5-C4	3.73	120.53	113.45
11	8	1502	CLA	C3C-C4C-NC	3.73	113.99	110.21
14	1	4008	BCR	C38-C26-C27	3.74	120.54	113.45
11	a	1111	CLA	CMC-C2C-C1C	3.74	130.69	125.02
11	A	1101	CLA	O2A-CGA-CBA	3.74	122.78	111.90
14	1	4008	BCR	C33-C5-C4	3.75	120.56	113.45
11	a	1123	CLA	O2A-CGA-CBA	3.75	122.82	111.90
11	A	1122	CLA	C4-C3-C5	3.76	121.81	115.29
11	a	1237	CLA	O2A-CGA-CBA	3.76	122.84	111.90
11	a	1106	CLA	O2A-CGA-CBA	3.76	122.84	111.90
11	A	1126	CLA	O2A-CGA-CBA	3.77	122.87	111.90
14	B	4017	BCR	C19-C18-C17	3.77	124.73	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	l	1501	CLA	C4-C3-C5	3.78	121.85	115.29
11	B	1230	CLA	O2A-CGA-CBA	3.78	122.91	111.90
11	A	1123	CLA	O2A-CGA-CBA	3.79	122.93	111.90
11	2	1215	CLA	O2A-CGA-CBA	3.79	122.94	111.90
11	b	1238	CLA	O2A-CGA-CBA	3.79	122.94	111.90
11	A	1125	CLA	O2A-CGA-CBA	3.80	122.94	111.90
14	a	4008	BCR	C38-C26-C27	3.80	120.67	113.45
11	a	1135	CLA	O2A-CGA-CBA	3.81	122.97	111.90
14	A	4001	BCR	C23-C22-C21	3.81	124.80	118.94
11	1	1123	CLA	O2A-CGA-CBA	3.82	123.02	111.90
11	B	1225	CLA	O2D-CGD-CBD	3.82	118.13	111.30
11	a	1132	CLA	O2A-CGA-CBA	3.82	123.03	111.90
11	A	1101	CLA	O2D-CGD-CBD	3.83	118.13	111.30
14	f	4018	BCR	C33-C5-C4	3.83	120.72	113.45
14	a	4008	BCR	C33-C5-C4	3.83	120.73	113.45
11	1	1103	CLA	O2A-CGA-CBA	3.83	123.06	111.90
11	1	1131	CLA	O2A-CGA-CBA	3.84	123.06	111.90
11	A	1022	CLA	O2A-CGA-CBA	3.84	123.08	111.90
11	b	1201	CLA	O2A-CGA-CBA	3.84	123.08	111.90
11	2	1213	CLA	C3C-C4C-NC	3.85	114.11	110.21
11	1	1128	CLA	O2A-CGA-CBA	3.85	123.09	111.90
11	B	1220	CLA	O2D-CGD-CBD	3.86	118.19	111.30
11	B	1221	CLA	O2A-CGA-CBA	3.86	123.13	111.90
11	B	1206	CLA	O2D-CGD-CBD	3.87	118.21	111.30
11	B	1203	CLA	O2A-CGA-CBA	3.89	123.23	111.90
11	a	1131	CLA	O2A-CGA-CBA	3.89	123.23	111.90
11	B	1013	CLA	C1-O2A-CGA	3.90	126.12	116.77
11	1	1125	CLA	CAC-C3C-C4C	3.90	130.33	124.83
11	2	1201	CLA	O2A-CGA-CBA	3.91	123.27	111.90
11	a	1237	CLA	O2D-CGD-CBD	3.91	118.29	111.30
11	2	1230	CLA	C1-O2A-CGA	3.92	126.17	116.77
14	A	4008	BCR	C38-C26-C27	3.92	120.89	113.45
11	8	1501	CLA	O2A-CGA-CBA	3.92	123.31	111.90
11	a	1128	CLA	O2A-CGA-CBA	3.92	123.31	111.90
11	2	1203	CLA	O2A-CGA-CBA	3.92	123.32	111.90
11	1	1126	CLA	O2A-CGA-CBA	3.93	123.33	111.90
11	A	1109	CLA	C4-C3-C5	3.93	122.11	115.29
11	A	1237	CLA	O2D-CGD-CBD	3.94	118.34	111.30
11	B	1213	CLA	O2A-CGA-CBA	3.94	123.37	111.90
11	1	1135	CLA	O2A-CGA-CBA	3.96	123.41	111.90
11	B	1216	CLA	O2A-CGA-CBA	3.96	123.43	111.90
11	2	1021	CLA	C4-C3-C5	3.96	122.17	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1012	CLA	C3C-C4C-NC	3.97	114.23	110.21
11	A	1128	CLA	O2A-CGA-CBA	3.97	123.44	111.90
11	b	1235	CLA	O2A-CGA-CBA	3.97	123.45	111.90
11	2	1220	CLA	O2D-CGD-CBD	3.98	118.40	111.30
11	a	1101	CLA	O2A-CGA-CBA	3.98	123.47	111.90
11	b	1021	CLA	C4-C3-C5	3.98	122.19	115.29
11	8	1503	CLA	CMB-C2B-C3B	3.98	132.28	124.89
11	A	1107	CLA	O2A-CGA-CBA	3.98	123.48	111.90
11	1	1237	CLA	O2D-CGD-CBD	3.98	118.42	111.30
11	8	1501	CLA	C4-C3-C5	3.98	122.20	115.29
11	b	1206	CLA	O2A-CGA-CBA	3.99	123.50	111.90
11	1	1107	CLA	O2A-CGA-CBA	4.00	123.55	111.90
11	a	1022	CLA	O2A-CGA-CBA	4.01	123.58	111.90
11	A	1132	CLA	O2A-CGA-CBA	4.01	123.58	111.90
11	2	1219	CLA	O2A-CGA-CBA	4.02	123.59	111.90
11	B	1023	CLA	O2D-CGD-CBD	4.03	118.50	111.30
11	b	1235	CLA	CMB-C2B-C3B	4.04	132.38	124.89
11	b	1229	CLA	O2A-CGA-CBA	4.04	123.66	111.90
11	b	1216	CLA	O2A-CGA-CBA	4.04	123.66	111.90
11	B	1223	CLA	O2A-CGA-CBA	4.04	123.67	111.90
14	2	4006	BCR	C33-C5-C4	4.04	121.12	113.45
11	B	1023	CLA	O2A-CGA-CBA	4.05	123.67	111.90
11	2	1213	CLA	C4-C3-C5	4.05	122.31	115.29
11	2	1234	CLA	O2D-CGD-CBD	4.05	118.53	111.30
11	B	1203	CLA	O2D-CGD-CBD	4.05	118.53	111.30
11	A	1139	CLA	O2A-CGA-CBA	4.05	123.68	111.90
11	B	1206	CLA	O2A-CGA-CBA	4.06	123.72	111.90
11	A	1106	CLA	O2A-CGA-CBA	4.06	123.72	111.90
11	b	1226	CLA	O2A-CGA-CBA	4.06	123.72	111.90
11	1	1101	CLA	O2A-CGA-CBA	4.06	123.72	111.90
11	1	1105	CLA	O2A-CGA-CBA	4.07	123.73	111.90
11	1	1102	CLA	O2D-CGD-CBD	4.07	118.58	111.30
11	1	1118	CLA	O2A-CGA-CBA	4.08	123.77	111.90
11	2	1235	CLA	O2A-CGA-CBA	4.09	123.79	111.90
11	1	1139	CLA	O2A-CGA-CBA	4.09	123.80	111.90
11	2	1202	CLA	O2A-CGA-CBA	4.10	123.82	111.90
11	B	1021	CLA	C4-C3-C5	4.10	122.40	115.29
11	2	1230	CLA	C4-C3-C5	4.10	122.40	115.29
11	a	1118	CLA	O2A-CGA-CBA	4.12	123.88	111.90
11	B	1202	CLA	O2A-CGA-CBA	4.12	123.89	111.90
11	A	1135	CLA	O2D-CGD-CBD	4.12	118.66	111.30
11	a	1012	CLA	C4-C3-C5	4.12	122.44	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	2	1223	CLA	O2A-CGA-CBA	4.13	123.91	111.90
14	B	4010	BCR	C23-C22-C21	4.13	125.27	118.94
15	a	5003	LHG	O7-C7-C8	4.13	120.13	111.55
11	a	1103	CLA	O2A-CGA-CBA	4.13	123.92	111.90
11	1	1106	CLA	O2A-CGA-CBA	4.13	123.93	111.90
11	1	1127	CLA	O2A-CGA-CBA	4.14	123.94	111.90
11	b	1213	CLA	O2A-CGA-CBA	4.14	123.96	111.90
14	b	4006	BCR	C33-C5-C4	4.14	121.31	113.45
11	b	1202	CLA	O2A-CGA-CBA	4.15	123.96	111.90
11	2	1226	CLA	O2A-CGA-CBA	4.15	123.99	111.90
14	6	4020	BCR	C38-C26-C27	4.15	121.33	113.45
11	A	1105	CLA	O2A-CGA-CBA	4.16	123.99	111.90
11	a	1139	CLA	O2A-CGA-CBA	4.16	124.00	111.90
11	b	1228	CLA	O2A-CGA-CBA	4.16	124.00	111.90
11	B	1229	CLA	O2A-CGA-CBA	4.16	124.01	111.90
11	K	1402	CLA	O2A-CGA-CBA	4.17	124.02	111.90
11	a	1109	CLA	C4-C3-C5	4.18	122.53	115.29
14	2	4010	BCR	C23-C22-C21	4.18	125.35	118.94
11	A	1126	CLA	C4-C3-C5	4.18	122.54	115.29
11	b	1023	CLA	O2A-CGA-CBA	4.18	124.08	111.90
11	8	1503	CLA	O2A-CGA-CBA	4.19	124.10	111.90
11	2	1213	CLA	O2A-CGA-CBA	4.19	124.10	111.90
11	A	1108	CLA	O2D-CGD-CBD	4.20	118.80	111.30
11	B	1215	CLA	O2A-CGA-CBA	4.20	124.12	111.90
11	2	1203	CLA	O2D-CGD-CBD	4.21	118.81	111.30
11	L	1503	CLA	O2A-CGA-CBA	4.21	124.15	111.90
15	2	5004	LHG	O7-C7-C8	4.22	120.32	111.55
11	2	1206	CLA	O2A-CGA-CBA	4.23	124.19	111.90
11	1	1022	CLA	O2A-CGA-CBA	4.23	124.20	111.90
11	2	1220	CLA	CAC-C3C-C4C	4.23	130.79	124.83
11	1	1124	CLA	O2A-CGA-CBA	4.23	124.21	111.90
11	1	1122	CLA	O2A-CGA-CBA	4.23	124.21	111.90
11	B	1214	CLA	O2A-CGA-CBA	4.23	124.22	111.90
14	A	4003	BCR	C23-C22-C21	4.23	125.44	118.94
11	1	1104	CLA	O2A-CGA-CBA	4.24	124.23	111.90
11	2	1229	CLA	O2A-CGA-CBA	4.24	124.25	111.90
11	b	1210	CLA	O2A-CGA-CBA	4.24	124.25	111.90
11	2	1219	CLA	O2D-CGD-CBD	4.25	118.89	111.30
11	2	1232	CLA	O2D-CGD-CBD	4.25	118.90	111.30
11	a	1140	CLA	O2A-CGA-CBA	4.26	124.29	111.90
11	a	1134	CLA	O2D-CGD-CBD	4.26	118.91	111.30
11	b	1203	CLA	O2A-CGA-CBA	4.26	124.30	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1801	CLA	O2D-CGD-CBD	4.27	118.92	111.30
11	A	1012	CLA	C4-C3-C5	4.27	122.70	115.29
11	a	1117	CLA	O2A-CGA-CBA	4.28	124.34	111.90
11	a	1119	CLA	O2A-CGA-CBA	4.28	124.35	111.90
11	A	1103	CLA	O2D-CGD-CBD	4.28	118.95	111.30
11	B	1240	CLA	O2D-CGD-CBD	4.29	118.96	111.30
15	b	5004	LHG	O7-C7-C8	4.29	120.46	111.55
11	a	1109	CLA	O2A-CGA-CBA	4.29	124.39	111.90
11	a	1104	CLA	O2A-CGA-CBA	4.30	124.40	111.90
11	L	1501	CLA	O2A-CGA-CBA	4.30	124.41	111.90
11	b	1201	CLA	CMB-C2B-C3B	4.31	132.88	124.89
11	2	1210	CLA	O2A-CGA-CBA	4.31	124.45	111.90
11	B	1214	CLA	C4-C3-C5	4.31	122.77	115.29
11	a	1124	CLA	O2A-CGA-CBA	4.31	124.45	111.90
11	B	1236	CLA	O2A-CGA-CBA	4.32	124.47	111.90
11	a	1012	CLA	O2A-CGA-CBA	4.32	124.48	111.90
11	1	1106	CLA	O2D-CGD-CBD	4.33	119.03	111.30
11	l	1503	CLA	O2A-CGA-CBA	4.33	124.49	111.90
11	b	1231	CLA	O2D-CGD-CBD	4.33	119.03	111.30
15	1	5003	LHG	O7-C7-C8	4.33	120.55	111.55
11	a	1110	CLA	O2A-CGA-CBA	4.34	124.52	111.90
11	A	1137	CLA	CMB-C2B-C3B	4.34	132.94	124.89
11	1	1137	CLA	C4-C3-C5	4.34	122.82	115.29
15	1	5001	LHG	O7-C7-C8	4.34	120.57	111.55
11	b	1023	CLA	O2D-CGD-CBD	4.35	119.07	111.30
11	b	1215	CLA	O2A-CGA-CBA	4.36	124.58	111.90
11	A	1114	CLA	O2D-CGD-CBD	4.36	119.08	111.30
11	B	1234	CLA	O2D-CGD-CBD	4.36	119.09	111.30
11	1	1117	CLA	O2A-CGA-CBA	4.36	124.59	111.90
11	A	1110	CLA	O2A-CGA-CBA	4.36	124.59	111.90
11	A	1139	CLA	O2D-CGD-CBD	4.36	119.10	111.30
11	B	1219	CLA	O2D-CGD-CBD	4.37	119.10	111.30
14	1	4002	BCR	C19-C18-C17	4.37	125.65	118.94
11	a	1109	CLA	O2D-CGD-CBD	4.38	119.12	111.30
11	b	1229	CLA	O2D-CGD-CBD	4.38	119.13	111.30
11	a	1107	CLA	C4-C3-C5	4.38	122.89	115.29
11	a	1111	CLA	O2A-CGA-CBA	4.39	124.67	111.90
11	2	1217	CLA	O2A-CGA-CBA	4.39	124.68	111.90
11	b	1223	CLA	O2A-CGA-CBA	4.39	124.69	111.90
11	a	1022	CLA	O2D-CGD-CBD	4.40	119.16	111.30
11	a	1011	CLA	CMB-C2B-C3B	4.40	133.05	124.89
15	a	5001	LHG	O7-C7-C8	4.40	120.68	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4017	BCR	C19-C18-C17	4.40	125.69	118.94
11	B	1210	CLA	O2A-CGA-CBA	4.40	124.71	111.90
11	1	1140	CLA	O2A-CGA-CBA	4.40	124.71	111.90
11	B	1226	CLA	O2A-CGA-CBA	4.42	124.76	111.90
11	A	1127	CLA	O2A-CGA-CBA	4.43	124.79	111.90
11	B	1230	CLA	C1-O2A-CGA	4.44	127.41	116.77
11	A	1111	CLA	O2A-CGA-CBA	4.44	124.81	111.90
11	2	1228	CLA	O2A-CGA-CBA	4.44	124.82	111.90
11	b	1213	CLA	C4-C3-C5	4.44	122.99	115.29
11	1	1102	CLA	O2A-CGA-CBA	4.44	124.83	111.90
11	b	1222	CLA	C4-C3-C5	4.44	123.00	115.29
11	1	1124	CLA	O2D-CGD-CBD	4.45	119.25	111.30
11	1	1801	CLA	O2A-CGA-CBA	4.45	124.85	111.90
11	b	1214	CLA	O2A-CGA-CBA	4.45	124.86	111.90
11	b	1219	CLA	O2A-CGA-CBA	4.46	124.87	111.90
11	A	1109	CLA	O2D-CGD-CBD	4.46	119.26	111.30
11	b	1219	CLA	CMB-C2B-C3B	4.46	133.16	124.89
11	2	1240	CLA	O2D-CGD-CBD	4.46	119.28	111.30
11	B	1222	CLA	O2A-CGA-CBA	4.47	124.90	111.90
11	B	1228	CLA	O2A-CGA-CBA	4.47	124.92	111.90
11	2	1222	CLA	O2A-CGA-CBA	4.48	124.92	111.90
11	A	1118	CLA	O2A-CGA-CBA	4.48	124.93	111.90
11	1	1109	CLA	C4-C3-C5	4.48	123.06	115.29
11	B	1219	CLA	O2A-CGA-CBA	4.48	124.94	111.90
11	1	1109	CLA	O2D-CGD-CBD	4.48	119.31	111.30
11	2	1208	CLA	O2D-CGD-CBD	4.48	119.31	111.30
11	K	1402	CLA	O2D-CGD-CBD	4.49	119.31	111.30
11	A	1127	CLA	O2D-CGD-CBD	4.49	119.32	111.30
11	2	1234	CLA	O2A-CGA-CBA	4.50	124.99	111.90
11	1	1012	CLA	C4-C3-C5	4.50	123.09	115.29
11	1	1127	CLA	O2D-CGD-CBD	4.50	119.34	111.30
11	l	1501	CLA	O2A-CGA-CBA	4.50	124.99	111.90
11	1	1108	CLA	O2D-CGD-CBD	4.50	119.34	111.30
11	a	1125	CLA	O2D-CGD-CBD	4.51	119.35	111.30
11	1	1110	CLA	O2A-CGA-CBA	4.51	125.02	111.90
11	b	1219	CLA	O2D-CGD-CBD	4.51	119.37	111.30
11	2	1205	CLA	O2A-CGA-CBA	4.52	125.04	111.90
11	k	1402	CLA	O2A-CGA-CBA	4.52	125.05	111.90
11	b	1230	CLA	C4-C3-C5	4.52	123.13	115.29
11	a	1127	CLA	O2A-CGA-CBA	4.53	125.07	111.90
11	A	1117	CLA	O2A-CGA-CBA	4.53	125.09	111.90
11	2	1013	CLA	O2D-CGD-CBD	4.54	119.41	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	1402	CLA	O2D-CGD-CBD	4.54	119.41	111.30
11	2	1236	CLA	O2A-CGA-CBA	4.55	125.12	111.90
11	b	1206	CLA	O2D-CGD-CBD	4.55	119.42	111.30
11	A	1134	CLA	O2D-CGD-CBD	4.55	119.43	111.30
11	a	1108	CLA	O2D-CGD-CBD	4.55	119.43	111.30
11	A	1124	CLA	O2A-CGA-CBA	4.55	125.15	111.90
11	A	1129	CLA	O2D-CGD-CBD	4.56	119.44	111.30
11	A	1113	CLA	O2D-CGD-CBD	4.56	119.45	111.30
11	1	1116	CLA	O2A-CGA-CBA	4.57	125.20	111.90
11	A	1116	CLA	O2A-CGA-CBA	4.57	125.20	111.90
11	a	1116	CLA	O2A-CGA-CBA	4.57	125.20	111.90
11	0	1402	CLA	O2A-CGA-CBA	4.57	125.21	111.90
11	2	1202	CLA	O2D-CGD-CBD	4.57	119.47	111.30
15	A	5001	LHG	O7-C7-C8	4.58	121.05	111.55
11	A	1104	CLA	O2A-CGA-CBA	4.58	125.22	111.90
11	b	1021	CLA	O2A-CGA-CBA	4.58	125.24	111.90
11	1	1113	CLA	O2D-CGD-CBD	4.58	119.49	111.30
11	A	1140	CLA	O2A-CGA-CBA	4.59	125.25	111.90
11	1	1121	CLA	O2D-CGD-CBD	4.59	119.50	111.30
16	b	5002	LMG	O7-C10-C11	4.59	121.08	111.55
11	b	1222	CLA	O2A-CGA-CBA	4.60	125.28	111.90
11	1	1011	CLA	O2A-CGA-CBA	4.60	125.29	111.90
11	0	1402	CLA	O2D-CGD-CBD	4.60	119.52	111.30
11	b	1223	CLA	O2D-CGD-CBD	4.60	119.52	111.30
11	b	1013	CLA	O2A-CGA-CBA	4.61	125.31	111.90
11	B	1205	CLA	O2A-CGA-CBA	4.61	125.32	111.90
11	1	1122	CLA	O2D-CGD-CBD	4.61	119.55	111.30
11	b	1205	CLA	O2A-CGA-CBA	4.62	125.35	111.90
11	a	1102	CLA	O2D-CGD-CBD	4.62	119.56	111.30
11	b	1013	CLA	O2D-CGD-CBD	4.62	119.56	111.30
11	A	1121	CLA	O2D-CGD-CBD	4.63	119.57	111.30
11	1	1119	CLA	O2A-CGA-CBA	4.64	125.41	111.90
11	L	1501	CLA	O2D-CGD-CBD	4.65	119.60	111.30
11	B	1210	CLA	O2D-CGD-CBD	4.65	119.60	111.30
11	A	1022	CLA	O2D-CGD-CBD	4.65	119.61	111.30
11	A	1135	CLA	O2A-CGA-CBA	4.65	125.43	111.90
11	A	1119	CLA	O2D-CGD-CBD	4.65	119.62	111.30
11	B	1202	CLA	CMB-C2B-C3B	4.66	133.53	124.89
11	a	1137	CLA	O2A-CGA-CBA	4.66	125.45	111.90
11	a	1103	CLA	O2D-CGD-CBD	4.66	119.63	111.30
11	a	1107	CLA	O2D-CGD-CBD	4.66	119.64	111.30
11	1	1140	CLA	O2D-CGD-CBD	4.66	119.64	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1125	CLA	CAC-C3C-C4C	4.67	131.41	124.83
11	a	1114	CLA	O2D-CGD-CBD	4.67	119.64	111.30
11	1	1111	CLA	O2A-CGA-CBA	4.67	125.49	111.90
11	2	1013	CLA	O2A-CGA-CBA	4.67	125.49	111.90
11	B	1217	CLA	O2D-CGD-CBD	4.68	119.66	111.30
11	b	1224	CLA	O2A-CGA-CBA	4.68	125.51	111.90
11	b	1234	CLA	O2A-CGA-CBA	4.68	125.53	111.90
11	b	1207	CLA	O2D-CGD-CBD	4.69	119.67	111.30
11	1	1138	CLA	O2D-CGD-CBD	4.69	119.68	111.30
11	b	1236	CLA	O2A-CGA-CBA	4.69	125.56	111.90
11	A	1102	CLA	O2A-CGA-CBA	4.69	125.56	111.90
11	2	1216	CLA	O2A-CGA-CBA	4.70	125.57	111.90
11	a	1122	CLA	O2A-CGA-CBA	4.70	125.57	111.90
11	2	1209	CLA	O2D-CGD-CBD	4.70	119.70	111.30
11	a	1102	CLA	O2A-CGA-CBA	4.71	125.60	111.90
11	a	1139	CLA	O2D-CGD-CBD	4.71	119.71	111.30
15	A	5003	LHG	O7-C7-C8	4.72	121.35	111.55
11	a	1113	CLA	O2D-CGD-CBD	4.72	119.73	111.30
11	B	1208	CLA	O2D-CGD-CBD	4.72	119.74	111.30
11	1	1109	CLA	O2A-CGA-CBA	4.73	125.65	111.90
11	a	1121	CLA	O2D-CGD-CBD	4.73	119.75	111.30
11	B	1210	CLA	CAC-C3C-C4C	4.73	131.51	124.83
11	B	1224	CLA	O2A-CGA-CBA	4.74	125.71	111.90
11	B	1013	CLA	O2A-CGA-CBA	4.75	125.71	111.90
11	A	1109	CLA	O2A-CGA-CBA	4.75	125.72	111.90
11	b	1234	CLA	O2D-CGD-CBD	4.75	119.78	111.30
11	B	1222	CLA	C4-C3-C5	4.75	123.53	115.29
11	1	1126	CLA	C4-C3-C5	4.76	123.54	115.29
11	B	1222	CLA	CMB-C2B-C3B	4.76	133.72	124.89
11	A	1122	CLA	O2A-CGA-CBA	4.76	125.77	111.90
11	B	1234	CLA	O2A-CGA-CBA	4.77	125.78	111.90
11	b	1230	CLA	O2A-CGA-CBA	4.77	125.79	111.90
11	B	1229	CLA	O2D-CGD-CBD	4.77	119.83	111.30
11	2	1023	CLA	O2A-CGA-CBA	4.78	125.80	111.90
11	k	1401	CLA	O2D-CGD-CBD	4.78	119.84	111.30
11	2	1207	CLA	O2D-CGD-CBD	4.78	119.84	111.30
11	K	1401	CLA	O2D-CGD-CBD	4.78	119.85	111.30
11	B	1013	CLA	O2D-CGD-CBD	4.79	119.85	111.30
11	a	1111	CLA	O2D-CGD-CBD	4.79	119.86	111.30
11	2	1219	CLA	CMB-C2B-C3B	4.79	133.78	124.89
11	b	1217	CLA	O2A-CGA-CBA	4.79	125.84	111.90
11	2	1228	CLA	O2D-CGD-CBD	4.79	119.87	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	5004	LHG	O7-C7-C8	4.80	121.51	111.55
11	0	1401	CLA	O2D-CGD-CBD	4.80	119.87	111.30
11	A	1137	CLA	O2A-CGA-CBA	4.80	125.86	111.90
11	B	1216	CLA	O2D-CGD-CBD	4.80	119.87	111.30
11	A	1138	CLA	O2D-CGD-CBD	4.80	119.88	111.30
11	1	1137	CLA	O2A-CGA-CBA	4.80	125.88	111.90
11	A	1117	CLA	CMB-C2B-C3B	4.81	133.81	124.89
11	A	1117	CLA	O2D-CGD-CBD	4.81	119.90	111.30
11	A	1120	CLA	O2D-CGD-CBD	4.82	119.91	111.30
11	A	1105	CLA	O2D-CGD-CBD	4.82	119.92	111.30
11	k	1401	CLA	O2A-CGA-CBA	4.83	125.95	111.90
11	a	1105	CLA	O2A-CGA-CBA	4.83	125.95	111.90
11	0	1401	CLA	O2A-CGA-CBA	4.83	125.96	111.90
11	K	1401	CLA	O2A-CGA-CBA	4.83	125.96	111.90
11	2	1212	CLA	O2D-CGD-CBD	4.85	119.96	111.30
11	b	1215	CLA	C4-C3-C5	4.85	123.70	115.29
11	b	1220	CLA	O2D-CGD-CBD	4.85	119.97	111.30
11	1	1139	CLA	O2D-CGD-CBD	4.85	119.97	111.30
11	b	1217	CLA	O2D-CGD-CBD	4.86	119.98	111.30
11	a	1117	CLA	O2D-CGD-CBD	4.86	119.99	111.30
11	a	1115	CLA	O2D-CGD-CBD	4.87	120.00	111.30
11	A	1124	CLA	O2D-CGD-CBD	4.87	120.01	111.30
11	2	1224	CLA	O2A-CGA-CBA	4.88	126.09	111.90
11	A	1107	CLA	O2D-CGD-CBD	4.88	120.03	111.30
11	a	1126	CLA	C4-C3-C5	4.88	123.76	115.29
11	2	1206	CLA	O2D-CGD-CBD	4.89	120.04	111.30
11	A	1128	CLA	O2D-CGD-CBD	4.90	120.05	111.30
11	2	1021	CLA	O2D-CGD-CBD	4.90	120.05	111.30
11	2	1023	CLA	O2D-CGD-CBD	4.91	120.08	111.30
11	1	1117	CLA	O2D-CGD-CBD	4.92	120.09	111.30
11	A	1011	CLA	O2A-CGA-CBA	4.93	126.24	111.90
11	a	1128	CLA	O2D-CGD-CBD	4.94	120.13	111.30
11	2	1201	CLA	O2D-CGD-CBD	4.94	120.13	111.30
11	A	1012	CLA	O2A-CGA-CBA	4.95	126.29	111.90
11	B	1217	CLA	O2A-CGA-CBA	4.95	126.30	111.90
11	1	1132	CLA	O2D-CGD-CBD	4.95	120.15	111.30
11	1	1133	CLA	O2D-CGD-CBD	4.95	120.15	111.30
11	B	1211	CLA	O2D-CGD-CBD	4.96	120.16	111.30
11	1	1128	CLA	O2D-CGD-CBD	4.96	120.17	111.30
11	a	1801	CLA	O2A-CGA-CBA	4.96	126.34	111.90
11	b	1210	CLA	O2D-CGD-CBD	4.97	120.17	111.30
14	b	4009	BCR	C19-C18-C17	4.97	126.56	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1801	CLA	O2A-CGA-CBA	4.97	126.35	111.90
11	a	1127	CLA	O2D-CGD-CBD	4.97	120.18	111.30
11	1	1022	CLA	O2D-CGD-CBD	4.97	120.18	111.30
11	a	1119	CLA	O2D-CGD-CBD	4.97	120.18	111.30
11	B	1232	CLA	O2D-CGD-CBD	4.98	120.19	111.30
11	b	1238	CLA	O2D-CGD-CBD	4.98	120.19	111.30
11	A	1123	CLA	O2D-CGD-CBD	4.99	120.22	111.30
11	b	1225	CLA	O2D-CGD-CBD	4.99	120.22	111.30
11	a	1011	CLA	O2A-CGA-CBA	4.99	126.43	111.90
11	a	1122	CLA	O2D-CGD-CBD	5.00	120.23	111.30
11	2	1239	CLA	O2D-CGD-CBD	5.01	120.26	111.30
11	2	1235	CLA	O2D-CGD-CBD	5.01	120.26	111.30
11	b	1021	CLA	O2D-CGD-CBD	5.01	120.26	111.30
11	b	1240	CLA	O2D-CGD-CBD	5.02	120.28	111.30
11	a	1101	CLA	O2D-CGD-CBD	5.03	120.29	111.30
16	2	5002	LMG	O7-C10-C11	5.03	122.00	111.55
11	A	1115	CLA	O2D-CGD-CBD	5.03	120.29	111.30
11	B	1236	CLA	O2D-CGD-CBD	5.04	120.31	111.30
11	b	1212	CLA	O2D-CGD-CBD	5.05	120.32	111.30
11	1	1119	CLA	O2D-CGD-CBD	5.05	120.33	111.30
11	1	1103	CLA	O2D-CGD-CBD	5.06	120.34	111.30
11	1	1012	CLA	O2A-CGA-CBA	5.06	126.63	111.90
11	b	1232	CLA	O2D-CGD-CBD	5.07	120.35	111.30
11	8	1503	CLA	O2D-CGD-CBD	5.07	120.36	111.30
11	A	1130	CLA	O2D-CGD-CBD	5.08	120.38	111.30
11	b	1216	CLA	O2D-CGD-CBD	5.08	120.38	111.30
11	1	1114	CLA	O2D-CGD-CBD	5.10	120.41	111.30
11	2	1238	CLA	O2D-CGD-CBD	5.10	120.42	111.30
11	B	1238	CLA	O2D-CGD-CBD	5.11	120.42	111.30
11	B	1202	CLA	O2D-CGD-CBD	5.11	120.43	111.30
11	B	1213	CLA	O2D-CGD-CBD	5.11	120.43	111.30
11	a	1140	CLA	O2D-CGD-CBD	5.11	120.43	111.30
11	1	1135	CLA	C4-C3-C5	5.12	121.91	115.85
11	2	1207	CLA	O2A-CGA-CBA	5.13	126.82	111.90
11	2	1223	CLA	O2D-CGD-CBD	5.13	120.47	111.30
11	2	1229	CLA	O2D-CGD-CBD	5.14	120.48	111.30
11	1	1107	CLA	O2D-CGD-CBD	5.14	120.48	111.30
11	a	1105	CLA	O2D-CGD-CBD	5.15	120.50	111.30
11	B	1239	CLA	O2D-CGD-CBD	5.15	120.50	111.30
11	B	1218	CLA	O2D-CGD-CBD	5.15	120.50	111.30
11	b	1207	CLA	O2A-CGA-CBA	5.16	126.92	111.90
11	b	1236	CLA	O2D-CGD-CBD	5.16	120.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1228	CLA	O2D-CGD-CBD	5.17	120.54	111.30
11	2	1214	CLA	O2D-CGD-CBD	5.17	120.54	111.30
11	1	1136	CLA	O2D-CGD-CBD	5.17	120.54	111.30
11	a	1131	CLA	O2D-CGD-CBD	5.18	120.56	111.30
11	B	1215	CLA	O2D-CGD-CBD	5.18	120.56	111.30
11	b	1203	CLA	O2D-CGD-CBD	5.18	120.56	111.30
11	b	1208	CLA	O2D-CGD-CBD	5.19	120.57	111.30
11	b	1201	CLA	O2D-CGD-CBD	5.19	120.58	111.30
11	B	1212	CLA	O2D-CGD-CBD	5.19	120.58	111.30
11	b	1218	CLA	O2D-CGD-CBD	5.19	120.58	111.30
11	B	1021	CLA	O2A-CGA-CBA	5.19	127.01	111.90
16	B	5002	LMG	O7-C10-C11	5.20	122.35	111.55
11	2	1215	CLA	C4-C3-C5	5.20	124.32	115.29
11	A	1140	CLA	O2D-CGD-CBD	5.21	120.60	111.30
11	B	1207	CLA	O2A-CGA-CBA	5.21	127.05	111.90
11	1	1104	CLA	O2D-CGD-CBD	5.21	120.61	111.30
11	1	1105	CLA	O2D-CGD-CBD	5.21	120.61	111.30
11	a	1123	CLA	O2D-CGD-CBD	5.22	120.63	111.30
11	a	1118	CLA	O2D-CGD-CBD	5.22	120.63	111.30
11	A	1118	CLA	O2D-CGD-CBD	5.22	120.63	111.30
11	A	1133	CLA	O2D-CGD-CBD	5.23	120.64	111.30
11	b	1204	CLA	O2D-CGD-CBD	5.23	120.64	111.30
11	A	1111	CLA	O2D-CGD-CBD	5.23	120.65	111.30
11	A	1136	CLA	O2D-CGD-CBD	5.24	120.66	111.30
11	B	1021	CLA	O2D-CGD-CBD	5.24	120.66	111.30
11	a	1104	CLA	O2D-CGD-CBD	5.26	120.70	111.30
11	a	1112	CLA	O2D-CGD-CBD	5.27	120.71	111.30
11	B	1228	CLA	O2D-CGD-CBD	5.27	120.71	111.30
11	b	1205	CLA	O2D-CGD-CBD	5.28	120.73	111.30
11	B	1230	CLA	O2D-CGD-CBD	5.28	120.74	111.30
11	a	1132	CLA	O2D-CGD-CBD	5.29	120.75	111.30
11	b	1235	CLA	O2D-CGD-CBD	5.30	120.77	111.30
11	A	1122	CLA	O2D-CGD-CBD	5.30	120.77	111.30
11	1	1131	CLA	O2D-CGD-CBD	5.30	120.77	111.30
11	b	1209	CLA	O2D-CGD-CBD	5.31	120.78	111.30
11	1	1135	CLA	O2D-CGD-CBD	5.31	120.79	111.30
11	A	1137	CLA	O2D-CGD-CBD	5.31	120.79	111.30
11	a	1130	CLA	O2D-CGD-CBD	5.32	120.80	111.30
11	1	1118	CLA	O2D-CGD-CBD	5.32	120.81	111.30
11	1	1130	CLA	O2D-CGD-CBD	5.33	120.82	111.30
11	1	1115	CLA	O2D-CGD-CBD	5.33	120.83	111.30
11	b	1202	CLA	O2D-CGD-CBD	5.33	120.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1213	CLA	O2D-CGD-CBD	5.34	120.84	111.30
11	a	1135	CLA	O2D-CGD-CBD	5.35	120.86	111.30
11	B	1235	CLA	O2D-CGD-CBD	5.35	120.87	111.30
11	b	1239	CLA	O2D-CGD-CBD	5.36	120.87	111.30
11	b	1221	CLA	C4-C3-C5	5.36	124.59	115.29
11	a	1801	CLA	O2D-CGD-CBD	5.36	120.88	111.30
11	2	1217	CLA	O2D-CGD-CBD	5.36	120.88	111.30
11	b	1214	CLA	O2D-CGD-CBD	5.36	120.88	111.30
11	b	1215	CLA	O2D-CGD-CBD	5.37	120.90	111.30
11	1	1111	CLA	O2D-CGD-CBD	5.38	120.91	111.30
11	2	1225	CLA	O2D-CGD-CBD	5.38	120.92	111.30
11	2	1230	CLA	O2D-CGD-CBD	5.38	120.92	111.30
11	1	1503	CLA	O2D-CGD-CBD	5.39	120.93	111.30
11	2	1216	CLA	O2D-CGD-CBD	5.40	120.95	111.30
11	2	1021	CLA	O2A-CGA-CBA	5.40	127.62	111.90
11	L	1503	CLA	O2D-CGD-CBD	5.41	120.96	111.30
11	b	1224	CLA	O2D-CGD-CBD	5.42	120.98	111.30
11	a	1120	CLA	O2D-CGD-CBD	5.42	120.98	111.30
11	2	1211	CLA	O2D-CGD-CBD	5.44	121.01	111.30
11	B	1209	CLA	O2D-CGD-CBD	5.44	121.03	111.30
11	a	1110	CLA	O2D-CGD-CBD	5.45	121.04	111.30
11	A	1102	CLA	O2D-CGD-CBD	5.45	121.04	111.30
11	1	1801	CLA	O2D-CGD-CBD	5.46	121.05	111.30
11	B	1204	CLA	O2D-CGD-CBD	5.46	121.06	111.30
11	A	1116	CLA	O2D-CGD-CBD	5.46	121.06	111.30
11	B	1223	CLA	O2D-CGD-CBD	5.48	121.10	111.30
11	2	1204	CLA	O2D-CGD-CBD	5.49	121.11	111.30
11	1	1134	CLA	O2D-CGD-CBD	5.50	121.12	111.30
11	2	1210	CLA	O2D-CGD-CBD	5.50	121.12	111.30
11	2	1218	CLA	O2D-CGD-CBD	5.50	121.13	111.30
11	1	1116	CLA	O2D-CGD-CBD	5.50	121.13	111.30
11	A	1112	CLA	O2D-CGD-CBD	5.50	121.14	111.30
11	1	1101	CLA	O2D-CGD-CBD	5.51	121.14	111.30
11	2	1227	CLA	O2D-CGD-CBD	5.51	121.15	111.30
11	a	1124	CLA	O2D-CGD-CBD	5.51	121.15	111.30
11	b	1211	CLA	O2D-CGD-CBD	5.52	121.16	111.30
11	2	1215	CLA	O2D-CGD-CBD	5.53	121.18	111.30
11	B	1215	CLA	C4-C3-C5	5.54	124.90	115.29
11	2	1221	CLA	O2D-CGD-CBD	5.54	121.20	111.30
11	A	1106	CLA	O2D-CGD-CBD	5.54	121.20	111.30
11	2	1231	CLA	O2D-CGD-CBD	5.55	121.21	111.30
11	1	1012	CLA	O2D-CGD-CBD	5.58	121.27	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1	1112	CLA	O2D-CGD-CBD	5.58	121.27	111.30
11	2	1224	CLA	O2D-CGD-CBD	5.59	121.28	111.30
11	a	1133	CLA	O2D-CGD-CBD	5.59	121.28	111.30
11	a	1129	CLA	O2D-CGD-CBD	5.59	121.29	111.30
14	B	4017	BCR	C20-C19-C18	5.61	142.16	126.42
11	a	1116	CLA	O2D-CGD-CBD	5.61	121.32	111.30
11	A	1104	CLA	O2D-CGD-CBD	5.61	121.33	111.30
11	l	1501	CLA	O2D-CGD-CBD	5.62	121.34	111.30
11	a	1136	CLA	O2D-CGD-CBD	5.65	121.39	111.30
11	1	1125	CLA	O2D-CGD-CBD	5.65	121.40	111.30
11	1	1126	CLA	O2D-CGD-CBD	5.66	121.41	111.30
11	B	1224	CLA	O2D-CGD-CBD	5.67	121.43	111.30
11	B	1231	CLA	O2D-CGD-CBD	5.67	121.44	111.30
11	b	1230	CLA	O2D-CGD-CBD	5.68	121.44	111.30
11	a	1012	CLA	O2D-CGD-CBD	5.68	121.45	111.30
11	A	1131	CLA	O2D-CGD-CBD	5.69	121.46	111.30
11	8	1502	CLA	O2D-CGD-CBD	5.70	121.49	111.30
11	b	1226	CLA	O2D-CGD-CBD	5.72	121.53	111.30
11	B	1207	CLA	O2D-CGD-CBD	5.74	121.55	111.30
11	l	1502	CLA	O2D-CGD-CBD	5.76	121.60	111.30
11	2	1222	CLA	O2D-CGD-CBD	5.77	121.61	111.30
11	A	1126	CLA	O2D-CGD-CBD	5.80	121.66	111.30
11	1	1120	CLA	O2D-CGD-CBD	5.81	121.69	111.30
14	2	4017	BCR	C20-C19-C18	5.82	142.77	126.42
11	a	1126	CLA	O2D-CGD-CBD	5.84	121.73	111.30
11	L	1502	CLA	O2D-CGD-CBD	5.90	121.84	111.30
11	1	1129	CLA	O2D-CGD-CBD	5.91	121.85	111.30
11	8	1501	CLA	O2D-CGD-CBD	5.91	121.86	111.30
11	a	1138	CLA	O2D-CGD-CBD	5.92	121.88	111.30
11	a	1137	CLA	O2D-CGD-CBD	5.93	121.89	111.30
11	A	1012	CLA	O2D-CGD-CBD	5.94	121.91	111.30
14	1	4003	BCR	C23-C22-C21	5.98	128.12	118.94
11	b	1227	CLA	O2D-CGD-CBD	6.00	122.02	111.30
11	b	1222	CLA	O2D-CGD-CBD	6.11	122.23	111.30
11	2	1226	CLA	O2D-CGD-CBD	6.12	122.23	111.30
11	B	1214	CLA	O2D-CGD-CBD	6.14	122.27	111.30
11	B	1227	CLA	O2D-CGD-CBD	6.14	122.27	111.30
14	F	4020	BCR	C20-C19-C18	6.14	143.68	126.42
11	2	1213	CLA	O2D-CGD-CBD	6.16	122.31	111.30
11	2	1236	CLA	O2D-CGD-CBD	6.18	122.34	111.30
14	b	4009	BCR	C20-C19-C18	6.18	143.77	126.42
11	1	1123	CLA	O2D-CGD-CBD	6.19	122.36	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1226	CLA	O2D-CGD-CBD	6.20	122.38	111.30
14	L	4022	BCR	C20-C19-C18	6.25	143.97	126.42
11	B	1222	CLA	O2D-CGD-CBD	6.27	122.50	111.30
14	f	4013	BCR	C11-C12-C13	6.27	144.04	126.42
11	A	1125	CLA	O2D-CGD-CBD	6.31	122.57	111.30
11	B	1201	CLA	O2D-CGD-CBD	6.33	122.61	111.30
14	L	4022	BCR	C11-C10-C9	6.34	136.36	127.31
11	1	1137	CLA	O2D-CGD-CBD	6.35	122.65	111.30
14	A	4003	BCR	C20-C19-C18	6.36	144.29	126.42
11	b	1221	CLA	O2D-CGD-CBD	6.41	122.75	111.30
14	8	4022	BCR	C20-C19-C18	6.44	144.52	126.42
14	l	4022	BCR	C20-C19-C18	6.50	144.66	126.42
11	A	1132	CLA	O2D-CGD-CBD	6.54	122.98	111.30
11	1	1110	CLA	O2D-CGD-CBD	6.54	122.98	111.30
14	b	4017	BCR	C20-C19-C18	6.56	144.85	126.42
11	a	1106	CLA	O2D-CGD-CBD	6.59	123.08	111.30
14	B	4014	BCR	C20-C19-C18	6.62	145.00	126.42
11	B	1221	CLA	O2D-CGD-CBD	6.63	123.15	111.30
14	1	4003	BCR	C20-C19-C18	6.64	145.07	126.42
14	6	4018	BCR	C20-C19-C18	6.69	145.22	126.42
11	A	1110	CLA	O2D-CGD-CBD	6.73	123.32	111.30
14	A	4001	BCR	C20-C19-C18	6.77	145.44	126.42
14	2	4010	BCR	C20-C19-C18	6.78	145.47	126.42
11	1	1111	CLA	C2C-C1C-NC	6.86	114.94	110.22
11	B	1205	CLA	O2D-CGD-CBD	6.87	123.58	111.30
14	8	4019	BCR	C20-C19-C18	6.92	145.84	126.42
14	2	4004	BCR	C20-C19-C18	6.93	145.89	126.42
14	a	4001	BCR	C20-C19-C18	6.93	145.89	126.42
11	A	1126	CLA	C2C-C1C-NC	6.96	115.01	110.22
11	2	1205	CLA	O2D-CGD-CBD	6.96	123.74	111.30
11	A	1103	CLA	C2C-C1C-NC	7.02	115.05	110.22
14	B	4010	BCR	C20-C19-C18	7.02	146.14	126.42
14	B	4004	BCR	C20-C19-C18	7.08	146.30	126.42
14	1	4002	BCR	C20-C19-C18	7.08	146.30	126.42
14	F	4018	BCR	C20-C19-C18	7.09	146.32	126.42
14	A	4008	BCR	C20-C19-C18	7.11	146.39	126.42
11	b	1202	CLA	C2C-C1C-NC	7.18	115.16	110.22
14	l	4019	BCR	C20-C19-C18	7.21	146.67	126.42
11	a	1126	CLA	C2C-C1C-NC	7.26	115.21	110.22
14	b	4004	BCR	C20-C19-C18	7.26	146.81	126.42
14	f	4020	BCR	C20-C19-C18	7.27	146.83	126.42
14	1	4001	BCR	C20-C19-C18	7.27	146.83	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	2	4014	BCR	C20-C19-C18	7.28	146.86	126.42
14	a	4003	BCR	C20-C19-C18	7.28	146.87	126.42
11	2	1218	CLA	C2C-C1C-NC	7.28	115.23	110.22
14	a	4002	BCR	C20-C19-C18	7.30	146.93	126.42
14	m	4021	BCR	C20-C19-C18	7.30	146.94	126.42
11	a	1115	CLA	C2C-C1C-NC	7.32	115.25	110.22
14	2	4011	BCR	C20-C19-C18	7.35	147.06	126.42
11	A	1111	CLA	C2C-C1C-NC	7.40	115.31	110.22
11	A	1112	CLA	C2C-C1C-NC	7.40	115.31	110.22
11	2	1210	CLA	C2C-C1C-NC	7.42	115.32	110.22
11	2	1235	CLA	C2C-C1C-NC	7.43	115.33	110.22
11	1	1126	CLA	C2C-C1C-NC	7.43	115.33	110.22
14	b	4005	BCR	C20-C19-C18	7.43	147.30	126.42
11	B	1013	CLA	C2C-C1C-NC	7.44	115.34	110.22
11	b	1210	CLA	C2C-C1C-NC	7.45	115.35	110.22
14	a	4003	BCR	C11-C10-C9	7.47	137.97	127.31
11	a	1112	CLA	C2C-C1C-NC	7.48	115.36	110.22
11	A	1116	CLA	C2C-C1C-NC	7.49	115.38	110.22
14	B	4005	BCR	C20-C19-C18	7.49	147.47	126.42
14	2	4006	BCR	C20-C19-C18	7.53	147.56	126.42
11	B	1210	CLA	C2C-C1C-NC	7.53	115.40	110.22
11	a	1104	CLA	C2C-C1C-NC	7.54	115.41	110.22
11	2	1223	CLA	C2C-C1C-NC	7.55	115.41	110.22
11	b	1214	CLA	C2C-C1C-NC	7.55	115.42	110.22
14	2	4005	BCR	C20-C19-C18	7.57	147.69	126.42
14	M	4021	BCR	C20-C19-C18	7.58	147.70	126.42
11	2	1013	CLA	C2C-C1C-NC	7.58	115.44	110.22
14	f	4018	BCR	C20-C19-C18	7.59	147.75	126.42
11	B	1214	CLA	C2C-C1C-NC	7.59	115.44	110.22
11	a	1111	CLA	C2C-C1C-NC	7.60	115.45	110.22
11	B	1202	CLA	C2C-C1C-NC	7.62	115.46	110.22
11	2	1219	CLA	C2C-C1C-NC	7.67	115.50	110.22
11	A	1022	CLA	C2C-C1C-NC	7.67	115.50	110.22
14	7	4021	BCR	C20-C19-C18	7.67	147.97	126.42
14	B	4009	BCR	C20-C19-C18	7.67	147.97	126.42
11	A	1117	CLA	C2C-C1C-NC	7.68	115.50	110.22
11	b	1013	CLA	C2C-C1C-NC	7.70	115.52	110.22
11	b	1221	CLA	C2C-C1C-NC	7.72	115.53	110.22
11	1	1118	CLA	C2C-C1C-NC	7.73	115.54	110.22
14	A	4002	BCR	C20-C19-C18	7.77	148.24	126.42
11	A	1115	CLA	C2C-C1C-NC	7.77	115.57	110.22
11	2	1205	CLA	C2C-C1C-NC	7.78	115.57	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	4014	BCR	C20-C19-C18	7.79	148.29	126.42
11	a	1122	CLA	C2C-C1C-NC	7.81	115.59	110.22
11	A	1109	CLA	C2C-C1C-NC	7.81	115.59	110.22
11	B	1224	CLA	C2C-C1C-NC	7.81	115.59	110.22
11	A	1120	CLA	C2C-C1C-NC	7.81	115.59	110.22
14	6	4020	BCR	C20-C19-C18	7.82	148.39	126.42
11	B	1212	CLA	C2C-C1C-NC	7.82	115.60	110.22
11	A	1139	CLA	C2C-C1C-NC	7.82	115.60	110.22
14	F	4013	BCR	C20-C19-C18	7.82	148.40	126.42
11	B	1208	CLA	C2C-C1C-NC	7.83	115.61	110.22
11	A	1119	CLA	C2C-C1C-NC	7.83	115.61	110.22
11	b	1236	CLA	C2C-C1C-NC	7.83	115.61	110.22
11	A	1104	CLA	C2C-C1C-NC	7.85	115.62	110.22
11	2	1202	CLA	C2C-C1C-NC	7.85	115.62	110.22
11	A	1128	CLA	C2C-C1C-NC	7.85	115.62	110.22
11	1	1138	CLA	C2C-C1C-NC	7.86	115.63	110.22
11	1	1125	CLA	C2C-C1C-NC	7.86	115.63	110.22
14	b	4011	BCR	C20-C19-C18	7.86	148.50	126.42
11	a	1132	CLA	C2C-C1C-NC	7.87	115.63	110.22
11	a	1117	CLA	C2C-C1C-NC	7.88	115.64	110.22
11	B	1218	CLA	C2C-C1C-NC	7.91	115.66	110.22
14	a	4008	BCR	C20-C19-C18	7.91	148.65	126.42
11	2	1229	CLA	C2C-C1C-NC	7.93	115.67	110.22
14	B	4011	BCR	C20-C19-C18	7.94	148.71	126.42
11	2	1236	CLA	C2C-C1C-NC	7.94	115.68	110.22
11	b	1201	CLA	C2C-C1C-NC	7.95	115.69	110.22
11	b	1231	CLA	C2C-C1C-NC	7.96	115.69	110.22
11	1	1119	CLA	C2C-C1C-NC	7.96	115.70	110.22
14	B	4006	BCR	C20-C19-C18	7.96	148.79	126.42
11	a	1116	CLA	C2C-C1C-NC	7.98	115.71	110.22
11	1	1136	CLA	C2C-C1C-NC	7.98	115.71	110.22
11	k	1402	CLA	C2C-C1C-NC	7.98	115.71	110.22
11	1	1112	CLA	C2C-C1C-NC	7.99	115.72	110.22
14	f	4013	BCR	C11-C10-C9	8.00	138.73	127.31
11	2	1231	CLA	C2C-C1C-NC	8.01	115.73	110.22
11	B	1238	CLA	C2C-C1C-NC	8.01	115.73	110.22
11	0	1402	CLA	C2C-C1C-NC	8.02	115.73	110.22
14	1	4007	BCR	C20-C19-C18	8.02	148.94	126.42
11	B	1236	CLA	C2C-C1C-NC	8.02	115.73	110.22
11	A	1105	CLA	C2C-C1C-NC	8.03	115.74	110.22
11	b	1218	CLA	C2C-C1C-NC	8.03	115.75	110.22
11	b	1235	CLA	C2C-C1C-NC	8.04	115.75	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1108	CLA	C2C-C1C-NC	8.04	115.75	110.22
11	A	1107	CLA	C2C-C1C-NC	8.06	115.76	110.22
11	B	1217	CLA	C2C-C1C-NC	8.06	115.76	110.22
11	2	1204	CLA	C2C-C1C-NC	8.06	115.76	110.22
11	B	1023	CLA	C2C-C1C-NC	8.06	115.77	110.22
11	a	1138	CLA	C2C-C1C-NC	8.06	115.77	110.22
11	1	1105	CLA	C2C-C1C-NC	8.06	115.77	110.22
11	A	1101	CLA	C2C-C1C-NC	8.07	115.77	110.22
11	B	1219	CLA	C2C-C1C-NC	8.07	115.77	110.22
11	1	1127	CLA	C2C-C1C-NC	8.07	115.78	110.22
11	B	1223	CLA	C2C-C1C-NC	8.08	115.78	110.22
11	A	1122	CLA	C2C-C1C-NC	8.08	115.78	110.22
11	B	1207	CLA	C2C-C1C-NC	8.08	115.78	110.22
11	l	1501	CLA	C2C-C1C-NC	8.08	115.78	110.22
11	A	1113	CLA	C2C-C1C-NC	8.08	115.78	110.22
11	B	1240	CLA	C2C-C1C-NC	8.09	115.78	110.22
11	2	1228	CLA	C2C-C1C-NC	8.09	115.78	110.22
11	1	1130	CLA	C2C-C1C-NC	8.09	115.78	110.22
11	b	1240	CLA	C2C-C1C-NC	8.09	115.79	110.22
11	a	1109	CLA	C2C-C1C-NC	8.10	115.79	110.22
11	b	1213	CLA	C2C-C1C-NC	8.10	115.79	110.22
11	1	1116	CLA	C2C-C1C-NC	8.10	115.79	110.22
11	L	1501	CLA	C2C-C1C-NC	8.11	115.80	110.22
11	B	1235	CLA	C2C-C1C-NC	8.11	115.80	110.22
11	A	1118	CLA	C2C-C1C-NC	8.11	115.80	110.22
11	1	1022	CLA	C2C-C1C-NC	8.12	115.80	110.22
11	K	1402	CLA	C2C-C1C-NC	8.13	115.81	110.22
11	B	1222	CLA	C2C-C1C-NC	8.13	115.81	110.22
11	1	1124	CLA	C2C-C1C-NC	8.14	115.82	110.22
14	6	4013	BCR	C20-C19-C18	8.17	149.38	126.42
14	1	4008	BCR	C20-C19-C18	8.17	149.38	126.42
11	a	1130	CLA	C2C-C1C-NC	8.18	115.85	110.22
11	a	1102	CLA	C2C-C1C-NC	8.19	115.85	110.22
11	2	1230	CLA	C2C-C1C-NC	8.19	115.86	110.22
11	B	1228	CLA	C2C-C1C-NC	8.20	115.86	110.22
11	A	1138	CLA	C2C-C1C-NC	8.21	115.87	110.22
11	a	1140	CLA	C2C-C1C-NC	8.22	115.87	110.22
11	2	1214	CLA	C2C-C1C-NC	8.22	115.87	110.22
11	1	1102	CLA	C2C-C1C-NC	8.22	115.87	110.22
11	2	1208	CLA	C2C-C1C-NC	8.22	115.88	110.22
11	2	1221	CLA	C2C-C1C-NC	8.23	115.88	110.22
11	b	1224	CLA	C2C-C1C-NC	8.23	115.88	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1203	CLA	C2C-C1C-NC	8.23	115.88	110.22
11	b	1204	CLA	C2C-C1C-NC	8.23	115.88	110.22
11	2	1222	CLA	C2C-C1C-NC	8.23	115.88	110.22
11	8	1503	CLA	C2C-C1C-NC	8.23	115.88	110.22
11	2	1232	CLA	C2C-C1C-NC	8.23	115.88	110.22
11	1	1131	CLA	C2C-C1C-NC	8.23	115.89	110.22
11	A	1121	CLA	C2C-C1C-NC	8.23	115.89	110.22
11	b	1217	CLA	C2C-C1C-NC	8.24	115.89	110.22
11	b	1229	CLA	C2C-C1C-NC	8.24	115.89	110.22
11	b	1238	CLA	C2C-C1C-NC	8.25	115.89	110.22
11	2	1211	CLA	C2C-C1C-NC	8.25	115.89	110.22
11	b	1215	CLA	C2C-C1C-NC	8.25	115.89	110.22
11	A	1012	CLA	C2C-C1C-NC	8.25	115.89	110.22
14	b	4010	BCR	C20-C19-C18	8.25	149.60	126.42
11	A	1102	CLA	C2C-C1C-NC	8.25	115.90	110.22
11	a	1123	CLA	C2C-C1C-NC	8.25	115.90	110.22
11	b	1232	CLA	C2C-C1C-NC	8.26	115.90	110.22
11	1	1011	CLA	O2D-CGD-CBD	8.26	126.06	111.30
11	b	1228	CLA	C2C-C1C-NC	8.27	115.91	110.22
11	B	1204	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	a	1134	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	1	1117	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	B	1239	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	B	1201	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	1	1109	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	B	1211	CLA	C2C-C1C-NC	8.28	115.92	110.22
11	A	1127	CLA	C2C-C1C-NC	8.29	115.92	110.22
11	b	1023	CLA	C2C-C1C-NC	8.29	115.92	110.22
11	B	1221	CLA	C2C-C1C-NC	8.29	115.92	110.22
11	1	1113	CLA	C2C-C1C-NC	8.29	115.92	110.22
11	a	1128	CLA	C2C-C1C-NC	8.29	115.93	110.22
11	A	1130	CLA	C2C-C1C-NC	8.30	115.93	110.22
11	1	1139	CLA	C2C-C1C-NC	8.30	115.93	110.22
11	1	1106	CLA	C2C-C1C-NC	8.30	115.93	110.22
11	a	1118	CLA	C2C-C1C-NC	8.30	115.93	110.22
11	1	1103	CLA	C2C-C1C-NC	8.31	115.94	110.22
14	6	4018	BCR	C11-C10-C9	8.31	139.17	127.31
11	1	1122	CLA	C2C-C1C-NC	8.31	115.94	110.22
11	b	1205	CLA	C2C-C1C-NC	8.31	115.94	110.22
11	A	1124	CLA	C2C-C1C-NC	8.31	115.94	110.22
11	1	1104	CLA	C2C-C1C-NC	8.31	115.94	110.22
11	2	1203	CLA	C2C-C1C-NC	8.32	115.94	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1216	CLA	C2C-C1C-NC	8.32	115.94	110.22
11	2	1238	CLA	C2C-C1C-NC	8.32	115.95	110.22
11	A	1135	CLA	C2C-C1C-NC	8.32	115.95	110.22
11	a	1106	CLA	C2C-C1C-NC	8.33	115.95	110.22
11	2	1201	CLA	C2C-C1C-NC	8.33	115.95	110.22
11	1	1140	CLA	C2C-C1C-NC	8.33	115.95	110.22
11	a	1113	CLA	C2C-C1C-NC	8.33	115.95	110.22
11	b	1203	CLA	C2C-C1C-NC	8.33	115.95	110.22
11	1	1120	CLA	C2C-C1C-NC	8.34	115.96	110.22
11	2	1023	CLA	C2C-C1C-NC	8.35	115.96	110.22
14	6	4013	BCR	C11-C10-C9	8.35	139.23	127.31
11	a	1131	CLA	C2C-C1C-NC	8.35	115.97	110.22
11	B	1213	CLA	C2C-C1C-NC	8.35	115.97	110.22
11	2	1220	CLA	C2C-C1C-NC	8.36	115.97	110.22
11	1	1129	CLA	C2C-C1C-NC	8.36	115.97	110.22
11	8	1502	CLA	C2C-C1C-NC	8.36	115.97	110.22
11	1	1137	CLA	C2C-C1C-NC	8.36	115.97	110.22
14	b	4006	BCR	C20-C19-C18	8.37	149.92	126.42
11	a	1012	CLA	C2C-C1C-NC	8.37	115.98	110.22
11	a	1124	CLA	C2C-C1C-NC	8.37	115.98	110.22
11	l	1502	CLA	C2C-C1C-NC	8.37	115.98	110.22
11	a	1801	CLA	C2C-C1C-NC	8.37	115.98	110.22
11	b	1226	CLA	C2C-C1C-NC	8.38	115.98	110.22
11	1	1108	CLA	C2C-C1C-NC	8.38	115.98	110.22
11	A	1137	CLA	C2C-C1C-NC	8.39	115.99	110.22
11	1	1135	CLA	C2C-C1C-NC	8.39	115.99	110.22
11	a	1120	CLA	C2C-C1C-NC	8.39	115.99	110.22
11	1	1101	CLA	C2C-C1C-NC	8.40	116.00	110.22
11	A	1129	CLA	C2C-C1C-NC	8.41	116.01	110.22
11	a	1137	CLA	C2C-C1C-NC	8.41	116.01	110.22
11	A	1132	CLA	C2C-C1C-NC	8.42	116.01	110.22
11	2	1226	CLA	C2C-C1C-NC	8.42	116.01	110.22
11	1	1132	CLA	C2C-C1C-NC	8.43	116.02	110.22
11	b	1212	CLA	C2C-C1C-NC	8.43	116.02	110.22
11	1	1121	CLA	C2C-C1C-NC	8.43	116.02	110.22
11	b	1222	CLA	C2C-C1C-NC	8.44	116.02	110.22
11	1	1128	CLA	C2C-C1C-NC	8.44	116.03	110.22
11	K	1401	CLA	C2C-C1C-NC	8.45	116.03	110.22
11	a	1108	CLA	C2C-C1C-NC	8.45	116.03	110.22
11	A	1011	CLA	C2C-C1C-NC	8.45	116.04	110.22
11	b	1209	CLA	C2C-C1C-NC	8.46	116.04	110.22
11	B	1216	CLA	C2C-C1C-NC	8.46	116.04	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	b	1225	CLA	C2C-C1C-NC	8.47	116.05	110.22
11	8	1501	CLA	C2C-C1C-NC	8.48	116.05	110.22
11	B	1205	CLA	C2C-C1C-NC	8.48	116.05	110.22
11	2	1217	CLA	C2C-C1C-NC	8.48	116.05	110.22
11	b	1211	CLA	C2C-C1C-NC	8.48	116.05	110.22
11	L	1502	CLA	C2C-C1C-NC	8.49	116.06	110.22
11	a	1237	CLA	C2C-C1C-NC	8.49	116.06	110.22
11	A	1131	CLA	C2C-C1C-NC	8.49	116.06	110.22
11	0	1401	CLA	C2C-C1C-NC	8.49	116.06	110.22
11	2	1224	CLA	C2C-C1C-NC	8.50	116.07	110.22
11	2	1209	CLA	C2C-C1C-NC	8.50	116.07	110.22
11	A	1106	CLA	C2C-C1C-NC	8.50	116.07	110.22
11	1	1237	CLA	C2C-C1C-NC	8.50	116.07	110.22
11	l	1503	CLA	C2C-C1C-NC	8.50	116.07	110.22
11	a	1121	CLA	C2C-C1C-NC	8.51	116.07	110.22
11	a	1129	CLA	C2C-C1C-NC	8.51	116.08	110.22
11	1	1123	CLA	C2C-C1C-NC	8.51	116.08	110.22
11	b	1227	CLA	C2C-C1C-NC	8.51	116.08	110.22
11	2	1225	CLA	C2C-C1C-NC	8.52	116.08	110.22
11	B	1209	CLA	C2C-C1C-NC	8.53	116.09	110.22
11	2	1240	CLA	C2C-C1C-NC	8.54	116.09	110.22
14	f	4013	BCR	C20-C19-C18	8.54	150.42	126.42
11	a	1136	CLA	C2C-C1C-NC	8.55	116.10	110.22
11	k	1401	CLA	C2C-C1C-NC	8.55	116.10	110.22
11	b	1230	CLA	C2C-C1C-NC	8.56	116.11	110.22
11	A	1136	CLA	C2C-C1C-NC	8.57	116.11	110.22
11	A	1140	CLA	C2C-C1C-NC	8.57	116.11	110.22
11	B	1220	CLA	C2C-C1C-NC	8.57	116.11	110.22
11	1	1134	CLA	C2C-C1C-NC	8.57	116.11	110.22
11	a	1125	CLA	C2C-C1C-NC	8.57	116.12	110.22
11	b	1220	CLA	C2C-C1C-NC	8.58	116.12	110.22
11	b	1223	CLA	C2C-C1C-NC	8.58	116.12	110.22
11	B	1225	CLA	C2C-C1C-NC	8.59	116.13	110.22
11	1	1114	CLA	C2C-C1C-NC	8.59	116.13	110.22
11	1	1012	CLA	C2C-C1C-NC	8.59	116.13	110.22
11	a	1022	CLA	C2C-C1C-NC	8.59	116.13	110.22
11	a	1110	CLA	C2C-C1C-NC	8.59	116.13	110.22
11	B	1226	CLA	C2C-C1C-NC	8.61	116.14	110.22
11	2	1216	CLA	C2C-C1C-NC	8.61	116.14	110.22
11	2	1207	CLA	C2C-C1C-NC	8.61	116.14	110.22
14	2	4014	BCR	C11-C12-C13	8.63	150.67	126.42
11	a	1105	CLA	C2C-C1C-NC	8.64	116.16	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	1101	CLA	C2C-C1C-NC	8.65	116.17	110.22
11	B	1230	CLA	C2C-C1C-NC	8.67	116.18	110.22
11	B	1215	CLA	C2C-C1C-NC	8.67	116.19	110.22
11	2	1021	CLA	C2C-C1C-NC	8.68	116.19	110.22
11	2	1234	CLA	C2C-C1C-NC	8.69	116.19	110.22
11	a	1119	CLA	C2C-C1C-NC	8.69	116.20	110.22
11	B	1229	CLA	C2C-C1C-NC	8.69	116.20	110.22
11	2	1215	CLA	C2C-C1C-NC	8.71	116.21	110.22
11	a	1107	CLA	C2C-C1C-NC	8.72	116.22	110.22
11	2	1227	CLA	C2C-C1C-NC	8.73	116.23	110.22
11	1	1801	CLA	C2C-C1C-NC	8.74	116.23	110.22
11	A	1110	CLA	C2C-C1C-NC	8.74	116.23	110.22
11	b	1208	CLA	C2C-C1C-NC	8.75	116.24	110.22
11	a	1114	CLA	C2C-C1C-NC	8.75	116.24	110.22
11	b	1021	CLA	C2C-C1C-NC	8.75	116.24	110.22
11	A	1237	CLA	C2C-C1C-NC	8.76	116.25	110.22
14	2	4009	BCR	C20-C19-C18	8.77	151.04	126.42
11	a	1103	CLA	C2C-C1C-NC	8.79	116.27	110.22
11	1	1110	CLA	C2C-C1C-NC	8.80	116.27	110.22
14	a	4007	BCR	C20-C19-C18	8.80	151.12	126.42
11	2	1212	CLA	C2C-C1C-NC	8.80	116.27	110.22
11	1	1107	CLA	C2C-C1C-NC	8.80	116.27	110.22
11	b	1219	CLA	C2C-C1C-NC	8.81	116.28	110.22
14	L	4019	BCR	C20-C19-C18	8.81	151.16	126.42
14	6	4013	BCR	C11-C12-C13	8.83	151.21	126.42
11	a	1011	CLA	C2C-C1C-NC	8.85	116.31	110.22
11	A	1114	CLA	C2C-C1C-NC	8.86	116.31	110.22
11	2	1239	CLA	C2C-C1C-NC	8.86	116.32	110.22
11	b	1206	CLA	C2C-C1C-NC	8.88	116.33	110.22
14	L	4022	BCR	C11-C12-C13	8.89	151.40	126.42
11	B	1021	CLA	C2C-C1C-NC	8.93	116.36	110.22
11	B	1227	CLA	C2C-C1C-NC	8.95	116.37	110.22
11	a	1127	CLA	C2C-C1C-NC	8.95	116.38	110.22
11	1	1115	CLA	C2C-C1C-NC	8.98	116.39	110.22
11	b	1234	CLA	C2C-C1C-NC	8.98	116.40	110.22
11	B	1232	CLA	C2C-C1C-NC	8.99	116.40	110.22
11	L	1503	CLA	C2C-C1C-NC	8.99	116.41	110.22
11	B	1231	CLA	C2C-C1C-NC	8.99	116.41	110.22
14	b	4005	BCR	C11-C12-C13	9.00	151.70	126.42
11	B	1206	CLA	C2C-C1C-NC	9.02	116.43	110.22
11	B	1234	CLA	C2C-C1C-NC	9.06	116.45	110.22
14	A	4002	BCR	C11-C10-C9	9.06	140.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4007	BCR	C20-C19-C18	9.07	151.90	126.42
11	a	1133	CLA	C2C-C1C-NC	9.09	116.47	110.22
14	a	4003	BCR	C11-C12-C13	9.09	151.94	126.42
11	2	1213	CLA	C2C-C1C-NC	9.09	116.47	110.22
14	6	4018	BCR	C11-C12-C13	9.10	151.98	126.42
11	2	1206	CLA	C2C-C1C-NC	9.11	116.48	110.22
11	A	1123	CLA	C2C-C1C-NC	9.15	116.51	110.22
14	b	4014	BCR	C11-C12-C13	9.15	152.13	126.42
11	a	1135	CLA	C2C-C1C-NC	9.15	116.52	110.22
11	a	1139	CLA	C2C-C1C-NC	9.18	116.54	110.22
11	A	1134	CLA	C2C-C1C-NC	9.19	116.54	110.22
14	f	4018	BCR	C11-C12-C13	9.22	152.31	126.42
11	1	1011	CLA	C2C-C1C-NC	9.23	116.57	110.22
11	b	1207	CLA	C2C-C1C-NC	9.24	116.58	110.22
11	1	1133	CLA	C2C-C1C-NC	9.26	116.59	110.22
11	b	1239	CLA	C2C-C1C-NC	9.27	116.59	110.22
14	1	4003	BCR	C11-C12-C13	9.37	152.75	126.42
14	F	4013	BCR	C11-C12-C13	9.39	152.80	126.42
14	A	4002	BCR	C11-C12-C13	9.47	153.02	126.42
11	A	1125	CLA	C2C-C1C-NC	9.48	116.74	110.22
11	A	1133	CLA	C2C-C1C-NC	9.52	116.77	110.22
14	a	4008	BCR	C11-C10-C9	9.59	141.00	127.31
14	A	4001	BCR	C11-C12-C13	9.61	153.41	126.42
14	8	4019	BCR	C11-C12-C13	9.71	153.70	126.42
11	A	1801	CLA	C2C-C1C-NC	9.76	116.93	110.22
14	2	4005	BCR	C11-C10-C9	9.92	141.47	127.31
14	f	4018	BCR	C11-C10-C9	9.94	141.50	127.31
14	B	4010	BCR	C11-C12-C13	9.97	154.44	126.42
14	B	4014	BCR	C11-C12-C13	9.99	154.47	126.42
14	8	4019	BCR	C11-C10-C9	9.99	141.56	127.31
14	b	4017	BCR	C11-C12-C13	9.99	154.49	126.42
14	A	4003	BCR	C11-C10-C9	10.01	141.60	127.31
14	f	4020	BCR	C11-C12-C13	10.03	154.60	126.42
14	A	4008	BCR	C11-C12-C13	10.04	154.62	126.42
14	b	4010	BCR	C11-C12-C13	10.05	154.66	126.42
14	A	4003	BCR	C11-C12-C13	10.06	154.68	126.42
14	2	4005	BCR	C11-C12-C13	10.07	154.71	126.42
14	2	4010	BCR	C11-C12-C13	10.13	154.88	126.42
14	B	4014	BCR	C11-C10-C9	10.17	141.83	127.31
14	2	4017	BCR	C11-C12-C13	10.22	155.13	126.42
14	B	4004	BCR	C11-C12-C13	10.25	155.20	126.42
14	6	4020	BCR	C11-C12-C13	10.26	155.24	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	4019	BCR	C11-C12-C13	10.33	155.44	126.42
14	l	4022	BCR	C11-C12-C13	10.34	155.47	126.42
14	b	4004	BCR	C11-C12-C13	10.40	155.62	126.42
14	8	4022	BCR	C11-C12-C13	10.40	155.64	126.42
14	2	4004	BCR	C11-C12-C13	10.43	155.72	126.42
14	L	4019	BCR	C11-C10-C9	10.44	142.21	127.31
14	L	4019	BCR	C11-C12-C13	10.48	155.84	126.42
14	1	4001	BCR	C11-C12-C13	10.58	156.13	126.42
14	B	4017	BCR	C11-C12-C13	10.60	156.18	126.42
14	2	4009	BCR	C11-C12-C13	10.60	156.19	126.42
14	1	4007	BCR	C11-C12-C13	10.64	156.32	126.42
14	B	4009	BCR	C11-C10-C9	10.66	142.53	127.31
14	B	4009	BCR	C11-C12-C13	10.78	156.69	126.42
14	a	4002	BCR	C11-C12-C13	10.78	156.70	126.42
14	a	4008	BCR	C11-C12-C13	10.82	156.82	126.42
14	7	4021	BCR	C11-C12-C13	10.83	156.84	126.42
14	F	4020	BCR	C11-C12-C13	10.85	156.89	126.42
14	6	4020	BCR	C11-C10-C9	10.86	142.80	127.31
14	a	4001	BCR	C11-C12-C13	10.88	156.97	126.42
14	m	4021	BCR	C11-C12-C13	10.91	157.06	126.42
14	B	4006	BCR	C11-C12-C13	10.95	157.17	126.42
14	a	4007	BCR	C11-C12-C13	10.97	157.23	126.42
14	1	4002	BCR	C11-C12-C13	11.00	157.31	126.42
14	b	4009	BCR	C11-C12-C13	11.01	157.33	126.42
14	A	4007	BCR	C11-C12-C13	11.06	157.48	126.42
14	1	4008	BCR	C11-C12-C13	11.06	157.50	126.42
14	1	4008	BCR	C11-C10-C9	11.20	143.29	127.31
14	F	4013	BCR	C21-C20-C19	11.23	157.68	123.23
14	B	4005	BCR	C11-C12-C13	11.25	158.03	126.42
14	F	4013	BCR	C11-C10-C9	11.31	143.45	127.31
14	6	4013	BCR	C21-C20-C19	11.32	157.96	123.23
14	l	4022	BCR	C11-C10-C9	11.35	143.50	127.31
14	1	4002	BCR	C16-C15-C14	11.39	147.78	123.46
14	F	4020	BCR	C16-C15-C14	11.44	147.88	123.46
14	b	4006	BCR	C11-C12-C13	11.45	158.57	126.42
14	A	4008	BCR	C21-C20-C19	11.47	158.43	123.23
14	F	4018	BCR	C11-C12-C13	11.47	158.65	126.42
14	f	4013	BCR	C21-C20-C19	11.49	158.47	123.23
14	m	4021	BCR	C11-C10-C9	11.53	143.76	127.31
14	b	4014	BCR	C11-C10-C9	11.53	143.77	127.31
14	b	4011	BCR	C11-C12-C13	11.55	158.87	126.42
14	l	4019	BCR	C11-C10-C9	11.58	143.84	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	4020	BCR	C16-C15-C14	11.67	148.38	123.46
14	2	4006	BCR	C11-C12-C13	11.69	159.24	126.42
14	M	4021	BCR	C16-C15-C14	11.70	148.44	123.46
14	1	4008	BCR	C21-C20-C19	11.71	159.15	123.23
14	1	4007	BCR	C21-C20-C19	11.72	159.18	123.23
14	2	4017	BCR	C16-C15-C14	11.72	148.49	123.46
14	M	4021	BCR	C11-C12-C13	11.78	159.50	126.42
14	b	4010	BCR	C21-C20-C19	11.80	159.44	123.23
14	B	4005	BCR	C11-C10-C9	11.89	144.27	127.31
14	a	4008	BCR	C21-C20-C19	11.90	159.75	123.23
14	b	4006	BCR	C21-C20-C19	11.91	159.78	123.23
14	f	4018	BCR	C16-C15-C14	11.96	148.98	123.46
14	2	4005	BCR	C16-C15-C14	11.99	149.06	123.46
14	B	4010	BCR	C11-C10-C9	12.00	144.44	127.31
14	2	4014	BCR	C11-C10-C9	12.02	144.46	127.31
14	2	4009	BCR	C21-C20-C19	12.03	160.13	123.23
14	B	4006	BCR	C21-C20-C19	12.05	160.19	123.23
14	L	4022	BCR	C16-C15-C14	12.07	149.22	123.46
14	B	4011	BCR	C11-C12-C13	12.09	160.38	126.42
14	2	4011	BCR	C11-C12-C13	12.13	160.51	126.42
14	1	4003	BCR	C11-C10-C9	12.18	144.69	127.31
14	b	4005	BCR	C16-C15-C14	12.19	149.47	123.46
14	l	4022	BCR	C16-C15-C14	12.22	149.55	123.46
14	m	4021	BCR	C16-C15-C14	12.22	149.55	123.46
14	6	4020	BCR	C21-C20-C19	12.26	160.86	123.23
14	6	4018	BCR	C16-C15-C14	12.29	149.69	123.46
14	B	4017	BCR	C16-C15-C14	12.32	149.76	123.46
14	2	4010	BCR	C11-C10-C9	12.32	144.90	127.31
14	2	4004	BCR	C11-C10-C9	12.33	144.90	127.31
14	a	4007	BCR	C21-C20-C19	12.35	161.12	123.23
14	1	4002	BCR	C11-C10-C9	12.40	145.01	127.31
14	B	4011	BCR	C21-C20-C19	12.44	161.40	123.23
14	6	4020	BCR	C16-C15-C14	12.44	150.02	123.46
14	B	4009	BCR	C21-C20-C19	12.48	161.52	123.23
14	B	4005	BCR	C16-C15-C14	12.50	150.15	123.46
14	f	4013	BCR	C16-C15-C14	12.51	150.16	123.46
14	2	4006	BCR	C16-C15-C14	12.51	150.17	123.46
14	2	4006	BCR	C21-C20-C19	12.52	161.63	123.23
14	8	4022	BCR	C16-C15-C14	12.54	150.22	123.46
14	f	4018	BCR	C21-C20-C19	12.58	161.82	123.23
14	b	4017	BCR	C16-C15-C14	12.59	150.33	123.46
14	A	4007	BCR	C21-C20-C19	12.61	161.90	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4003	BCR	C16-C15-C14	12.66	150.48	123.46
14	b	4011	BCR	C21-C20-C19	12.68	162.14	123.23
14	2	4005	BCR	C21-C20-C19	12.70	162.19	123.23
14	2	4009	BCR	C11-C10-C9	12.70	145.44	127.31
14	A	4008	BCR	C11-C10-C9	12.71	145.45	127.31
14	F	4018	BCR	C16-C15-C14	12.72	150.62	123.46
14	2	4004	BCR	C16-C15-C14	12.75	150.67	123.46
14	f	4020	BCR	C21-C20-C19	12.76	162.37	123.23
14	a	4003	BCR	C16-C15-C14	12.77	150.73	123.46
14	8	4022	BCR	C11-C10-C9	12.77	145.54	127.31
14	A	4002	BCR	C21-C20-C19	12.79	162.48	123.23
14	7	4021	BCR	C16-C15-C14	12.80	150.77	123.46
14	F	4018	BCR	C11-C10-C9	12.80	145.57	127.31
14	7	4021	BCR	C11-C10-C9	12.83	145.61	127.31
14	B	4014	BCR	C16-C15-C14	12.83	150.85	123.46
14	b	4004	BCR	C21-C20-C19	12.84	162.61	123.23
14	B	4005	BCR	C21-C20-C19	12.84	162.63	123.23
14	7	4021	BCR	C21-C20-C19	12.85	162.65	123.23
14	2	4011	BCR	C16-C15-C14	12.88	150.96	123.46
14	A	4001	BCR	C11-C10-C9	12.91	145.73	127.31
14	1	4002	BCR	C21-C20-C19	12.91	162.84	123.23
14	b	4014	BCR	C21-C20-C19	12.91	162.85	123.23
14	b	4004	BCR	C11-C10-C9	12.92	145.75	127.31
14	a	4002	BCR	C11-C10-C9	12.94	145.77	127.31
14	a	4007	BCR	C16-C15-C14	12.98	151.17	123.46
14	b	4011	BCR	C16-C15-C14	12.98	151.18	123.46
14	F	4018	BCR	C21-C20-C19	13.00	163.10	123.23
14	2	4011	BCR	C21-C20-C19	13.00	163.11	123.23
14	6	4013	BCR	C16-C15-C14	13.01	151.24	123.46
14	b	4005	BCR	C21-C20-C19	13.02	163.18	123.23
14	2	4017	BCR	C11-C10-C9	13.03	145.91	127.31
14	b	4010	BCR	C11-C10-C9	13.04	145.93	127.31
14	B	4004	BCR	C21-C20-C19	13.05	163.25	123.23
14	A	4002	BCR	C16-C15-C14	13.06	151.33	123.46
14	B	4006	BCR	C11-C10-C9	13.08	145.98	127.31
14	2	4014	BCR	C16-C15-C14	13.10	151.42	123.46
14	b	4017	BCR	C21-C20-C19	13.13	163.51	123.23
14	l	4019	BCR	C21-C20-C19	13.14	163.54	123.23
14	b	4014	BCR	C16-C15-C14	13.14	151.52	123.46
14	M	4021	BCR	C21-C20-C19	13.18	163.66	123.23
14	F	4020	BCR	C11-C10-C9	13.18	146.12	127.31
14	a	4003	BCR	C21-C20-C19	13.19	163.70	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	4019	BCR	C21-C20-C19	13.20	163.73	123.23
14	A	4007	BCR	C16-C15-C14	13.20	151.64	123.46
14	a	4001	BCR	C16-C15-C14	13.21	151.65	123.46
14	m	4021	BCR	C21-C20-C19	13.21	163.75	123.23
14	6	4018	BCR	C21-C20-C19	13.22	163.78	123.23
14	f	4020	BCR	C11-C10-C9	13.23	146.20	127.31
14	B	4004	BCR	C16-C15-C14	13.29	151.82	123.46
14	a	4002	BCR	C21-C20-C19	13.32	164.09	123.23
14	2	4004	BCR	C21-C20-C19	13.33	164.13	123.23
14	1	4001	BCR	C21-C20-C19	13.34	164.16	123.23
14	8	4019	BCR	C21-C20-C19	13.35	164.17	123.23
14	B	4004	BCR	C11-C10-C9	13.36	146.38	127.31
14	B	4006	BCR	C16-C15-C14	13.42	152.10	123.46
14	A	4001	BCR	C16-C15-C14	13.42	152.10	123.46
14	2	4010	BCR	C16-C15-C14	13.44	152.16	123.46
14	b	4004	BCR	C16-C15-C14	13.50	152.28	123.46
14	a	4001	BCR	C21-C20-C19	13.52	164.71	123.23
14	2	4014	BCR	C21-C20-C19	13.53	164.74	123.23
14	B	4017	BCR	C11-C10-C9	13.54	146.63	127.31
14	B	4010	BCR	C16-C15-C14	13.54	152.37	123.46
14	a	4002	BCR	C16-C15-C14	13.61	152.51	123.46
14	1	4007	BCR	C11-C10-C9	13.64	146.77	127.31
14	2	4017	BCR	C21-C20-C19	13.65	165.10	123.23
14	8	4022	BCR	C21-C20-C19	13.66	165.15	123.23
14	b	4006	BCR	C16-C15-C14	13.68	152.66	123.46
14	1	4001	BCR	C11-C10-C9	13.68	146.84	127.31
14	1	4007	BCR	C16-C15-C14	13.70	152.71	123.46
14	B	4010	BCR	C21-C20-C19	13.71	165.30	123.23
14	b	4006	BCR	C11-C10-C9	13.73	146.91	127.31
14	L	4022	BCR	C21-C20-C19	13.76	165.44	123.23
14	1	4003	BCR	C16-C15-C14	13.77	152.85	123.46
14	b	4009	BCR	C11-C10-C9	13.80	147.01	127.31
14	A	4001	BCR	C21-C20-C19	13.82	165.62	123.23
14	1	4001	BCR	C16-C15-C14	13.84	153.00	123.46
14	l	4022	BCR	C21-C20-C19	13.84	165.70	123.23
14	B	4014	BCR	C21-C20-C19	13.86	165.75	123.23
14	A	4008	BCR	C16-C15-C14	13.87	153.06	123.46
14	a	4008	BCR	C16-C15-C14	13.88	153.09	123.46
14	2	4010	BCR	C21-C20-C19	13.89	165.84	123.23
14	F	4013	BCR	C16-C15-C14	13.89	153.11	123.46
14	F	4020	BCR	C21-C20-C19	13.89	165.86	123.23
14	a	4001	BCR	C11-C10-C9	13.91	147.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	4021	BCR	C11-C10-C9	13.94	147.20	127.31
14	2	4006	BCR	C11-C10-C9	13.99	147.27	127.31
14	b	4017	BCR	C11-C10-C9	14.00	147.28	127.31
14	L	4022	BCR	C10-C11-C12	14.00	166.17	123.23
14	b	4009	BCR	C21-C20-C19	14.00	166.19	123.23
14	B	4011	BCR	C16-C15-C14	14.04	153.43	123.46
14	B	4017	BCR	C21-C20-C19	14.04	166.30	123.23
14	b	4010	BCR	C16-C15-C14	14.08	153.51	123.46
14	a	4007	BCR	C11-C10-C9	14.11	147.45	127.31
14	1	4002	BCR	C15-C16-C17	14.13	153.63	123.46
14	B	4009	BCR	C16-C15-C14	14.19	153.74	123.46
14	b	4005	BCR	C11-C10-C9	14.21	147.60	127.31
14	1	4003	BCR	C21-C20-C19	14.24	166.91	123.23
14	A	4003	BCR	C21-C20-C19	14.28	167.04	123.23
14	L	4019	BCR	C16-C15-C14	14.40	154.19	123.46
14	A	4007	BCR	C11-C10-C9	14.55	148.07	127.31
14	1	4019	BCR	C16-C15-C14	14.55	154.52	123.46
14	2	4009	BCR	C16-C15-C14	14.70	154.83	123.46
14	1	4008	BCR	C16-C15-C14	14.71	154.86	123.46
14	a	4003	BCR	C10-C11-C12	14.85	168.78	123.23
14	b	4009	BCR	C16-C15-C14	14.89	155.24	123.46
14	f	4013	BCR	C10-C11-C12	14.93	169.04	123.23
14	8	4019	BCR	C16-C15-C14	14.98	155.44	123.46
14	B	4011	BCR	C11-C10-C9	15.10	148.86	127.31
14	2	4011	BCR	C11-C10-C9	15.31	149.16	127.31
14	6	4018	BCR	C10-C11-C12	15.50	170.77	123.23
14	1	4003	BCR	C20-C21-C22	15.55	149.50	127.31
14	6	4013	BCR	C10-C11-C12	15.59	171.05	123.23
14	A	4002	BCR	C10-C11-C12	15.65	171.23	123.23
14	B	4014	BCR	C10-C11-C12	15.76	171.57	123.23
14	f	4018	BCR	C10-C11-C12	15.78	171.64	123.23
14	b	4009	BCR	C15-C16-C17	15.92	157.44	123.46
14	A	4001	BCR	C10-C11-C12	15.93	172.11	123.23
14	2	4005	BCR	C10-C11-C12	16.00	172.32	123.23
14	B	4011	BCR	C10-C11-C12	16.28	173.17	123.23
14	2	4011	BCR	C10-C11-C12	16.35	173.38	123.23
14	1	4008	BCR	C10-C11-C12	16.36	173.41	123.23
14	b	4011	BCR	C11-C10-C9	16.40	150.72	127.31
14	A	4003	BCR	C20-C21-C22	16.43	150.76	127.31
14	A	4002	BCR	C15-C16-C17	16.44	158.55	123.46
14	a	4008	BCR	C10-C11-C12	16.48	173.78	123.23
14	b	4011	BCR	C10-C11-C12	16.54	173.98	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	8	4019	BCR	C10-C11-C12	16.55	174.00	123.23
14	a	4002	BCR	C15-C16-C17	16.57	158.82	123.46
14	B	4009	BCR	C10-C11-C12	16.59	174.13	123.23
14	F	4013	BCR	C10-C11-C12	16.64	174.27	123.23
14	b	4014	BCR	C10-C11-C12	16.64	174.28	123.23
14	l	4019	BCR	C15-C16-C17	16.72	159.16	123.46
14	1	4003	BCR	C10-C11-C12	16.76	174.63	123.23
14	A	4003	BCR	C10-C11-C12	16.77	174.68	123.23
14	b	4009	BCR	C10-C11-C12	16.80	174.76	123.23
14	8	4019	BCR	C15-C16-C17	16.82	159.37	123.46
14	B	4010	BCR	C10-C11-C12	16.86	174.96	123.23
14	2	4006	BCR	C10-C11-C12	16.87	174.98	123.23
14	A	4007	BCR	C10-C11-C12	16.98	175.32	123.23
14	b	4006	BCR	C10-C11-C12	17.09	175.65	123.23
14	L	4019	BCR	C15-C16-C17	17.10	159.95	123.46
14	A	4008	BCR	C10-C11-C12	17.10	175.70	123.23
14	1	4008	BCR	C15-C16-C17	17.11	159.98	123.46
14	2	4014	BCR	C10-C11-C12	17.18	175.94	123.23
14	B	4011	BCR	C15-C16-C17	17.20	160.18	123.46
14	M	4021	BCR	C10-C11-C12	17.25	176.16	123.23
14	l	4022	BCR	C10-C11-C12	17.26	176.17	123.23
14	b	4017	BCR	C10-C11-C12	17.28	176.24	123.23
14	8	4022	BCR	C10-C11-C12	17.28	176.26	123.23
14	a	4001	BCR	C10-C11-C12	17.29	176.27	123.23
14	a	4007	BCR	C10-C11-C12	17.29	176.27	123.23
14	a	4002	BCR	C10-C11-C12	17.33	176.38	123.23
14	b	4004	BCR	C10-C11-C12	17.33	176.39	123.23
14	2	4004	BCR	C10-C11-C12	17.33	176.40	123.23
14	F	4018	BCR	C10-C11-C12	17.36	176.48	123.23
14	B	4004	BCR	C10-C11-C12	17.38	176.55	123.23
14	b	4006	BCR	C15-C16-C17	17.39	160.59	123.46
14	2	4017	BCR	C10-C11-C12	17.40	176.60	123.23
14	m	4021	BCR	C10-C11-C12	17.40	176.62	123.23
14	b	4010	BCR	C15-C16-C17	17.40	160.61	123.46
14	b	4010	BCR	C10-C11-C12	17.41	176.63	123.23
14	2	4010	BCR	C10-C11-C12	17.47	176.83	123.23
14	2	4009	BCR	C15-C16-C17	17.54	160.90	123.46
14	B	4005	BCR	C10-C11-C12	17.55	177.09	123.23
14	2	4017	BCR	C16-C17-C18	17.56	152.38	127.31
14	6	4020	BCR	C10-C11-C12	17.57	177.12	123.23
14	b	4005	BCR	C10-C11-C12	17.61	177.26	123.23
14	7	4021	BCR	C10-C11-C12	17.61	177.26	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4006	BCR	C10-C11-C12	17.62	177.28	123.23
14	2	4010	BCR	C20-C21-C22	17.63	152.47	127.31
14	l	4019	BCR	C10-C11-C12	17.64	177.36	123.23
14	f	4020	BCR	C10-C11-C12	17.66	177.41	123.23
14	1	4001	BCR	C10-C11-C12	17.67	177.43	123.23
14	1	4007	BCR	C10-C11-C12	17.67	177.44	123.23
14	F	4020	BCR	C10-C11-C12	17.67	177.45	123.23
14	2	4009	BCR	C10-C11-C12	17.68	177.49	123.23
14	2	4011	BCR	C15-C16-C17	17.78	161.42	123.46
14	B	4017	BCR	C10-C11-C12	17.81	177.86	123.23
14	1	4002	BCR	C10-C11-C12	17.82	177.91	123.23
14	A	4007	BCR	C15-C16-C17	17.86	161.57	123.46
14	1	4007	BCR	C15-C16-C17	17.89	161.66	123.46
14	a	4008	BCR	C15-C16-C17	17.93	161.73	123.46
14	L	4019	BCR	C10-C11-C12	17.96	178.32	123.23
14	F	4013	BCR	C15-C16-C17	18.00	161.88	123.46
14	b	4011	BCR	C15-C16-C17	18.01	161.90	123.46
14	1	4003	BCR	C15-C16-C17	18.07	162.03	123.46
14	b	4004	BCR	C15-C16-C17	18.12	162.14	123.46
14	B	4010	BCR	C15-C16-C17	18.12	162.15	123.46
14	6	4013	BCR	C15-C16-C17	18.20	162.31	123.46
14	F	4018	BCR	C15-C16-C17	18.21	162.32	123.46
14	2	4010	BCR	C15-C16-C17	18.24	162.40	123.46
14	B	4014	BCR	C20-C21-C22	18.26	153.36	127.31
14	1	4001	BCR	C15-C16-C17	18.29	162.50	123.46
14	B	4004	BCR	C15-C16-C17	18.29	162.51	123.46
14	B	4006	BCR	C15-C16-C17	18.31	162.54	123.46
14	f	4013	BCR	C15-C16-C17	18.34	162.60	123.46
14	B	4010	BCR	C20-C21-C22	18.44	153.63	127.31
14	a	4007	BCR	C15-C16-C17	18.45	162.85	123.46
14	B	4009	BCR	C15-C16-C17	18.52	162.99	123.46
14	A	4008	BCR	C15-C16-C17	18.58	163.11	123.46
14	F	4020	BCR	C20-C21-C22	18.62	153.88	127.31
14	a	4001	BCR	C15-C16-C17	18.62	163.21	123.46
14	a	4003	BCR	C15-C16-C17	18.63	163.22	123.46
14	A	4001	BCR	C20-C21-C22	18.68	153.97	127.31
14	b	4014	BCR	C15-C16-C17	18.75	163.49	123.46
14	8	4022	BCR	C15-C16-C17	18.77	163.52	123.46
14	6	4020	BCR	C15-C16-C17	18.79	163.56	123.46
14	A	4003	BCR	C15-C16-C17	18.80	163.59	123.46
14	2	4014	BCR	C15-C16-C17	18.85	163.70	123.46
14	l	4022	BCR	C15-C16-C17	18.89	163.78	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	4022	BCR	C20-C21-C22	18.90	154.29	127.31
14	6	4018	BCR	C15-C16-C17	18.92	163.85	123.46
14	2	4004	BCR	C15-C16-C17	19.00	164.02	123.46
14	b	4017	BCR	C15-C16-C17	19.00	164.03	123.46
14	a	4003	BCR	C20-C21-C22	19.02	154.46	127.31
14	A	4001	BCR	C15-C16-C17	19.04	164.11	123.46
14	f	4018	BCR	C15-C16-C17	19.05	164.12	123.46
14	L	4022	BCR	C15-C16-C17	19.09	164.22	123.46
14	B	4014	BCR	C15-C16-C17	19.14	164.31	123.46
14	B	4005	BCR	C15-C16-C17	19.18	164.39	123.46
14	1	4001	BCR	C20-C21-C22	19.19	154.70	127.31
14	7	4021	BCR	C15-C16-C17	19.20	164.44	123.46
14	b	4017	BCR	C16-C17-C18	19.23	154.76	127.31
14	2	4006	BCR	C15-C16-C17	19.27	164.59	123.46
14	2	4014	BCR	C20-C21-C22	19.29	154.83	127.31
14	a	4001	BCR	C20-C21-C22	19.30	154.86	127.31
14	L	4019	BCR	C20-C21-C22	19.31	154.87	127.31
14	L	4022	BCR	C20-C21-C22	19.34	154.92	127.31
14	F	4020	BCR	C16-C17-C18	19.43	155.03	127.31
14	m	4021	BCR	C15-C16-C17	19.43	164.94	123.46
14	b	4009	BCR	C20-C21-C22	19.44	155.05	127.31
14	A	4008	BCR	C16-C17-C18	19.49	155.12	127.31
14	B	4017	BCR	C15-C16-C17	19.56	165.20	123.46
14	M	4021	BCR	C16-C17-C18	19.58	155.25	127.31
14	B	4014	BCR	C16-C17-C18	19.62	155.31	127.31
14	A	4001	BCR	C16-C17-C18	19.62	155.32	127.31
14	2	4005	BCR	C15-C16-C17	19.65	165.41	123.46
14	b	4005	BCR	C15-C16-C17	19.66	165.43	123.46
14	2	4004	BCR	C20-C21-C22	19.69	155.41	127.31
14	B	4017	BCR	C16-C17-C18	19.71	155.43	127.31
14	m	4021	BCR	C16-C17-C18	19.85	155.64	127.31
14	6	4018	BCR	C16-C17-C18	19.86	155.66	127.31
14	8	4022	BCR	C20-C21-C22	19.87	155.67	127.31
14	2	4014	BCR	C16-C17-C18	19.97	155.82	127.31
14	f	4020	BCR	C15-C16-C17	19.98	166.11	123.46
14	f	4020	BCR	C16-C17-C18	20.02	155.88	127.31
14	A	4003	BCR	C16-C17-C18	20.16	156.09	127.31
14	2	4004	BCR	C16-C17-C18	20.19	156.12	127.31
14	f	4018	BCR	C16-C17-C18	20.19	156.13	127.31
14	F	4020	BCR	C15-C16-C17	20.28	166.76	123.46
14	2	4006	BCR	C16-C17-C18	20.31	156.30	127.31
14	B	4011	BCR	C20-C21-C22	20.32	156.31	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	4021	BCR	C15-C16-C17	20.37	166.93	123.46
14	m	4021	BCR	C20-C21-C22	20.44	156.48	127.31
14	2	4011	BCR	C20-C21-C22	20.45	156.50	127.31
14	2	4010	BCR	C16-C17-C18	20.47	156.53	127.31
14	B	4004	BCR	C20-C21-C22	20.48	156.53	127.31
14	L	4022	BCR	C16-C17-C18	20.48	156.54	127.31
14	a	4002	BCR	C20-C21-C22	20.54	156.63	127.31
14	a	4001	BCR	C16-C17-C18	20.57	156.67	127.31
14	B	4017	BCR	C20-C21-C22	20.60	156.71	127.31
14	B	4005	BCR	C16-C17-C18	20.61	156.72	127.31
14	6	4020	BCR	C16-C17-C18	20.65	156.78	127.31
14	8	4022	BCR	C16-C17-C18	20.69	156.84	127.31
14	M	4021	BCR	C20-C21-C22	20.70	156.85	127.31
14	A	4002	BCR	C20-C21-C22	20.71	156.87	127.31
14	2	4017	BCR	C15-C16-C17	20.72	167.68	123.46
14	a	4003	BCR	C16-C17-C18	20.73	156.90	127.31
14	6	4018	BCR	C20-C21-C22	20.74	156.91	127.31
14	b	4004	BCR	C20-C21-C22	20.77	156.95	127.31
14	B	4005	BCR	C20-C21-C22	20.78	156.97	127.31
14	2	4005	BCR	C16-C17-C18	20.81	157.01	127.31
14	F	4018	BCR	C16-C17-C18	20.82	157.02	127.31
14	b	4005	BCR	C20-C21-C22	20.86	157.08	127.31
14	b	4014	BCR	C16-C17-C18	20.90	157.13	127.31
14	7	4021	BCR	C16-C17-C18	20.91	157.15	127.31
14	F	4018	BCR	C20-C21-C22	20.92	157.16	127.31
14	l	4022	BCR	C16-C17-C18	20.93	157.19	127.31
14	b	4005	BCR	C16-C17-C18	20.94	157.20	127.31
14	1	4003	BCR	C16-C17-C18	20.98	157.25	127.31
14	1	4001	BCR	C16-C17-C18	21.00	157.29	127.31
14	7	4021	BCR	C20-C21-C22	21.02	157.31	127.31
14	f	4018	BCR	C20-C21-C22	21.03	157.33	127.31
14	b	4014	BCR	C20-C21-C22	21.05	157.35	127.31
14	6	4020	BCR	C20-C21-C22	21.05	157.35	127.31
14	B	4010	BCR	C16-C17-C18	21.05	157.35	127.31
14	B	4004	BCR	C16-C17-C18	21.13	157.46	127.31
14	B	4006	BCR	C16-C17-C18	21.16	157.50	127.31
14	b	4004	BCR	C16-C17-C18	21.34	157.76	127.31
14	l	4019	BCR	C16-C17-C18	21.36	157.79	127.31
14	a	4008	BCR	C16-C17-C18	21.37	157.80	127.31
14	2	4005	BCR	C20-C21-C22	21.50	157.99	127.31
14	8	4019	BCR	C16-C17-C18	21.59	158.12	127.31
14	a	4007	BCR	C16-C17-C18	21.60	158.13	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4007	BCR	C20-C21-C22	21.63	158.18	127.31
14	b	4011	BCR	C20-C21-C22	21.63	158.18	127.31
14	6	4013	BCR	C16-C17-C18	21.72	158.30	127.31
14	f	4020	BCR	C20-C21-C22	21.79	158.41	127.31
14	F	4013	BCR	C16-C17-C18	21.81	158.44	127.31
14	1	4007	BCR	C16-C17-C18	21.95	158.63	127.31
14	2	4009	BCR	C20-C21-C22	22.02	158.74	127.31
14	B	4011	BCR	C16-C17-C18	22.07	158.80	127.31
14	2	4017	BCR	C20-C21-C22	22.10	158.86	127.31
14	b	4011	BCR	C16-C17-C18	22.13	158.90	127.31
14	a	4002	BCR	C16-C17-C18	22.14	158.91	127.31
14	b	4010	BCR	C20-C21-C22	22.17	158.95	127.31
14	B	4009	BCR	C20-C21-C22	22.21	159.01	127.31
14	b	4017	BCR	C20-C21-C22	22.29	159.12	127.31
14	A	4002	BCR	C16-C17-C18	22.35	159.21	127.31
14	A	4007	BCR	C16-C17-C18	22.41	159.30	127.31
14	1	4002	BCR	C20-C21-C22	22.46	159.37	127.31
14	L	4019	BCR	C16-C17-C18	22.53	159.47	127.31
14	a	4008	BCR	C20-C21-C22	22.55	159.49	127.31
14	1	4008	BCR	C16-C17-C18	22.75	159.78	127.31
14	b	4010	BCR	C16-C17-C18	22.94	160.05	127.31
14	a	4007	BCR	C20-C21-C22	22.98	160.10	127.31
14	f	4013	BCR	C16-C17-C18	23.12	160.30	127.31
14	2	4009	BCR	C16-C17-C18	23.20	160.42	127.31
14	b	4006	BCR	C16-C17-C18	23.23	160.47	127.31
14	A	4008	BCR	C20-C21-C22	23.32	160.59	127.31
14	2	4011	BCR	C16-C17-C18	23.47	160.81	127.31
14	A	4007	BCR	C20-C21-C22	23.50	160.84	127.31
14	B	4009	BCR	C16-C17-C18	23.84	161.34	127.31
14	2	4006	BCR	C20-C21-C22	24.08	161.67	127.31
14	1	4008	BCR	C20-C21-C22	24.11	161.72	127.31
14	B	4006	BCR	C20-C21-C22	24.38	162.10	127.31
14	8	4019	BCR	C20-C21-C22	24.42	162.16	127.31
14	b	4006	BCR	C20-C21-C22	24.66	162.51	127.31
14	l	4019	BCR	C20-C21-C22	24.80	162.70	127.31
14	f	4013	BCR	C20-C21-C22	25.36	163.51	127.31
14	F	4013	BCR	C20-C21-C22	25.73	164.03	127.31
14	6	4013	BCR	C20-C21-C22	26.01	164.43	127.31
14	b	4009	BCR	C16-C17-C18	27.86	167.07	127.31
14	1	4002	BCR	C16-C17-C18	28.55	168.05	127.31

All (748) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	2	1218	CLA	NC
11	2	1218	CLA	ND
11	2	1218	CLA	NA
11	a	1122	CLA	NC
11	a	1122	CLA	ND
11	a	1122	CLA	NA
11	A	1101	CLA	ND
11	A	1101	CLA	NA
11	b	1218	CLA	NC
11	b	1218	CLA	ND
11	b	1218	CLA	NA
11	1	1801	CLA	NC
11	1	1801	CLA	ND
11	1	1801	CLA	NA
11	A	1125	CLA	ND
11	A	1125	CLA	NA
11	b	1222	CLA	NC
11	b	1222	CLA	ND
11	b	1222	CLA	NA
11	2	1224	CLA	NC
11	2	1224	CLA	NA
11	2	1224	CLA	ND
11	K	1401	CLA	NC
11	K	1401	CLA	NA
11	K	1401	CLA	ND
11	a	1124	CLA	NC
11	a	1124	CLA	ND
11	a	1124	CLA	NA
11	1	1133	CLA	NC
11	1	1133	CLA	ND
11	1	1133	CLA	NA
11	1	1139	CLA	NC
11	1	1139	CLA	ND
11	1	1139	CLA	NA
11	2	1208	CLA	NC
11	2	1208	CLA	ND
11	2	1208	CLA	NA
11	1	1111	CLA	NC
11	1	1111	CLA	NA
11	1	1111	CLA	ND
11	a	1114	CLA	ND
11	a	1114	CLA	NA
11	b	1213	CLA	NC

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Mol	Chain	Res	Type	Atom
11	b	1213	CLA	ND
11	b	1213	CLA	NA
11	B	1210	CLA	NC
11	B	1210	CLA	ND
11	B	1210	CLA	NA
11	b	1240	CLA	NC
11	b	1240	CLA	ND
11	b	1240	CLA	NA
11	a	1022	CLA	ND
11	a	1022	CLA	NA
11	A	1120	CLA	NC
11	A	1120	CLA	ND
11	A	1120	CLA	NA
11	8	1501	CLA	NC
11	8	1501	CLA	ND
11	8	1501	CLA	NA
11	B	1216	CLA	NC
11	B	1216	CLA	ND
11	B	1216	CLA	NA
11	B	1213	CLA	NC
11	B	1213	CLA	ND
11	B	1213	CLA	NA
11	1	1120	CLA	NC
11	1	1120	CLA	ND
11	1	1120	CLA	NA
11	2	1217	CLA	NC
11	2	1217	CLA	ND
11	2	1217	CLA	NA
11	K	1402	CLA	NC
11	K	1402	CLA	ND
11	K	1402	CLA	NA
11	1	1108	CLA	NC
11	1	1108	CLA	ND
11	1	1108	CLA	NA
11	2	1204	CLA	ND
11	2	1204	CLA	NA
11	B	1215	CLA	ND
11	B	1215	CLA	NA
11	A	1133	CLA	NC
11	A	1133	CLA	ND
11	A	1133	CLA	NA
11	1	1138	CLA	NC

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Mol	Chain	Res	Type	Atom
11	1	1138	CLA	ND
11	1	1138	CLA	NA
11	b	1220	CLA	NC
11	b	1220	CLA	ND
11	b	1220	CLA	NA
11	b	1216	CLA	NC
11	b	1216	CLA	NA
11	b	1216	CLA	ND
11	b	1234	CLA	NC
11	b	1234	CLA	ND
11	b	1234	CLA	NA
11	B	1207	CLA	ND
11	B	1207	CLA	NA
11	a	1103	CLA	NC
11	a	1103	CLA	NA
11	a	1103	CLA	ND
11	1	1129	CLA	NC
11	1	1129	CLA	ND
11	1	1129	CLA	NA
11	b	1239	CLA	NC
11	b	1239	CLA	ND
11	b	1239	CLA	NA
11	1	1109	CLA	NC
11	1	1109	CLA	NA
11	1	1132	CLA	NC
11	1	1132	CLA	ND
11	1	1132	CLA	NA
11	A	1126	CLA	NC
11	A	1126	CLA	ND
11	A	1126	CLA	NA
11	1	1103	CLA	NC
11	1	1103	CLA	ND
11	1	1103	CLA	NA
11	A	1109	CLA	NC
11	A	1109	CLA	NA
11	B	1202	CLA	NC
11	B	1202	CLA	NA
11	B	1202	CLA	ND
11	k	1402	CLA	NC
11	k	1402	CLA	ND
11	k	1402	CLA	NA
11	B	1203	CLA	NA

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Mol	Chain	Res	Type	Atom
11	8	1502	CLA	NC
11	8	1502	CLA	ND
11	8	1502	CLA	NA
11	A	1119	CLA	NC
11	A	1119	CLA	ND
11	A	1119	CLA	NA
11	A	1113	CLA	NC
11	A	1113	CLA	NA
11	A	1113	CLA	ND
11	L	1502	CLA	NC
11	L	1502	CLA	ND
11	L	1502	CLA	NA
11	A	1131	CLA	ND
11	A	1131	CLA	NA
11	1	1022	CLA	NC
11	1	1022	CLA	ND
11	1	1022	CLA	NA
11	a	1112	CLA	NC
11	a	1112	CLA	ND
11	a	1112	CLA	NA
11	1	1123	CLA	ND
11	1	1123	CLA	NA
11	a	1115	CLA	NC
11	a	1115	CLA	NA
11	0	1401	CLA	NC
11	0	1401	CLA	NA
11	0	1401	CLA	ND
11	b	1225	CLA	NC
11	b	1225	CLA	ND
11	b	1225	CLA	NA
11	a	1012	CLA	ND
11	a	1012	CLA	NA
11	1	1106	CLA	ND
11	1	1106	CLA	NA
11	A	1127	CLA	NC
11	A	1127	CLA	ND
11	A	1127	CLA	NA
11	A	1114	CLA	NC
11	A	1114	CLA	ND
11	A	1114	CLA	NA
11	2	1221	CLA	NC
11	2	1221	CLA	NA

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Mol	Chain	Res	Type	Atom
11	2	1221	CLA	ND
11	B	1223	CLA	ND
11	B	1223	CLA	NA
11	a	1140	CLA	NC
11	a	1140	CLA	ND
11	a	1140	CLA	NA
11	A	1134	CLA	NC
11	A	1134	CLA	ND
11	A	1134	CLA	NA
11	1	1114	CLA	NC
11	1	1114	CLA	ND
11	1	1114	CLA	NA
11	b	1235	CLA	NC
11	b	1235	CLA	NA
11	b	1235	CLA	ND
11	a	1116	CLA	NC
11	a	1116	CLA	ND
11	a	1116	CLA	NA
11	A	1117	CLA	NC
11	A	1117	CLA	ND
11	A	1117	CLA	NA
11	a	1119	CLA	NC
11	a	1119	CLA	ND
11	a	1119	CLA	NA
11	B	1231	CLA	NC
11	B	1231	CLA	ND
11	B	1231	CLA	NA
11	2	1231	CLA	NC
11	2	1231	CLA	ND
11	2	1231	CLA	NA
11	A	1128	CLA	NC
11	A	1128	CLA	ND
11	A	1128	CLA	NA
11	B	1224	CLA	NC
11	B	1224	CLA	NA
11	B	1224	CLA	ND
11	1	1137	CLA	NC
11	1	1137	CLA	NA
11	1	1137	CLA	ND
11	1	1130	CLA	NA
11	B	1206	CLA	ND
11	B	1206	CLA	NA

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Mol	Chain	Res	Type	Atom
11	a	1102	CLA	NC
11	a	1102	CLA	ND
11	a	1102	CLA	NA
11	b	1219	CLA	NC
11	b	1219	CLA	ND
11	b	1219	CLA	NA
11	a	1120	CLA	NC
11	a	1120	CLA	ND
11	a	1120	CLA	NA
11	b	1230	CLA	NC
11	b	1230	CLA	ND
11	b	1230	CLA	NA
11	0	1402	CLA	NC
11	0	1402	CLA	ND
11	0	1402	CLA	NA
11	1	1124	CLA	NC
11	1	1124	CLA	ND
11	1	1124	CLA	NA
11	L	1503	CLA	ND
11	L	1503	CLA	NA
11	B	1234	CLA	NC
11	B	1234	CLA	ND
11	B	1234	CLA	NA
11	a	1106	CLA	NC
11	a	1106	CLA	ND
11	a	1106	CLA	NA
11	2	1229	CLA	NC
11	2	1229	CLA	ND
11	2	1229	CLA	NA
11	a	1801	CLA	NC
11	a	1801	CLA	ND
11	a	1801	CLA	NA
11	B	1205	CLA	NC
11	B	1205	CLA	ND
11	B	1205	CLA	NA
11	2	1201	CLA	NC
11	2	1201	CLA	ND
11	2	1201	CLA	NA
11	a	1136	CLA	NC
11	a	1136	CLA	NA
11	a	1136	CLA	ND
11	2	1236	CLA	NC

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Mol	Chain	Res	Type	Atom
11	2	1236	CLA	ND
11	2	1236	CLA	NA
11	2	1219	CLA	NC
11	2	1219	CLA	ND
11	2	1219	CLA	NA
11	1	1237	CLA	NC
11	1	1237	CLA	ND
11	1	1237	CLA	NA
11	2	1212	CLA	NC
11	2	1212	CLA	ND
11	2	1212	CLA	NA
11	1	1135	CLA	ND
11	1	1135	CLA	NA
11	1	1116	CLA	NC
11	1	1116	CLA	ND
11	1	1116	CLA	NA
11	2	1232	CLA	ND
11	2	1232	CLA	NA
11	a	1117	CLA	NC
11	a	1117	CLA	ND
11	a	1117	CLA	NA
11	b	1228	CLA	NC
11	b	1228	CLA	ND
11	b	1228	CLA	NA
11	2	1227	CLA	NC
11	2	1227	CLA	NA
11	A	1011	CLA	NC
11	A	1011	CLA	NA
11	b	1227	CLA	NC
11	b	1227	CLA	NA
11	l	1501	CLA	NC
11	l	1501	CLA	NA
11	a	1105	CLA	NC
11	a	1105	CLA	ND
11	a	1105	CLA	NA
11	2	1235	CLA	NC
11	2	1235	CLA	ND
11	2	1235	CLA	NA
11	b	1201	CLA	NC
11	b	1201	CLA	ND
11	b	1201	CLA	NA
11	B	1239	CLA	NC

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Mol	Chain	Res	Type	Atom
11	B	1239	CLA	ND
11	B	1239	CLA	NA
11	A	1237	CLA	NC
11	A	1237	CLA	ND
11	A	1237	CLA	NA
11	B	1209	CLA	NC
11	B	1209	CLA	ND
11	B	1209	CLA	NA
11	a	1118	CLA	NC
11	a	1118	CLA	ND
11	a	1118	CLA	NA
11	A	1116	CLA	NC
11	A	1116	CLA	ND
11	A	1116	CLA	NA
11	2	1209	CLA	NC
11	2	1209	CLA	ND
11	2	1209	CLA	NA
11	k	1401	CLA	NC
11	k	1401	CLA	NA
11	k	1401	CLA	ND
11	A	1022	CLA	ND
11	A	1022	CLA	NA
11	1	1136	CLA	NC
11	1	1136	CLA	NA
11	1	1136	CLA	ND
11	b	1212	CLA	NC
11	b	1212	CLA	ND
11	b	1212	CLA	NA
11	A	1106	CLA	NC
11	A	1106	CLA	ND
11	A	1106	CLA	NA
11	2	1238	CLA	NC
11	2	1238	CLA	ND
11	2	1238	CLA	NA
11	a	1139	CLA	NC
11	a	1139	CLA	ND
11	a	1139	CLA	NA
11	a	1125	CLA	ND
11	a	1125	CLA	NA
11	A	1801	CLA	NC
11	A	1801	CLA	ND
11	A	1801	CLA	NA

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Mol	Chain	Res	Type	Atom
11	b	1224	CLA	NC
11	b	1224	CLA	ND
11	b	1224	CLA	NA
11	2	1214	CLA	NC
11	2	1214	CLA	ND
11	2	1214	CLA	NA
11	B	1217	CLA	NC
11	B	1217	CLA	ND
11	B	1217	CLA	NA
11	8	1503	CLA	NC
11	8	1503	CLA	ND
11	8	1503	CLA	NA
11	B	1204	CLA	ND
11	B	1204	CLA	NA
11	a	1134	CLA	NC
11	a	1134	CLA	NA
11	a	1134	CLA	ND
11	1	1127	CLA	NC
11	1	1127	CLA	ND
11	1	1127	CLA	NA
11	1	1126	CLA	NC
11	1	1126	CLA	ND
11	1	1126	CLA	NA
11	a	1107	CLA	NC
11	a	1107	CLA	ND
11	a	1107	CLA	NA
11	A	1129	CLA	NC
11	A	1129	CLA	ND
11	A	1129	CLA	NA
11	a	1237	CLA	NC
11	a	1237	CLA	ND
11	a	1237	CLA	NA
11	A	1115	CLA	NC
11	A	1115	CLA	ND
11	A	1115	CLA	NA
11	a	1113	CLA	NC
11	a	1113	CLA	ND
11	a	1113	CLA	NA
11	a	1128	CLA	NC
11	a	1128	CLA	ND
11	a	1128	CLA	NA
11	1	1122	CLA	NC

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Mol	Chain	Res	Type	Atom
11	1	1122	CLA	ND
11	1	1122	CLA	NA
11	a	1110	CLA	ND
11	a	1110	CLA	NA
11	B	1212	CLA	NC
11	B	1212	CLA	ND
11	B	1212	CLA	NA
11	L	1501	CLA	NC
11	L	1501	CLA	ND
11	L	1501	CLA	NA
11	1	1140	CLA	NC
11	1	1140	CLA	ND
11	1	1140	CLA	NA
11	b	1215	CLA	ND
11	b	1215	CLA	NA
11	A	1123	CLA	ND
11	A	1123	CLA	NA
11	b	1226	CLA	NC
11	b	1226	CLA	ND
11	b	1226	CLA	NA
11	a	1108	CLA	NC
11	a	1108	CLA	ND
11	a	1108	CLA	NA
11	2	1234	CLA	ND
11	2	1234	CLA	NA
11	2	1213	CLA	NC
11	2	1213	CLA	ND
11	2	1213	CLA	NA
11	A	1130	CLA	ND
11	A	1130	CLA	NA
11	B	1232	CLA	NC
11	B	1232	CLA	ND
11	B	1232	CLA	NA
11	A	1012	CLA	NC
11	A	1012	CLA	ND
11	A	1012	CLA	NA
11	A	1103	CLA	NC
11	A	1103	CLA	NA
11	A	1103	CLA	ND
11	b	1238	CLA	NC
11	b	1238	CLA	ND
11	b	1238	CLA	NA

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Mol	Chain	Res	Type	Atom
11	a	1011	CLA	NA
11	b	1204	CLA	ND
11	b	1204	CLA	NA
11	b	1223	CLA	NC
11	b	1223	CLA	ND
11	b	1223	CLA	NA
11	b	1229	CLA	NC
11	b	1229	CLA	ND
11	b	1229	CLA	NA
11	b	1023	CLA	NC
11	b	1023	CLA	ND
11	b	1023	CLA	NA
11	a	1104	CLA	NC
11	a	1104	CLA	ND
11	a	1104	CLA	NA
11	B	1222	CLA	NC
11	B	1222	CLA	ND
11	B	1222	CLA	NA
11	b	1232	CLA	NC
11	b	1232	CLA	ND
11	b	1232	CLA	NA
11	A	1132	CLA	NC
11	A	1132	CLA	ND
11	A	1132	CLA	NA
11	b	1231	CLA	NC
11	b	1231	CLA	ND
11	b	1231	CLA	NA
11	B	1236	CLA	NC
11	B	1236	CLA	ND
11	B	1236	CLA	NA
11	l	1502	CLA	NC
11	l	1502	CLA	ND
11	l	1502	CLA	NA
11	a	1126	CLA	NC
11	a	1126	CLA	ND
11	a	1126	CLA	NA
11	B	1235	CLA	NC
11	B	1235	CLA	ND
11	B	1235	CLA	NA
11	A	1104	CLA	NC
11	A	1104	CLA	ND
11	A	1104	CLA	NA

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Mol	Chain	Res	Type	Atom
11	2	1230	CLA	NC
11	2	1230	CLA	NA
11	2	1203	CLA	NC
11	2	1203	CLA	ND
11	2	1203	CLA	NA
11	A	1137	CLA	NC
11	A	1137	CLA	NA
11	A	1137	CLA	ND
11	1	1125	CLA	ND
11	1	1125	CLA	NA
11	B	1021	CLA	NC
11	B	1021	CLA	NA
11	B	1021	CLA	ND
11	A	1122	CLA	NC
11	A	1122	CLA	ND
11	A	1122	CLA	NA
11	B	1221	CLA	NC
11	B	1221	CLA	NA
11	B	1221	CLA	ND
11	1	1101	CLA	ND
11	1	1101	CLA	NA
11	A	1138	CLA	NC
11	A	1138	CLA	ND
11	A	1138	CLA	NA
11	b	1021	CLA	NC
11	b	1021	CLA	ND
11	b	1021	CLA	NA
11	2	1215	CLA	NC
11	2	1215	CLA	ND
11	2	1215	CLA	NA
11	b	1207	CLA	ND
11	b	1207	CLA	NA
11	b	1214	CLA	NC
11	b	1214	CLA	ND
11	b	1214	CLA	NA
11	1	1115	CLA	ND
11	1	1115	CLA	NA
11	b	1013	CLA	NA
11	1	1121	CLA	ND
11	1	1121	CLA	NA
11	b	1217	CLA	NC
11	b	1217	CLA	ND

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Mol	Chain	Res	Type	Atom
11	b	1217	CLA	NA
11	b	1205	CLA	NC
11	b	1205	CLA	ND
11	b	1205	CLA	NA
11	A	1140	CLA	ND
11	A	1140	CLA	NA
11	2	1225	CLA	NC
11	2	1225	CLA	ND
11	2	1225	CLA	NA
11	a	1123	CLA	ND
11	a	1123	CLA	NA
11	B	1023	CLA	NC
11	B	1023	CLA	ND
11	B	1023	CLA	NA
11	b	1202	CLA	NC
11	b	1202	CLA	NA
11	b	1202	CLA	ND
11	2	1226	CLA	NC
11	2	1226	CLA	ND
11	2	1226	CLA	NA
11	B	1238	CLA	NC
11	B	1238	CLA	ND
11	B	1238	CLA	NA
11	A	1111	CLA	NC
11	A	1111	CLA	ND
11	A	1111	CLA	NA
11	1	1131	CLA	ND
11	1	1131	CLA	NA
11	a	1135	CLA	ND
11	a	1135	CLA	NA
11	1	1119	CLA	NC
11	1	1119	CLA	ND
11	1	1119	CLA	NA
11	B	1226	CLA	NC
11	B	1226	CLA	ND
11	B	1226	CLA	NA
11	A	1112	CLA	NC
11	A	1112	CLA	NA
11	A	1112	CLA	ND
11	1	1118	CLA	NC
11	1	1118	CLA	ND
11	1	1118	CLA	NA

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Mol	Chain	Res	Type	Atom
11	a	1133	CLA	NC
11	a	1133	CLA	ND
11	a	1133	CLA	NA
11	A	1124	CLA	NC
11	A	1124	CLA	ND
11	A	1124	CLA	NA
11	2	1023	CLA	NC
11	2	1023	CLA	NA
11	2	1023	CLA	ND
11	2	1211	CLA	NC
11	2	1211	CLA	ND
11	2	1211	CLA	NA
11	B	1214	CLA	NC
11	B	1214	CLA	ND
11	B	1214	CLA	NA
11	B	1220	CLA	NA
11	A	1136	CLA	NC
11	A	1136	CLA	ND
11	A	1136	CLA	NA
11	a	1127	CLA	NC
11	a	1127	CLA	ND
11	a	1127	CLA	NA
11	1	1110	CLA	ND
11	1	1110	CLA	NA
11	l	1503	CLA	ND
11	l	1503	CLA	NA
11	A	1118	CLA	NC
11	A	1118	CLA	ND
11	A	1118	CLA	NA
11	B	1218	CLA	NC
11	B	1218	CLA	ND
11	B	1218	CLA	NA
11	a	1132	CLA	NC
11	a	1132	CLA	ND
11	a	1132	CLA	NA
11	1	1112	CLA	NC
11	1	1112	CLA	ND
11	1	1112	CLA	NA
11	A	1139	CLA	NC
11	A	1139	CLA	ND
11	A	1139	CLA	NA
11	2	1202	CLA	NC

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Mol	Chain	Res	Type	Atom
11	2	1202	CLA	NA
11	2	1202	CLA	ND
11	B	1208	CLA	ND
11	B	1208	CLA	NA
11	B	1227	CLA	NC
11	B	1227	CLA	ND
11	B	1227	CLA	NA
11	1	1011	CLA	NA
11	B	1228	CLA	NC
11	B	1228	CLA	ND
11	B	1228	CLA	NA
11	B	1240	CLA	NC
11	B	1240	CLA	ND
11	B	1240	CLA	NA
11	A	1135	CLA	NC
11	A	1135	CLA	ND
11	A	1135	CLA	NA
11	1	1134	CLA	NC
11	1	1134	CLA	NA
11	1	1134	CLA	ND
11	B	1219	CLA	NC
11	B	1219	CLA	ND
11	B	1219	CLA	NA
11	1	1012	CLA	ND
11	1	1012	CLA	NA
11	1	1104	CLA	ND
11	1	1104	CLA	NA
11	2	1206	CLA	NC
11	2	1206	CLA	ND
11	2	1206	CLA	NA
11	2	1240	CLA	NC
11	2	1240	CLA	ND
11	2	1240	CLA	NA
11	2	1220	CLA	ND
11	2	1220	CLA	NA
11	2	1239	CLA	NC
11	2	1239	CLA	ND
11	2	1239	CLA	NA
11	A	1105	CLA	NC
11	A	1105	CLA	ND
11	A	1105	CLA	NA
11	A	1121	CLA	NC

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Mol	Chain	Res	Type	Atom
11	A	1121	CLA	ND
11	A	1121	CLA	NA
11	A	1107	CLA	NC
11	A	1107	CLA	ND
11	A	1107	CLA	NA
11	b	1208	CLA	NC
11	b	1208	CLA	ND
11	b	1208	CLA	NA
11	a	1101	CLA	ND
11	a	1101	CLA	NA
11	B	1013	CLA	NC
11	B	1013	CLA	NA
11	B	1225	CLA	NC
11	B	1225	CLA	ND
11	B	1225	CLA	NA
11	a	1111	CLA	NC
11	a	1111	CLA	ND
11	a	1111	CLA	NA
11	2	1021	CLA	NC
11	2	1021	CLA	ND
11	2	1021	CLA	NA
11	2	1223	CLA	NC
11	2	1223	CLA	ND
11	2	1223	CLA	NA
11	B	1201	CLA	NC
11	B	1201	CLA	ND
11	B	1201	CLA	NA
11	B	1211	CLA	NC
11	B	1211	CLA	ND
11	B	1211	CLA	NA
11	B	1230	CLA	NC
11	B	1230	CLA	NA
11	b	1221	CLA	NC
11	b	1221	CLA	NA
11	b	1221	CLA	ND
11	b	1209	CLA	NC
11	b	1209	CLA	ND
11	b	1209	CLA	NA
11	b	1203	CLA	NC
11	b	1203	CLA	ND
11	b	1203	CLA	NA
11	2	1205	CLA	NC

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Mol	Chain	Res	Type	Atom
11	2	1205	CLA	ND
11	2	1205	CLA	NA
11	A	1108	CLA	NC
11	A	1108	CLA	ND
11	A	1108	CLA	NA
11	1	1113	CLA	NC
11	1	1113	CLA	ND
11	1	1113	CLA	NA
11	2	1210	CLA	NC
11	2	1210	CLA	ND
11	2	1210	CLA	NA
11	a	1131	CLA	NC
11	a	1131	CLA	ND
11	a	1131	CLA	NA
11	1	1107	CLA	NC
11	1	1107	CLA	ND
11	1	1107	CLA	NA
11	a	1109	CLA	NC
11	a	1109	CLA	NA
11	b	1236	CLA	NC
11	b	1236	CLA	NA
11	b	1236	CLA	ND
11	a	1137	CLA	NC
11	a	1137	CLA	NA
11	a	1137	CLA	ND
11	1	1105	CLA	NC
11	1	1105	CLA	ND
11	1	1105	CLA	NA
11	2	1216	CLA	NC
11	2	1216	CLA	ND
11	2	1216	CLA	NA
11	1	1102	CLA	NC
11	1	1102	CLA	ND
11	1	1102	CLA	NA
11	b	1206	CLA	NC
11	b	1206	CLA	ND
11	b	1206	CLA	NA
11	1	1117	CLA	NC
11	1	1117	CLA	ND
11	1	1117	CLA	NA
11	A	1102	CLA	ND
11	A	1102	CLA	NA

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Mol	Chain	Res	Type	Atom
11	a	1129	CLA	NC
11	a	1129	CLA	ND
11	a	1129	CLA	NA
11	2	1013	CLA	NA
11	2	1207	CLA	NA
11	b	1211	CLA	NC
11	b	1211	CLA	ND
11	b	1211	CLA	NA
11	2	1228	CLA	NC
11	2	1228	CLA	ND
11	2	1228	CLA	NA
11	a	1130	CLA	NC
11	a	1130	CLA	NA
11	B	1229	CLA	ND
11	B	1229	CLA	NA
11	a	1138	CLA	NC
11	a	1138	CLA	ND
11	a	1138	CLA	NA
11	b	1210	CLA	NC
11	b	1210	CLA	ND
11	b	1210	CLA	NA
11	2	1222	CLA	NC
11	2	1222	CLA	ND
11	2	1222	CLA	NA
11	A	1110	CLA	NC
11	A	1110	CLA	ND
11	A	1110	CLA	NA
11	1	1128	CLA	NC
11	1	1128	CLA	ND
11	1	1128	CLA	NA
11	a	1121	CLA	NC
11	a	1121	CLA	ND
11	a	1121	CLA	NA

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	a	4008	BCR	C10-C11-C12-C13
14	b	4004	BCR	C11-C10-C9-C8
14	B	4017	BCR	C11-C10-C9-C34
14	1	4008	BCR	C11-C10-C9-C34
14	2	4017	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
14	2	4017	BCR	C11-C10-C9-C34
14	A	4008	BCR	C10-C11-C12-C13
14	A	4008	BCR	C11-C10-C9-C8
14	A	4008	BCR	C11-C10-C9-C34
14	6	4020	BCR	C10-C11-C12-C13
14	B	4006	BCR	C11-C10-C9-C8
14	b	4006	BCR	C11-C10-C9-C8
14	b	4014	BCR	C11-C10-C9-C8
14	b	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C11-C10-C9-C34
14	b	4014	BCR	C11-C10-C9-C34
14	b	4017	BCR	C10-C11-C12-C13

There are no ring outliers.

208 monomers are involved in 696 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	0	1401	CLA	3	0
11	0	1402	CLA	1	0
11	1	1011	CLA	1	0
11	1	1012	CLA	5	0
11	1	1022	CLA	5	0
11	1	1101	CLA	3	0
11	1	1102	CLA	1	0
11	1	1103	CLA	2	0
11	1	1104	CLA	1	0
11	1	1105	CLA	1	0
11	1	1106	CLA	8	0
11	1	1107	CLA	3	0
11	1	1109	CLA	2	0
11	1	1110	CLA	2	0
11	1	1111	CLA	1	0
11	1	1112	CLA	3	0
11	1	1113	CLA	3	0
11	1	1115	CLA	4	0
11	1	1117	CLA	2	0
11	1	1118	CLA	2	0
11	1	1119	CLA	4	0
11	1	1121	CLA	1	0
11	1	1122	CLA	1	0
11	1	1123	CLA	5	0
11	1	1124	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	1125	CLA	2	0
11	1	1126	CLA	4	0
11	1	1127	CLA	4	0
11	1	1128	CLA	9	0
11	1	1129	CLA	2	0
11	1	1130	CLA	2	0
11	1	1131	CLA	2	0
11	1	1132	CLA	3	0
11	1	1133	CLA	2	0
11	1	1134	CLA	3	0
11	1	1137	CLA	4	0
11	1	1140	CLA	2	0
11	1	1237	CLA	3	0
11	1	1801	CLA	5	0
12	1	2001	PQN	1	0
13	1	3001	SF4	1	0
14	1	4001	BCR	8	0
14	1	4002	BCR	5	0
14	1	4003	BCR	2	0
14	1	4007	BCR	7	0
14	1	4008	BCR	4	0
15	1	5001	LHG	10	0
15	1	5003	LHG	6	0
11	2	1013	CLA	5	0
11	2	1021	CLA	6	0
11	2	1023	CLA	3	0
11	2	1201	CLA	2	0
11	2	1202	CLA	3	0
11	2	1203	CLA	1	0
11	2	1204	CLA	3	0
11	2	1205	CLA	4	0
11	2	1206	CLA	6	0
11	2	1207	CLA	4	0
11	2	1208	CLA	1	0
11	2	1209	CLA	1	0
11	2	1210	CLA	2	0
11	2	1211	CLA	2	0
11	2	1212	CLA	4	0
11	2	1214	CLA	2	0
11	2	1220	CLA	1	0
11	2	1222	CLA	3	0
11	2	1223	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	2	1225	CLA	1	0
11	2	1227	CLA	3	0
11	2	1229	CLA	5	0
11	2	1230	CLA	3	0
11	2	1231	CLA	8	0
11	2	1232	CLA	3	0
11	2	1234	CLA	4	0
11	2	1235	CLA	2	0
11	2	1238	CLA	5	0
11	2	1239	CLA	4	0
11	2	1240	CLA	2	0
12	2	2002	PQN	3	0
14	2	4004	BCR	2	0
14	2	4005	BCR	3	0
14	2	4006	BCR	1	0
14	2	4009	BCR	5	0
14	2	4010	BCR	6	0
14	2	4011	BCR	7	0
14	2	4014	BCR	7	0
14	2	4017	BCR	9	0
16	2	5002	LMG	1	0
15	2	5004	LHG	7	0
13	3	3002	SF4	9	0
13	3	3003	SF4	12	0
14	6	4013	BCR	7	0
14	6	4018	BCR	9	0
14	6	4020	BCR	4	0
14	7	4021	BCR	6	0
11	8	1501	CLA	6	0
11	8	1503	CLA	3	0
14	8	4019	BCR	7	0
14	8	4022	BCR	8	0
11	A	1011	CLA	3	0
11	A	1012	CLA	5	0
11	A	1022	CLA	6	0
11	A	1101	CLA	4	0
11	A	1102	CLA	4	0
11	A	1103	CLA	20	0
11	A	1104	CLA	8	0
11	A	1105	CLA	1	0
11	A	1106	CLA	6	0
11	A	1107	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1108	CLA	2	0
11	A	1109	CLA	1	0
11	A	1110	CLA	2	0
11	A	1111	CLA	4	0
11	A	1112	CLA	7	0
11	A	1113	CLA	2	0
11	A	1114	CLA	2	0
11	A	1115	CLA	2	0
11	A	1116	CLA	2	0
11	A	1117	CLA	2	0
11	A	1118	CLA	5	0
11	A	1119	CLA	11	0
11	A	1121	CLA	4	0
11	A	1122	CLA	2	0
11	A	1123	CLA	6	0
11	A	1124	CLA	3	0
11	A	1125	CLA	7	0
11	A	1126	CLA	9	0
11	A	1127	CLA	3	0
11	A	1128	CLA	6	0
11	A	1129	CLA	4	0
11	A	1131	CLA	4	0
11	A	1132	CLA	4	0
11	A	1133	CLA	4	0
11	A	1134	CLA	1	0
11	A	1135	CLA	1	0
11	A	1136	CLA	4	0
11	A	1137	CLA	5	0
11	A	1138	CLA	6	0
11	A	1140	CLA	1	0
11	A	1237	CLA	4	0
11	A	1801	CLA	8	0
12	A	2001	PQN	5	0
13	A	3001	SF4	4	0
14	A	4001	BCR	6	0
14	A	4002	BCR	9	0
14	A	4003	BCR	9	0
14	A	4007	BCR	9	0
14	A	4008	BCR	5	0
15	A	5001	LHG	5	0
15	A	5003	LHG	10	0
11	B	1013	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1021	CLA	7	0
11	B	1023	CLA	8	0
11	B	1201	CLA	4	0
11	B	1202	CLA	1	0
11	B	1203	CLA	2	0
11	B	1204	CLA	3	0
11	B	1205	CLA	5	0
11	B	1206	CLA	5	0
11	B	1207	CLA	3	0
11	B	1208	CLA	3	0
11	B	1209	CLA	6	0
11	B	1210	CLA	3	0
11	B	1211	CLA	5	0
11	B	1212	CLA	5	0
11	B	1214	CLA	2	0
11	B	1215	CLA	1	0
11	B	1217	CLA	2	0
11	B	1219	CLA	2	0
11	B	1220	CLA	3	0
11	B	1221	CLA	4	0
11	B	1222	CLA	7	0
11	B	1223	CLA	20	0
11	B	1224	CLA	1	0
11	B	1225	CLA	3	0
11	B	1226	CLA	1	0
11	B	1227	CLA	4	0
11	B	1228	CLA	2	0
11	B	1229	CLA	6	0
11	B	1230	CLA	5	0
11	B	1231	CLA	3	0
11	B	1234	CLA	2	0
11	B	1235	CLA	3	0
11	B	1238	CLA	7	0
11	B	1240	CLA	1	0
12	B	2002	PQN	4	0
14	B	4004	BCR	4	0
14	B	4005	BCR	7	0
14	B	4006	BCR	3	0
14	B	4009	BCR	7	0
14	B	4010	BCR	15	0
14	B	4011	BCR	10	0
14	B	4014	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	4017	BCR	10	0
16	B	5002	LMG	1	0
15	B	5004	LHG	8	0
13	C	3002	SF4	11	0
13	C	3003	SF4	11	0
14	F	4013	BCR	6	0
14	F	4018	BCR	11	0
14	F	4020	BCR	7	0
11	K	1401	CLA	4	0
11	K	1402	CLA	4	0
11	L	1501	CLA	8	0
11	L	1503	CLA	3	0
14	L	4019	BCR	13	0
14	L	4022	BCR	9	0
14	M	4021	BCR	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	739/751 (98%)	-0.34	17 (2%) 61 51	100, 203, 296, 388	0
1	A	739/751 (98%)	-0.45	1 (0%) 95 94	80, 113, 176, 250	0
1	a	739/751 (98%)	-0.30	27 (3%) 42 34	125, 205, 289, 372	0
2	2	728/731 (99%)	-0.44	2 (0%) 93 91	91, 133, 197, 293	0
2	B	728/731 (99%)	-0.40	3 (0%) 92 88	81, 133, 213, 297	0
2	b	728/731 (99%)	-0.38	17 (2%) 61 51	112, 221, 302, 414	0
3	3	80/81 (98%)	-0.52	1 (1%) 77 69	143, 185, 231, 268	0
3	C	80/81 (98%)	-0.42	0 100 100	100, 116, 140, 196	0
3	c	80/81 (98%)	-0.41	0 100 100	149, 205, 255, 292	0
4	4	138/141 (97%)	-0.10	4 (2%) 52 42	93, 195, 240, 290	0
4	D	138/141 (97%)	-0.52	0 100 100	88, 119, 165, 202	0
4	d	138/141 (97%)	-0.42	1 (0%) 87 82	83, 185, 253, 282	0
5	5	68/74 (91%)	0.44	4 (5%) 23 17	175, 220, 285, 372	0
5	E	68/74 (91%)	-0.10	4 (5%) 23 17	111, 151, 185, 210	0
5	e	68/74 (91%)	0.55	10 (14%) 3 3	198, 253, 319, 365	0
6	6	125/125 (100%)	1.43	39 (31%) 0 1	188, 307, 389, 486	0
6	F	125/125 (100%)	0.26	14 (11%) 6 6	154, 241, 336, 388	0
6	f	125/125 (100%)	1.59	41 (32%) 0 1	245, 333, 408, 478	0
7	8	151/157 (96%)	-0.26	2 (1%) 77 69	97, 125, 211, 294	0
7	L	151/157 (96%)	-0.43	0 100 100	89, 109, 163, 229	0
7	l	151/157 (96%)	-0.44	1 (0%) 87 82	107, 122, 165, 258	0
8	7	31/31 (100%)	-0.46	0 100 100	89, 95, 139, 147	0
8	M	31/31 (100%)	-0.53	0 100 100	108, 124, 158, 172	0
8	m	31/31 (100%)	-0.51	0 100 100	150, 174, 211, 233	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
9	9	38/40 (95%)	-0.47	0 100 100	89, 97, 152, 208	0
9	I	38/40 (95%)	-0.35	1 (2%) 56 46	92, 112, 198, 208	0
9	i	38/40 (95%)	-0.35	1 (2%) 56 46	125, 151, 224, 233	0
10	0	80/128 (62%)	0.27	10 (12%) 4 5	220, 289, 383, 449	0
10	K	80/128 (62%)	-0.57	1 (1%) 77 69	118, 160, 246, 314	0
10	k	80/128 (62%)	0.56	11 (13%) 3 4	189, 227, 344, 404	0
All	All	6534/6777 (96%)	-0.26	212 (3%) 48 38	80, 168, 303, 486	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	132	GLY	12.4
6	f	50	PRO	11.5
10	k	92	GLN	10.6
6	f	125	ARG	10.4
6	f	51	SER	9.8
10	k	91	PRO	9.7
6	6	12	PRO	9.6
6	6	75	SER	8.9
6	6	77	ASN	8.8
6	6	121	PRO	8.7
6	6	11	ALA	8.7
10	k	127	ILE	8.4
6	f	20	THR	8.1
6	f	21	PHE	8.1
6	f	23	ALA	7.8
1	a	131	GLY	7.8
6	f	49	ILE	7.2
6	f	116	LYS	7.1
6	f	19	LEU	7.1
10	k	90	LEU	6.9
6	f	48	LEU	6.8
6	f	22	THR	6.5
5	e	32	GLY	6.4
6	6	62	GLY	6.2
5	e	31	SER	6.1
10	k	79	ILE	5.8
5	e	34	LEU	5.6
1	a	207	LEU	5.6
5	e	30	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
6	6	71	GLU	5.4
1	1	22	PRO	5.3
6	f	24	GLY	5.3
6	f	58	ALA	5.2
1	1	19	ASN	5.1
6	f	111	GLY	5.1
6	F	86	ASN	5.0
6	6	69	LEU	4.9
10	0	91	PRO	4.9
2	b	617	PHE	4.9
10	k	93	LEU	4.9
6	6	122	THR	4.8
6	f	76	LYS	4.8
1	a	133	GLY	4.7
6	f	54	PHE	4.7
6	6	78	PRO	4.6
6	6	60	TRP	4.6
10	k	96	LYS	4.4
5	5	32	GLY	4.3
2	b	226	PHE	4.3
1	a	134	PHE	4.3
6	6	76	LYS	4.2
5	5	3	LEU	4.2
6	6	38	PHE	4.2
6	f	52	ILE	4.1
10	k	95	SER	4.0
5	e	33	ILE	4.0
6	6	72	ILE	3.9
6	f	11	ALA	3.8
6	6	61	ILE	3.8
5	E	3	LEU	3.8
7	8	153	ARG	3.7
2	b	506	PHE	3.7
6	f	53	ILE	3.7
1	1	317	ILE	3.7
6	6	81	GLN	3.7
6	6	37	LEU	3.7
10	0	127	ILE	3.6
1	1	243	ILE	3.6
5	E	4	ASN	3.6
6	f	18	LEU	3.6
5	e	29	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
6	6	89	LEU	3.5
6	f	12	PRO	3.5
6	f	75	SER	3.5
6	F	5	LYS	3.5
6	F	88	PRO	3.5
6	f	117	ASP	3.5
9	I	38	GLY	3.5
6	6	25	ILE	3.4
6	f	110	SER	3.4
1	a	208	GLY	3.4
1	a	696	LEU	3.4
6	6	59	GLY	3.3
2	b	205	GLN	3.3
6	F	20	THR	3.3
4	4	63	GLU	3.3
6	f	47	PHE	3.2
1	a	368	GLN	3.2
6	6	24	GLY	3.2
2	b	227	THR	3.2
10	0	84	LYS	3.2
2	b	225	PHE	3.1
6	F	1	MET	3.1
1	a	623	PRO	3.1
6	f	124	PRO	3.0
1	a	205	LEU	3.0
6	f	17	ALA	3.0
1	a	689	GLY	3.0
6	F	41	CYS	3.0
3	3	81	TYR	3.0
6	f	74	GLU	3.0
1	a	31	PRO	3.0
6	f	1	MET	2.9
2	b	396	TYR	2.9
6	6	119	GLU	2.9
5	E	63	GLU	2.9
6	f	115	MET	2.9
6	F	121	PRO	2.9
6	6	10	THR	2.9
1	a	19	ASN	2.9
6	f	57	ILE	2.9
6	6	70	ILE	2.8
1	1	712	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	1	62	THR	2.8
2	b	352	SER	2.8
5	e	8	LYS	2.8
1	1	21	VAL	2.8
6	6	67	SER	2.8
4	4	138	PRO	2.8
1	a	717	ALA	2.8
1	1	190	PHE	2.8
9	i	1	MET	2.7
1	1	731	TYR	2.7
6	F	85	ILE	2.7
10	k	80	GLN	2.7
5	E	2	ALA	2.7
1	1	316	GLY	2.7
10	k	89	ALA	2.7
2	b	92	TRP	2.6
5	e	63	GLU	2.6
6	f	119	GLU	2.6
6	6	73	ARG	2.6
10	0	92	GLN	2.6
4	d	110	GLU	2.6
1	a	478	LEU	2.6
6	f	55	LEU	2.6
6	6	40	PRO	2.6
6	f	40	PRO	2.5
1	A	712	ALA	2.5
6	6	58	ALA	2.5
1	a	249	MET	2.5
6	F	40	PRO	2.5
1	1	713	ILE	2.5
10	0	102	PRO	2.5
2	B	255	LEU	2.5
1	a	690	ARG	2.4
6	f	78	PRO	2.4
1	a	321	MET	2.4
6	f	15	ILE	2.4
1	1	20	PRO	2.4
5	5	2	ALA	2.4
7	l	109	GLY	2.4
2	b	222	LEU	2.4
4	4	60	ALA	2.4
5	e	7	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
6	6	27	ILE	2.4
6	f	16	MET	2.4
1	1	705	ASN	2.3
2	B	472	PHE	2.3
1	a	18	ASN	2.3
6	F	83	VAL	2.3
2	b	307	ALA	2.3
6	6	90	ALA	2.3
6	F	89	LEU	2.3
10	K	58	LEU	2.3
1	a	697	ILE	2.3
4	4	64	GLN	2.2
1	a	184	ALA	2.2
2	2	549	ASP	2.2
1	a	203	GLY	2.2
6	F	22	THR	2.2
6	6	64	VAL	2.2
7	8	152	PHE	2.2
2	2	542	LYS	2.2
6	f	25	ILE	2.2
6	6	88	PRO	2.2
6	6	22	THR	2.1
1	a	94	GLY	2.1
6	6	74	GLU	2.1
10	0	83	GLY	2.1
1	1	527	LEU	2.1
2	b	501	GLY	2.1
5	5	63	GLU	2.1
6	6	28	GLU	2.1
1	a	109	HIS	2.1
1	a	210	LEU	2.1
1	a	515	ALA	2.1
2	b	136	TYR	2.1
6	6	106	GLY	2.1
6	6	42	SER	2.1
2	b	351	TYR	2.1
1	a	20	PRO	2.1
2	b	551	GLY	2.1
6	f	79	GLU	2.1
6	6	105	VAL	2.1
10	0	55	GLY	2.1
6	F	90	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
10	0	98	THR	2.0
1	1	567	ASN	2.0
2	b	621	LEU	2.0
2	B	563	GLY	2.0
1	1	15	SER	2.0
6	f	123	SER	2.0
10	0	54	ALA	2.0
10	0	57	SER	2.0
2	b	65	LEU	2.0
10	k	75	GLY	2.0
5	e	69	VAL	2.0
6	F	6	SER	2.0
1	1	593	LEU	2.0
6	f	61	ILE	2.0
6	6	117	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	BCR	1	4003	40/40	0.62	1.31	15.39	193,227,269,270	0
14	BCR	2	4014	40/40	0.55	1.01	15.04	184,206,223,228	0
14	BCR	f	4018	40/40	0.90	0.73	14.02	132,138,152,154	0
14	BCR	b	4010	40/40	0.82	1.16	12.05	230,257,283,284	0
14	BCR	2	4011	40/40	0.68	1.23	10.17	187,207,215,220	0
15	LHG	2	5004	49/49	0.93	0.62	9.82	183,200,224,236	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	BCR	1	4002	40/40	0.53	1.04	8.67	220,241,266,270	0
14	BCR	F	4018	40/40	0.91	0.41	8.54	94,101,113,114	0
14	BCR	l	4019	40/40	0.85	0.97	8.40	122,133,149,151	0
16	LMG	B	5002	55/55	0.88	0.71	7.85	110,116,120,125	0
14	BCR	B	4014	40/40	0.81	0.91	7.63	138,157,191,200	0
14	BCR	B	4005	40/40	0.81	0.85	7.55	118,135,161,162	0
14	BCR	8	4019	40/40	0.89	0.85	7.35	125,129,144,154	0
14	BCR	b	4005	40/40	0.62	1.20	7.26	193,207,227,230	0
15	LHG	1	5003	49/49	0.91	0.49	6.86	154,173,196,198	0
14	BCR	6	4018	40/40	0.94	0.51	6.48	93,97,107,113	0
14	BCR	b	4011	40/40	0.67	0.96	6.46	204,219,248,251	0
15	LHG	a	5003	49/49	0.94	0.35	6.36	144,147,154,158	0
14	BCR	2	4010	40/40	0.88	0.69	5.82	132,140,147,150	0
14	BCR	1	4007	40/40	0.82	0.75	5.80	202,218,231,231	0
14	BCR	a	4007	40/40	0.82	0.61	5.58	144,153,167,170	0
11	CLA	2	1223	65/65	0.93	0.44	5.49	131,134,148,153	0
14	BCR	m	4021	40/40	0.74	0.76	5.48	175,183,191,194	0
12	PQN	2	2002	33/33	0.94	0.48	5.41	106,118,130,131	0
14	BCR	L	4019	40/40	0.92	0.79	5.31	87,90,93,93	0
14	BCR	A	4008	40/40	0.92	0.49	5.21	82,86,94,95	0
11	CLA	2	1234	60/65	0.92	0.51	5.16	151,164,196,206	0
11	CLA	1	1104	65/65	0.94	0.44	5.13	205,230,242,264	0
14	BCR	2	4017	40/40	0.90	0.59	5.08	96,102,117,117	0
11	CLA	2	1227	45/65	0.77	0.50	5.01	197,210,223,231	0
14	BCR	7	4021	40/40	0.86	0.47	5.01	106,110,121,131	0
14	BCR	M	4021	40/40	0.81	0.36	4.98	103,111,125,126	0
14	BCR	b	4017	40/40	0.87	0.62	4.97	143,150,160,162	0
14	BCR	B	4011	40/40	0.91	0.59	4.90	108,121,138,141	0
14	BCR	A	4003	40/40	0.87	0.54	4.73	100,112,129,132	0
14	BCR	f	4020	40/40	0.89	0.67	4.53	113,119,125,126	0
14	BCR	8	4022	40/40	0.85	0.54	4.46	123,131,145,146	0
11	CLA	a	1137	65/65	0.91	0.58	4.40	153,164,174,179	0
12	PQN	b	2002	33/33	0.91	0.57	4.22	140,146,156,158	0
12	PQN	B	2002	33/33	0.93	0.41	4.20	86,88,98,133	0
14	BCR	2	4005	40/40	0.81	0.66	4.16	102,108,118,120	0
14	BCR	l	4022	40/40	0.79	0.65	4.14	121,122,124,124	0
14	BCR	1	4008	40/40	0.89	0.57	4.04	169,180,189,192	0
14	BCR	B	4017	40/40	0.90	0.42	3.92	80,85,96,96	0
14	BCR	2	4004	40/40	0.78	0.65	3.84	123,137,161,163	0
14	BCR	a	4001	40/40	0.83	0.82	3.83	173,199,227,229	0
11	CLA	1	1127	65/65	0.95	0.57	3.81	214,223,233,237	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	b	1221	54/65	0.87	0.52	3.80	241,253,261,266	0
11	CLA	1	1102	65/65	0.88	0.53	3.79	199,219,239,246	0
14	BCR	B	4010	40/40	0.88	0.52	3.60	128,141,167,171	0
16	LMG	b	5002	55/55	0.89	0.56	3.60	149,160,167,167	0
12	PQN	A	2001	33/33	0.90	0.44	3.53	104,115,128,137	0
12	PQN	a	2001	33/33	0.71	1.19	3.47	181,201,225,229	0
11	CLA	B	1225	65/65	0.95	0.47	3.47	110,123,143,148	0
14	BCR	2	4006	40/40	0.88	0.37	3.47	98,105,120,122	0
11	CLA	b	1202	65/65	0.90	0.60	3.37	169,187,198,202	0
14	BCR	b	4006	40/40	0.54	0.75	3.36	193,210,237,241	0
16	LMG	2	5002	55/55	0.84	0.42	3.36	122,136,148,155	0
15	LHG	1	5001	49/49	0.89	0.41	3.33	182,196,208,213	0
11	CLA	B	1203	65/65	0.95	0.37	3.32	104,109,117,121	0
11	CLA	B	1240	45/65	0.83	0.53	3.30	211,230,239,242	0
11	CLA	A	1012	65/65	0.94	0.44	3.26	105,116,126,129	0
14	BCR	f	4013	40/40	0.71	1.73	3.23	275,292,321,326	0
11	CLA	A	1140	65/65	0.94	0.51	3.18	124,136,172,178	0
11	CLA	1	1107	65/65	0.90	0.44	3.18	207,232,269,282	0
11	CLA	b	1206	65/65	0.94	0.64	3.16	135,142,149,151	0
15	LHG	B	5004	49/49	0.90	0.47	3.13	158,169,178,183	0
11	CLA	a	1128	65/65	0.94	0.45	3.08	185,196,213,224	0
14	BCR	1	4001	40/40	0.84	0.80	3.04	241,254,269,271	0
11	CLA	B	1209	45/65	0.90	0.36	3.02	149,160,170,173	0
11	CLA	B	1219	55/65	0.94	0.31	3.01	158,173,186,192	0
11	CLA	B	1239	46/65	0.95	0.34	3.01	87,91,94,95	0
11	CLA	B	1226	65/65	0.94	0.43	2.97	104,114,121,124	0
11	CLA	A	1111	60/65	0.94	0.31	2.97	106,111,121,124	0
11	CLA	1	1106	65/65	0.94	0.41	2.95	187,201,212,222	0
11	CLA	b	1210	65/65	0.83	0.64	2.91	207,221,229,232	0
11	CLA	A	1127	65/65	0.96	0.46	2.89	94,101,108,110	0
11	CLA	A	1117	65/65	0.96	0.46	2.83	92,103,111,114	0
14	BCR	b	4014	40/40	0.42	2.06	2.83	230,259,294,299	0
11	CLA	1	1137	65/65	0.92	0.40	2.82	155,167,185,189	0
14	BCR	L	4022	40/40	0.78	0.59	2.76	110,121,132,133	0
11	CLA	A	1118	61/65	0.90	0.35	2.74	130,138,152,163	0
11	CLA	b	1225	65/65	0.92	0.50	2.73	183,198,210,214	0
11	CLA	1	1131	65/65	0.93	0.34	2.61	108,119,126,130	0
11	CLA	A	1125	52/65	0.94	0.38	2.61	95,99,105,127	0
11	CLA	1	1117	65/65	0.93	0.47	2.56	185,202,216,219	0
11	CLA	2	1235	60/65	0.91	0.34	2.55	154,169,185,191	0
14	BCR	A	4001	40/40	0.85	0.41	2.54	110,115,129,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	a	1131	65/65	0.95	0.36	2.54	121,124,131,134	0
11	CLA	a	1134	46/65	0.89	0.22	2.52	160,175,184,187	0
11	CLA	A	1124	55/65	0.96	0.34	2.52	85,89,93,93	0
11	CLA	A	1103	65/65	0.93	0.38	2.52	93,100,116,120	0
11	CLA	1	1128	65/65	0.95	0.39	2.52	197,213,223,224	0
11	CLA	1	1012	65/65	0.93	0.62	2.51	147,161,195,201	0
11	CLA	a	1126	65/65	0.89	0.42	2.50	210,232,258,266	0
11	CLA	b	1214	59/65	0.92	0.41	2.49	229,247,262,266	0
11	CLA	a	1132	65/65	0.94	0.37	2.49	113,128,133,136	0
11	CLA	B	1228	50/65	0.89	0.33	2.48	181,188,206,208	0
11	CLA	2	1222	56/65	0.92	0.42	2.46	141,153,179,185	0
14	BCR	a	4002	40/40	0.75	1.15	2.46	214,227,233,235	0
11	CLA	B	1227	45/65	0.87	0.28	2.44	168,175,199,212	0
11	CLA	b	1216	65/65	0.91	0.42	2.42	221,239,260,264	0
11	CLA	2	1225	65/65	0.95	0.34	2.39	100,105,110,112	0
11	CLA	b	1208	45/65	0.74	0.57	2.38	227,240,247,250	0
11	CLA	2	1013	65/65	0.94	0.54	2.37	153,169,194,196	0
15	LHG	a	5001	49/49	0.90	0.49	2.35	181,190,210,212	0
15	LHG	A	5001	49/49	0.93	0.37	2.33	94,99,108,110	0
14	BCR	6	4020	40/40	0.88	0.37	2.30	93,104,116,117	0
11	CLA	B	1206	65/65	0.94	0.41	2.30	94,99,104,106	0
11	CLA	b	1222	56/65	0.93	0.35	2.29	230,254,284,293	0
11	CLA	l	1501	65/65	0.88	0.47	2.27	137,139,157,168	0
11	CLA	2	1207	65/65	0.93	0.36	2.26	99,103,107,121	0
11	CLA	a	1117	65/65	0.89	0.67	2.23	167,191,206,211	0
11	CLA	B	1207	65/65	0.94	0.38	2.22	99,106,116,180	0
11	CLA	B	1223	65/65	0.92	0.41	2.22	154,166,176,183	0
15	LHG	b	5004	49/49	0.89	0.37	2.20	270,283,301,308	0
11	CLA	B	1222	56/65	0.91	0.37	2.19	121,136,161,169	0
11	CLA	1	1125	52/65	0.88	0.37	2.12	168,181,193,200	0
11	CLA	2	1211	46/65	0.94	0.34	2.10	98,104,109,112	0
14	BCR	a	4003	40/40	0.78	1.13	2.10	192,210,235,238	0
11	CLA	2	1204	65/65	0.94	0.34	2.10	88,90,94,99	0
11	CLA	B	1210	65/65	0.92	0.51	2.08	126,135,144,149	0
11	CLA	A	1126	65/65	0.92	0.41	2.05	95,105,125,130	0
14	BCR	A	4007	40/40	0.88	0.36	2.00	91,93,99,109	0
11	CLA	0	1401	65/65	0.80	0.43	1.99	251,268,277,306	0
11	CLA	b	1203	65/65	0.92	0.54	1.97	169,178,189,193	0
14	BCR	B	4004	40/40	0.77	0.54	1.97	168,175,187,190	0
11	CLA	b	1240	45/65	0.84	0.59	1.96	286,304,319,324	0
11	CLA	B	1235	60/65	0.95	0.37	1.91	141,154,163,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	B	1229	65/65	0.87	0.47	1.91	151,164,176,181	0
11	CLA	A	1133	46/65	0.94	0.35	1.89	89,96,101,103	0
11	CLA	B	1238	65/65	0.93	0.40	1.87	82,86,90,93	0
11	CLA	1	1103	65/65	0.95	0.42	1.87	218,234,261,272	0
11	CLA	1	1124	55/65	0.94	0.34	1.87	176,181,188,196	0
11	CLA	0	1402	50/65	0.86	0.52	1.86	282,304,319,325	0
11	CLA	A	1106	65/65	0.93	0.45	1.86	123,134,140,152	0
11	CLA	1	1129	46/65	0.93	0.41	1.86	166,179,190,191	0
11	CLA	A	1130	46/65	0.93	0.35	1.84	88,90,93,107	0
11	CLA	2	1206	65/65	0.95	0.34	1.84	91,95,98,100	0
14	BCR	A	4002	40/40	0.92	0.39	1.83	118,122,130,131	0
11	CLA	A	1129	46/65	0.94	0.34	1.82	82,85,88,89	0
11	CLA	2	1215	65/65	0.94	0.39	1.82	107,116,134,140	0
11	CLA	b	1219	55/65	0.91	0.53	1.81	267,284,296,299	0
11	CLA	B	1204	65/65	0.94	0.28	1.81	100,109,115,117	0
11	CLA	A	1134	46/65	0.93	0.28	1.77	98,106,111,113	0
11	CLA	A	1110	54/65	0.95	0.23	1.74	113,119,131,135	0
11	CLA	B	1224	55/65	0.95	0.35	1.74	116,122,128,136	0
11	CLA	L	1503	65/65	0.94	0.36	1.72	106,116,134,148	0
11	CLA	b	1205	55/65	0.96	0.30	1.72	146,156,165,167	0
11	CLA	2	1021	65/65	0.95	0.49	1.72	122,129,148,156	0
11	CLA	2	1238	65/65	0.94	0.38	1.71	93,106,113,116	0
11	CLA	B	1021	65/65	0.95	0.33	1.69	110,119,135,150	0
11	CLA	a	1130	46/65	0.95	0.27	1.68	117,123,125,128	0
11	CLA	b	1013	65/65	0.85	0.61	1.67	201,226,239,244	0
11	CLA	2	1213	65/65	0.88	0.46	1.66	142,149,160,181	0
11	CLA	1	1133	46/65	0.93	0.33	1.63	179,192,203,206	0
11	CLA	A	1011	65/65	0.95	0.37	1.62	85,97,106,141	0
11	CLA	8	1501	65/65	0.94	0.33	1.60	131,138,145,158	0
11	CLA	B	1221	54/65	0.94	0.43	1.60	126,134,140,146	0
11	CLA	B	1202	65/65	0.96	0.42	1.60	107,117,127,130	0
11	CLA	l	1503	65/65	0.92	0.32	1.59	125,130,137,187	0
11	CLA	b	1239	46/65	0.97	0.29	1.59	155,159,164,171	0
11	CLA	1	1126	65/65	0.93	0.44	1.58	179,200,211,215	0
11	CLA	a	1104	65/65	0.94	0.40	1.58	189,200,213,217	0
11	CLA	a	1113	45/65	0.81	0.47	1.56	233,253,273,278	0
11	CLA	2	1228	50/65	0.91	0.31	1.54	191,205,224,232	0
11	CLA	K	1401	65/65	0.85	0.36	1.54	141,148,155,157	0
11	CLA	b	1238	65/65	0.94	0.32	1.53	121,126,133,135	0
11	CLA	B	1216	65/65	0.88	0.38	1.52	151,164,179,185	0
11	CLA	a	1129	46/65	0.94	0.31	1.52	141,147,154,156	0
11	CLA	A	1135	51/65	0.95	0.31	1.50	90,94,97,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	1	1116	54/65	0.93	0.38	1.50	201,212,225,236	0
11	CLA	B	1234	60/65	0.88	0.32	1.50	124,143,166,172	0
11	CLA	b	1220	46/65	0.93	0.32	1.50	254,281,294,297	0
11	CLA	A	1102	65/65	0.96	0.27	1.49	123,130,142,144	0
11	CLA	a	1237	55/65	0.95	0.30	1.48	116,121,126,128	0
11	CLA	A	1128	65/65	0.95	0.34	1.46	102,108,118,128	0
11	CLA	2	1210	65/65	0.90	0.47	1.46	104,112,120,123	0
11	CLA	A	1116	54/65	0.94	0.34	1.46	96,102,108,123	0
11	CLA	2	1221	54/65	0.90	0.38	1.44	120,128,140,143	0
11	CLA	1	1132	65/65	0.95	0.34	1.44	99,105,118,123	0
11	CLA	2	1224	55/65	0.93	0.41	1.42	103,107,124,141	0
11	CLA	a	1123	65/65	0.92	0.53	1.42	159,181,191,193	0
11	CLA	1	1109	65/65	0.87	0.57	1.41	239,261,278,283	0
11	CLA	b	1217	47/65	0.89	0.28	1.41	240,259,267,270	0
11	CLA	2	1216	65/65	0.93	0.34	1.41	141,156,169,176	0
14	BCR	F	4020	40/40	0.93	0.28	1.40	84,87,94,94	0
11	CLA	B	1023	65/65	0.96	0.31	1.39	80,82,87,88	0
11	CLA	B	1205	55/65	0.95	0.34	1.38	97,104,114,127	0
11	CLA	b	1226	65/65	0.95	0.39	1.38	165,186,192,194	0
11	CLA	A	1237	55/65	0.95	0.30	1.31	80,83,86,87	0
11	CLA	b	1218	45/65	0.85	0.23	1.31	273,286,303,305	0
11	CLA	2	1214	59/65	0.95	0.31	1.30	120,130,139,145	0
11	CLA	L	1501	65/65	0.92	0.39	1.29	116,126,140,160	0
11	CLA	A	1120	46/65	0.94	0.27	1.28	99,107,111,112	0
11	CLA	a	1106	65/65	0.94	0.37	1.28	212,222,232,234	0
11	CLA	a	1102	65/65	0.90	0.34	1.28	213,223,246,250	0
15	LHG	A	5003	49/49	0.92	0.32	1.27	92,97,104,115	0
11	CLA	2	1218	45/65	0.89	0.24	1.25	164,178,189,194	0
11	CLA	b	1023	65/65	0.93	0.34	1.25	135,142,156,159	0
11	CLA	B	1201	54/65	0.93	0.32	1.24	99,107,110,111	0
11	CLA	A	1137	65/65	0.94	0.30	1.24	81,83,91,110	0
14	BCR	a	4008	40/40	0.78	0.42	1.24	150,152,155,155	0
11	CLA	a	1109	65/65	0.84	0.41	1.22	224,238,254,259	0
11	CLA	1	1112	45/65	0.88	0.48	1.20	263,286,301,303	0
11	CLA	A	1123	65/65	0.94	0.31	1.19	89,95,99,100	0
11	CLA	a	1124	55/65	0.94	0.43	1.19	156,166,174,176	0
11	CLA	a	1127	65/65	0.94	0.48	1.19	186,200,211,220	0
11	CLA	1	1113	45/65	0.87	0.51	1.18	235,255,277,284	0
11	CLA	2	1202	65/65	0.95	0.47	1.18	114,123,128,130	0
11	CLA	8	1503	65/65	0.93	0.42	1.17	137,142,156,177	0
11	CLA	2	1239	46/65	0.97	0.28	1.16	103,112,115,119	0
11	CLA	B	1236	47/65	0.96	0.33	1.15	136,145,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	B	1215	65/65	0.94	0.39	1.14	135,141,147,154	0
14	BCR	B	4006	40/40	0.80	0.39	1.14	128,148,172,176	0
11	CLA	1	1118	61/65	0.88	0.52	1.13	279,308,317,321	0
11	CLA	b	1207	65/65	0.93	0.40	1.13	120,127,132,133	0
11	CLA	A	1119	65/65	0.94	0.35	1.13	82,95,99,109	0
11	CLA	b	1209	45/65	0.78	0.32	1.13	226,238,250,254	0
11	CLA	2	1231	45/65	0.93	0.24	1.11	139,147,159,168	0
11	CLA	1	1123	65/65	0.94	0.44	1.11	208,227,237,242	0
11	CLA	k	1402	50/65	0.88	0.37	1.10	225,232,238,242	0
11	CLA	1	1119	65/65	0.92	0.39	1.10	197,237,248,254	0
11	CLA	a	1801	52/65	0.92	0.27	1.09	156,164,182,184	0
11	CLA	A	1801	52/65	0.92	0.25	1.07	89,95,98,103	0
11	CLA	A	1132	65/65	0.94	0.30	1.06	90,92,97,100	0
11	CLA	A	1121	46/65	0.93	0.29	1.06	97,103,120,155	0
14	BCR	6	4013	40/40	0.47	1.32	1.06	254,275,285,291	0
11	CLA	a	1118	61/65	0.93	0.58	1.06	202,218,238,243	0
11	CLA	B	1213	65/65	0.70	0.43	1.06	190,205,222,228	0
11	CLA	A	1104	65/65	0.95	0.33	1.04	93,99,105,107	0
11	CLA	A	1131	65/65	0.94	0.33	1.03	81,84,88,109	0
11	CLA	A	1122	59/65	0.95	0.34	0.99	83,88,92,94	0
11	CLA	A	1109	65/65	0.94	0.26	0.99	111,119,129,132	0
11	CLA	l	1502	46/65	0.95	0.40	0.99	111,114,119,120	0
11	CLA	b	1213	65/65	0.78	0.40	0.98	261,273,288,291	0
12	PQN	1	2001	33/33	0.91	0.60	0.97	184,204,226,230	0
11	CLA	B	1217	47/65	0.90	0.30	0.96	159,172,182,186	0
11	CLA	1	1105	48/65	0.90	0.30	0.96	208,225,238,242	0
11	CLA	a	1103	65/65	0.94	0.34	0.95	199,214,239,246	0
11	CLA	1	1237	55/65	0.93	0.29	0.94	113,120,130,133	0
11	CLA	b	1204	65/65	0.94	0.39	0.94	163,169,175,177	0
11	CLA	B	1220	46/65	0.94	0.25	0.93	133,148,155,158	0
11	CLA	2	1023	65/65	0.94	0.37	0.91	117,135,145,149	0
11	CLA	a	1107	65/65	0.91	0.34	0.91	235,255,266,271	0
11	CLA	1	1122	59/65	0.94	0.34	0.91	168,189,205,209	0
11	CLA	1	1111	60/65	0.91	0.40	0.90	229,246,266,273	0
11	CLA	b	1227	45/65	0.85	0.19	0.89	277,302,310,314	0
11	CLA	B	1013	65/65	0.96	0.28	0.89	99,112,120,139	0
11	CLA	a	1022	65/65	0.92	0.35	0.88	142,156,166,168	0
11	CLA	2	1201	54/65	0.92	0.31	0.87	91,100,104,107	0
11	CLA	1	1135	51/65	0.94	0.40	0.87	174,178,184,187	0
11	CLA	a	1121	46/65	0.87	0.29	0.87	162,173,180,183	0
11	CLA	2	1236	47/65	0.91	0.35	0.84	149,159,173,177	0
11	CLA	A	1139	50/65	0.93	0.42	0.83	112,126,138,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	a	1111	60/65	0.95	0.36	0.83	198,205,225,229	0
11	CLA	A	1022	65/65	0.95	0.33	0.82	82,88,92,93	0
11	CLA	a	1138	46/65	0.91	0.28	0.81	226,242,255,260	0
11	CLA	a	1105	48/65	0.91	0.41	0.81	249,270,280,285	0
11	CLA	2	1226	65/65	0.94	0.31	0.81	99,113,120,122	0
11	CLA	2	1220	46/65	0.95	0.31	0.80	145,153,163,167	0
11	CLA	k	1401	65/65	0.87	0.32	0.79	196,201,206,207	0
11	CLA	b	1234	60/65	0.84	0.46	0.79	220,242,268,270	0
13	SF4	A	3001	8/8	0.97	0.24	0.76	50,62,210,290	0
11	CLA	L	1502	46/65	0.94	0.33	0.76	86,91,96,114	0
11	CLA	A	1138	46/65	0.94	0.28	0.76	121,131,139,143	0
11	CLA	b	1235	60/65	0.93	0.24	0.73	235,252,263,268	0
11	CLA	a	1136	46/65	0.95	0.30	0.71	140,148,157,173	0
11	CLA	a	1135	51/65	0.93	0.39	0.71	140,155,162,167	0
11	CLA	a	1116	54/65	0.95	0.30	0.70	170,177,186,189	0
11	CLA	1	1011	65/65	0.95	0.36	0.69	124,133,140,142	0
11	CLA	A	1101	65/65	0.94	0.39	0.68	143,151,160,175	0
11	CLA	A	1107	65/65	0.92	0.38	0.67	122,130,137,141	0
14	BCR	b	4004	40/40	0.77	0.56	0.66	242,256,279,281	0
11	CLA	K	1402	50/65	0.90	0.34	0.66	169,178,200,223	0
11	CLA	a	1140	65/65	0.93	0.53	0.64	203,218,260,267	0
11	CLA	b	1201	54/65	0.90	0.27	0.64	150,157,164,166	0
11	CLA	b	1215	65/65	0.95	0.30	0.63	226,238,256,265	0
11	CLA	a	1011	65/65	0.92	0.41	0.63	161,188,194,198	0
11	CLA	a	1122	59/65	0.94	0.29	0.63	134,144,153,156	0
11	CLA	1	1130	46/65	0.91	0.29	0.60	131,140,148,150	0
11	CLA	A	1113	45/65	0.92	0.27	0.56	121,133,146,148	0
11	CLA	1	1022	65/65	0.94	0.39	0.53	101,124,132,137	0
11	CLA	b	1228	50/65	0.90	0.22	0.53	262,267,290,297	0
11	CLA	a	1012	65/65	0.93	0.41	0.52	185,204,226,230	0
11	CLA	A	1136	46/65	0.95	0.25	0.52	82,86,88,89	0
11	CLA	b	1224	55/65	0.93	0.28	0.52	163,171,178,179	0
11	CLA	8	1502	46/65	0.95	0.27	0.51	153,164,178,197	0
11	CLA	a	1110	54/65	0.83	0.27	0.51	211,224,241,244	0
11	CLA	A	1115	46/65	0.95	0.26	0.48	111,121,126,126	0
11	CLA	2	1205	55/65	0.96	0.28	0.43	92,96,98,99	0
11	CLA	1	1140	65/65	0.94	0.48	0.43	180,188,218,225	0
11	CLA	b	1236	47/65	0.93	0.20	0.43	239,254,268,270	0
11	CLA	b	1021	65/65	0.94	0.37	0.41	185,193,223,226	0
11	CLA	a	1119	65/65	0.92	0.42	0.40	143,162,172,177	0
11	CLA	a	1133	46/65	0.93	0.26	0.38	158,171,178,183	0
11	CLA	1	1121	46/65	0.87	0.23	0.38	195,211,221,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	a	1112	45/65	0.85	0.29	0.36	233,251,261,266	0
11	CLA	b	1231	45/65	0.91	0.37	0.36	275,294,305,311	0
11	CLA	b	1223	65/65	0.94	0.47	0.35	218,233,240,242	0
11	CLA	B	1230	58/65	0.85	0.34	0.34	159,178,203,214	0
13	SF4	1	3001	8/8	0.98	0.19	0.34	50,62,210,290	0
11	CLA	a	1101	65/65	0.93	0.39	0.33	236,245,257,265	0
13	SF4	C	3003	8/8	0.98	0.21	0.29	60,67,100,115	0
11	CLA	2	1209	45/65	0.91	0.21	0.27	124,135,140,143	0
11	CLA	2	1230	58/65	0.88	0.37	0.27	222,240,273,278	0
11	CLA	2	1203	65/65	0.94	0.24	0.26	97,104,108,110	0
11	CLA	1	1134	46/65	0.90	0.21	0.26	212,228,242,244	0
11	CLA	B	1211	46/65	0.95	0.26	0.19	137,146,156,161	0
11	CLA	A	1112	45/65	0.97	0.21	0.17	132,143,149,153	0
11	CLA	1	1101	65/65	0.93	0.47	0.17	214,232,245,253	0
11	CLA	b	1230	58/65	0.84	0.38	0.16	250,275,310,317	0
11	CLA	B	1212	45/65	0.92	0.27	0.15	160,174,184,187	0
11	CLA	1	1136	46/65	0.95	0.27	0.14	154,164,170,176	0
11	CLA	B	1218	45/65	0.94	0.23	0.14	168,176,189,196	0
11	CLA	2	1217	47/65	0.94	0.20	0.14	127,139,146,149	0
11	CLA	B	1232	45/65	0.91	0.23	0.11	168,184,196,202	0
11	CLA	2	1229	65/65	0.87	0.33	0.11	177,187,202,209	0
11	CLA	a	1125	52/65	0.92	0.34	0.11	157,167,173,177	0
11	CLA	A	1114	46/65	0.93	0.26	0.10	150,165,173,175	0
11	CLA	B	1214	59/65	0.92	0.24	0.08	143,159,171,177	0
11	CLA	B	1231	45/65	0.92	0.24	0.07	154,169,180,185	0
11	CLA	a	1114	46/65	0.85	0.25	0.06	248,267,279,284	0
11	CLA	b	1211	46/65	0.87	0.25	0.06	210,224,234,240	0
11	CLA	B	1208	45/65	0.94	0.27	0.05	128,136,143,147	0
11	CLA	1	1115	46/65	0.90	0.24	0.04	236,256,261,267	0
11	CLA	A	1105	48/65	0.92	0.28	0.04	118,132,139,142	0
11	CLA	A	1108	45/65	0.93	0.23	0.01	111,120,127,130	0
11	CLA	1	1801	52/65	0.91	0.24	-0.01	199,212,225,231	0
13	SF4	C	3002	8/8	0.95	0.24	-0.11	60,88,151,152	0
11	CLA	1	1138	46/65	0.92	0.29	-0.13	175,188,205,208	0
11	CLA	a	1120	46/65	0.93	0.28	-0.16	190,204,214,230	0
11	CLA	1	1120	46/65	0.90	0.32	-0.16	227,248,258,262	0
11	CLA	1	1114	46/65	0.80	0.40	-0.20	262,279,288,293	0
11	CLA	1	1139	50/65	0.93	0.27	-0.20	181,204,222,225	0
11	CLA	a	1139	50/65	0.83	0.23	-0.23	210,233,255,263	0
11	CLA	2	1212	45/65	0.94	0.25	-0.28	114,120,125,126	0
11	CLA	a	1115	46/65	0.92	0.19	-0.30	188,200,211,232	0
11	CLA	b	1229	65/65	0.88	0.50	-0.32	249,269,282,289	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	1	1108	45/65	0.83	0.19	-0.41	247,270,284,289	0
11	CLA	a	1108	45/65	0.87	0.21	-0.47	215,233,245,250	0
11	CLA	b	1212	45/65	0.88	0.22	-0.50	248,260,269,270	0
13	SF4	3	3002	8/8	0.97	0.19	-0.54	60,88,151,152	0
11	CLA	1	1110	54/65	0.89	0.27	-0.56	258,268,295,299	0
11	CLA	2	1208	45/65	0.93	0.28	-0.73	102,111,118,120	0
13	SF4	c	3002	8/8	0.97	0.16	-0.83	60,88,151,152	0
13	SF4	a	3001	8/8	0.98	0.16	-1.19	50,62,210,290	0
13	SF4	3	3003	8/8	0.97	0.10	-1.38	60,67,100,115	0
13	SF4	c	3003	8/8	0.97	0.11	-1.47	60,67,100,115	0
14	BCR	F	4013	40/40	0.65	1.11	-	163,191,214,225	0
14	BCR	B	4009	40/40	0.75	1.11	-	169,203,225,226	0
11	CLA	2	1232	45/65	0.94	0.23	-	148,157,170,176	0
14	BCR	b	4009	40/40	0.82	1.31	-	254,280,313,316	0
14	BCR	2	4009	40/40	0.60	1.70	-	189,224,256,263	0
11	CLA	2	1219	55/65	0.91	0.30	-	177,196,211,233	0
11	CLA	b	1232	45/65	0.90	0.28	-	249,265,277,284	0
11	CLA	2	1240	45/65	0.85	0.34	-	224,246,269,289	0

6.5 Other polymers [i](#)

There are no such residues in this entry.