



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:58 am GMT

PDB ID : 1QZV
Title : Crystal structure of plant photosystem I
Authors : Ben-Shem, A.; Frolow, F.; Nelson, N.
Deposited on : 2003-09-18
Resolution : 4.44 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

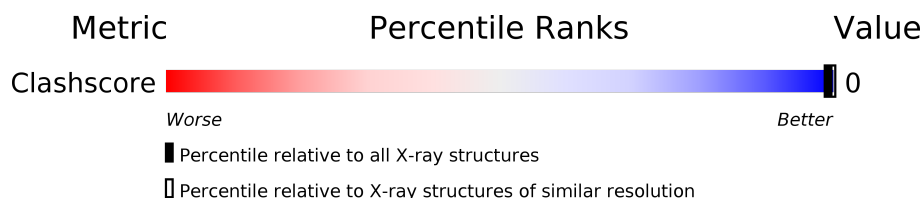
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.44 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))
Clashscore	112137	1021 (5.08-3.70)
















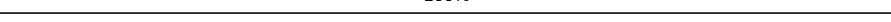
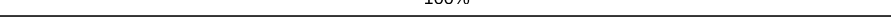
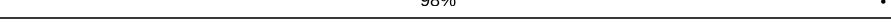
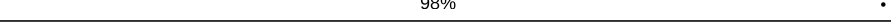
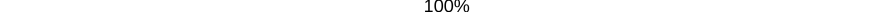
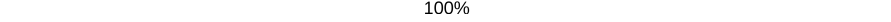
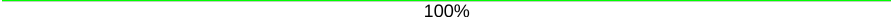
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	726	 100%
1	P	726	 100%
2	B	732	 100%
2	Q	732	 100%
3	C	80	 100%
3	R	80	 100%
4	D	154	 100%
4	S	154	 100%
5	E	64	 100%
5	T	64	 100%

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Mol	Chain	Length	Quality of chain
6	F	154	 100%
6	U	154	 100%
7	G	74	 100%
7	V	74	 100%
8	H	52	 100%
8	W	52	 100%
9	I	30	 100%
9	Y	30	 100%
10	J	41	 100%
10	Z	41	 100%
11	5	42	 100%
11	K	42	 100%
12	6	135	 100%
12	L	135	 100%
13	1	109	 100%
13	7	109	 100%
14	2	115	 98%
14	8	115	 98%
15	3	117	 100%
15	9	117	 100%
16	0	119	 100%
16	4	119	 100%

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
17	CLA	0	1011	X	-	-	-
17	CLA	0	1012	X	-	-	-
17	CLA	0	1013	X	-	-	-
17	CLA	0	1014	X	-	-	-
17	CLA	0	1015	X	-	-	-
17	CLA	0	1016	X	-	-	-
17	CLA	0	1017	X	-	-	-
17	CLA	0	1021	X	-	-	-
17	CLA	0	1022	X	-	-	-
17	CLA	0	1023	X	-	-	-
17	CLA	0	1025	X	-	-	-
17	CLA	0	1026	X	-	-	-
17	CLA	0	1031	X	-	-	-
17	CLA	0	1032	X	-	-	-
17	CLA	0	1033	X	-	-	-
17	CLA	0	8002	X	-	-	-
17	CLA	1	1011	X	-	-	-
17	CLA	1	1012	X	-	-	-
17	CLA	1	1013	X	-	-	-
17	CLA	1	1014	X	-	-	-
17	CLA	1	1015	X	-	-	-
17	CLA	1	1016	X	-	-	-
17	CLA	1	1017	X	-	-	-
17	CLA	1	1021	X	-	-	-
17	CLA	1	1022	X	-	-	-
17	CLA	1	1023	X	-	-	-
17	CLA	1	1025	X	-	-	-
17	CLA	1	1026	X	-	-	-
17	CLA	1	1031	X	-	-	-
17	CLA	2	1011	X	-	-	-
17	CLA	2	1012	X	-	-	-
17	CLA	2	1013	X	-	-	-
17	CLA	2	1014	X	-	-	-
17	CLA	2	1015	X	-	-	-
17	CLA	2	1016	X	-	-	-
17	CLA	2	1017	X	-	-	-
17	CLA	2	1021	X	-	-	-
17	CLA	2	1022	X	-	-	-
17	CLA	2	1023	X	-	-	-
17	CLA	2	1025	X	-	-	-
17	CLA	2	1026	X	-	-	-
17	CLA	2	1031	X	-	-	-
17	CLA	2	1033	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	4007	X	-	-	-
17	CLA	3	1011	X	-	-	-
17	CLA	3	1012	X	-	-	-
17	CLA	3	1014	X	-	-	-
17	CLA	3	1015	X	-	-	-
17	CLA	3	1016	X	-	-	-
17	CLA	3	1017	X	-	-	-
17	CLA	3	1021	X	-	-	-
17	CLA	3	1022	X	-	-	-
17	CLA	3	1025	X	-	-	-
17	CLA	3	1026	X	-	-	-
17	CLA	3	1031	X	-	-	-
17	CLA	3	1032	X	-	-	-
17	CLA	3	1033	X	-	-	-
17	CLA	3	1041	X	-	-	-
17	CLA	4	1011	X	-	-	-
17	CLA	4	1012	X	-	-	-
17	CLA	4	1013	X	-	-	-
17	CLA	4	1014	X	-	-	-
17	CLA	4	1015	X	-	-	-
17	CLA	4	1016	X	-	-	-
17	CLA	4	1017	X	-	-	-
17	CLA	4	1021	X	-	-	-
17	CLA	4	1022	X	-	-	-
17	CLA	4	1023	X	-	-	-
17	CLA	4	1025	X	-	-	-
17	CLA	4	1026	X	-	-	-
17	CLA	4	1031	X	-	-	-
17	CLA	4	1032	X	-	-	-
17	CLA	4	1033	X	-	-	-
17	CLA	4	4002	X	-	-	-
17	CLA	5	5401	X	-	-	-
17	CLA	5	5403	X	-	-	-
17	CLA	5	5404	X	-	-	-
17	CLA	6	5501	X	-	-	-
17	CLA	6	5502	X	-	-	-
17	CLA	6	5503	X	-	-	-
17	CLA	6	5504	X	-	-	-
17	CLA	7	1011	X	-	-	-
17	CLA	7	1012	X	-	-	-
17	CLA	7	1013	X	-	-	-
17	CLA	7	1014	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	7	1015	X	-	-	-
17	CLA	7	1016	X	-	-	-
17	CLA	7	1017	X	-	-	-
17	CLA	7	1021	X	-	-	-
17	CLA	7	1022	X	-	-	-
17	CLA	7	1023	X	-	-	-
17	CLA	7	1025	X	-	-	-
17	CLA	7	1026	X	-	-	-
17	CLA	7	1031	X	-	-	-
17	CLA	8	1011	X	-	-	-
17	CLA	8	1012	X	-	-	-
17	CLA	8	1013	X	-	-	-
17	CLA	8	1014	X	-	-	-
17	CLA	8	1015	X	-	-	-
17	CLA	8	1016	X	-	-	-
17	CLA	8	1017	X	-	-	-
17	CLA	8	1021	X	-	-	-
17	CLA	8	1022	X	-	-	-
17	CLA	8	1023	X	-	-	-
17	CLA	8	1025	X	-	-	-
17	CLA	8	1026	X	-	-	-
17	CLA	8	1031	X	-	-	-
17	CLA	8	1033	X	-	-	-
17	CLA	8	8007	X	-	-	-
17	CLA	9	1011	X	-	-	-
17	CLA	9	1012	X	-	-	-
17	CLA	9	1014	X	-	-	-
17	CLA	9	1015	X	-	-	-
17	CLA	9	1016	X	-	-	-
17	CLA	9	1017	X	-	-	-
17	CLA	9	1021	X	-	-	-
17	CLA	9	1022	X	-	-	-
17	CLA	9	1025	X	-	-	-
17	CLA	9	1026	X	-	-	-
17	CLA	9	1031	X	-	-	-
17	CLA	9	1032	X	-	-	-
17	CLA	9	1033	X	-	-	-
17	CLA	9	1041	X	-	-	-
17	CLA	A	1011	X	-	-	-
17	CLA	A	1012	X	-	-	-
17	CLA	A	1013	X	-	-	-
17	CLA	A	1102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	1103	X	-	-	-
17	CLA	A	1104	X	-	-	-
17	CLA	A	1105	X	-	-	-
17	CLA	A	1106	X	-	-	-
17	CLA	A	1107	X	-	-	-
17	CLA	A	1108	X	-	-	-
17	CLA	A	1109	X	-	-	-
17	CLA	A	1110	X	-	-	-
17	CLA	A	1111	X	-	-	-
17	CLA	A	1112	X	-	-	-
17	CLA	A	1113	X	-	-	-
17	CLA	A	1114	X	-	-	-
17	CLA	A	1115	X	-	-	-
17	CLA	A	1116	X	-	-	-
17	CLA	A	1117	X	-	-	-
17	CLA	A	1118	X	-	-	-
17	CLA	A	1119	X	-	-	-
17	CLA	A	1120	X	-	-	-
17	CLA	A	1121	X	-	-	-
17	CLA	A	1122	X	-	-	-
17	CLA	A	1123	X	-	-	-
17	CLA	A	1124	X	-	-	-
17	CLA	A	1125	X	-	-	-
17	CLA	A	1126	X	-	-	-
17	CLA	A	1127	X	-	-	-
17	CLA	A	1128	X	-	-	-
17	CLA	A	1129	X	-	-	-
17	CLA	A	1131	X	-	-	-
17	CLA	A	1132	X	-	-	-
17	CLA	A	1133	X	-	-	-
17	CLA	A	1134	X	-	-	-
17	CLA	A	1135	X	-	-	-
17	CLA	A	1136	X	-	-	-
17	CLA	A	1137	X	-	-	-
17	CLA	A	1138	X	-	-	-
17	CLA	A	1139	X	-	-	-
17	CLA	A	1140	X	-	-	-
17	CLA	A	1402	X	-	-	-
17	CLA	A	1901	X	-	-	-
17	CLA	A	4009	X	-	-	-
17	CLA	A	4010	X	-	-	-
17	CLA	B	1021	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	1022	X	-	-	-
17	CLA	B	1023	X	-	-	-
17	CLA	B	1130	X	-	-	-
17	CLA	B	1201	X	-	-	-
17	CLA	B	1202	X	-	-	-
17	CLA	B	1203	X	-	-	-
17	CLA	B	1204	X	-	-	-
17	CLA	B	1205	X	-	-	-
17	CLA	B	1206	X	-	-	-
17	CLA	B	1207	X	-	-	-
17	CLA	B	1208	X	-	-	-
17	CLA	B	1209	X	-	-	-
17	CLA	B	1210	X	-	-	-
17	CLA	B	1211	X	-	-	-
17	CLA	B	1212	X	-	-	-
17	CLA	B	1213	X	-	-	-
17	CLA	B	1214	X	-	-	-
17	CLA	B	1215	X	-	-	-
17	CLA	B	1216	X	-	-	-
17	CLA	B	1217	X	-	-	-
17	CLA	B	1218	X	-	-	-
17	CLA	B	1219	X	-	-	-
17	CLA	B	1220	X	-	-	-
17	CLA	B	1221	X	-	-	-
17	CLA	B	1222	X	-	-	-
17	CLA	B	1223	X	-	-	-
17	CLA	B	1224	X	-	-	-
17	CLA	B	1225	X	-	-	-
17	CLA	B	1226	X	-	-	-
17	CLA	B	1227	X	-	-	-
17	CLA	B	1228	X	-	-	-
17	CLA	B	1230	X	-	-	-
17	CLA	B	1231	X	-	-	-
17	CLA	B	1232	X	-	-	-
17	CLA	B	1234	X	-	-	-
17	CLA	B	1235	X	-	-	-
17	CLA	B	1236	X	-	-	-
17	CLA	B	1237	X	-	-	-
17	CLA	B	1238	X	-	-	-
17	CLA	B	1239	X	-	-	-
17	CLA	B	1240	X	-	-	-
17	CLA	B	1241	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	1242	X	-	-	-
17	CLA	B	4001	X	-	-	-
17	CLA	F	1229	X	-	-	-
17	CLA	F	1301	X	-	-	-
17	CLA	F	4003	X	-	-	-
17	CLA	F	4004	X	-	-	-
17	CLA	F	4005	X	-	-	-
17	CLA	F	4006	X	-	-	-
17	CLA	G	1233	X	-	-	-
17	CLA	G	1701	X	-	-	-
17	CLA	H	1801	X	-	-	-
17	CLA	J	1101	X	-	-	-
17	CLA	J	1302	X	-	-	-
17	CLA	J	4008	X	-	-	-
17	CLA	K	1401	X	-	-	-
17	CLA	K	1403	X	-	-	-
17	CLA	K	1404	X	-	-	-
17	CLA	L	1501	X	-	-	-
17	CLA	L	1502	X	-	-	-
17	CLA	L	1503	X	-	-	-
17	CLA	L	1504	X	-	-	-
17	CLA	P	5011	X	-	-	-
17	CLA	P	5012	X	-	-	-
17	CLA	P	5013	X	-	-	-
17	CLA	P	5102	X	-	-	-
17	CLA	P	5103	X	-	-	-
17	CLA	P	5104	X	-	-	-
17	CLA	P	5105	X	-	-	-
17	CLA	P	5106	X	-	-	-
17	CLA	P	5107	X	-	-	-
17	CLA	P	5108	X	-	-	-
17	CLA	P	5109	X	-	-	-
17	CLA	P	5110	X	-	-	-
17	CLA	P	5111	X	-	-	-
17	CLA	P	5112	X	-	-	-
17	CLA	P	5113	X	-	-	-
17	CLA	P	5114	X	-	-	-
17	CLA	P	5115	X	-	-	-
17	CLA	P	5116	X	-	-	-
17	CLA	P	5117	X	-	-	-
17	CLA	P	5118	X	-	-	-
17	CLA	P	5119	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	P	5120	X	-	-	-
17	CLA	P	5121	X	-	-	-
17	CLA	P	5122	X	-	-	-
17	CLA	P	5123	X	-	-	-
17	CLA	P	5124	X	-	-	-
17	CLA	P	5125	X	-	-	-
17	CLA	P	5126	X	-	-	-
17	CLA	P	5127	X	-	-	-
17	CLA	P	5128	X	-	-	-
17	CLA	P	5129	X	-	-	-
17	CLA	P	5131	X	-	-	-
17	CLA	P	5132	X	-	-	-
17	CLA	P	5133	X	-	-	-
17	CLA	P	5134	X	-	-	-
17	CLA	P	5135	X	-	-	-
17	CLA	P	5136	X	-	-	-
17	CLA	P	5137	X	-	-	-
17	CLA	P	5138	X	-	-	-
17	CLA	P	5139	X	-	-	-
17	CLA	P	5140	X	-	-	-
17	CLA	P	5402	X	-	-	-
17	CLA	P	5901	X	-	-	-
17	CLA	P	8009	X	-	-	-
17	CLA	P	8010	X	-	-	-
17	CLA	Q	5021	X	-	-	-
17	CLA	Q	5022	X	-	-	-
17	CLA	Q	5023	X	-	-	-
17	CLA	Q	5130	X	-	-	-
17	CLA	Q	5201	X	-	-	-
17	CLA	Q	5202	X	-	-	-
17	CLA	Q	5203	X	-	-	-
17	CLA	Q	5204	X	-	-	-
17	CLA	Q	5205	X	-	-	-
17	CLA	Q	5206	X	-	-	-
17	CLA	Q	5207	X	-	-	-
17	CLA	Q	5208	X	-	-	-
17	CLA	Q	5209	X	-	-	-
17	CLA	Q	5210	X	-	-	-
17	CLA	Q	5211	X	-	-	-
17	CLA	Q	5212	X	-	-	-
17	CLA	Q	5213	X	-	-	-
17	CLA	Q	5214	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	Q	5215	X	-	-	-
17	CLA	Q	5216	X	-	-	-
17	CLA	Q	5217	X	-	-	-
17	CLA	Q	5218	X	-	-	-
17	CLA	Q	5219	X	-	-	-
17	CLA	Q	5220	X	-	-	-
17	CLA	Q	5221	X	-	-	-
17	CLA	Q	5222	X	-	-	-
17	CLA	Q	5223	X	-	-	-
17	CLA	Q	5224	X	-	-	-
17	CLA	Q	5225	X	-	-	-
17	CLA	Q	5226	X	-	-	-
17	CLA	Q	5227	X	-	-	-
17	CLA	Q	5228	X	-	-	-
17	CLA	Q	5230	X	-	-	-
17	CLA	Q	5231	X	-	-	-
17	CLA	Q	5232	X	-	-	-
17	CLA	Q	5234	X	-	-	-
17	CLA	Q	5235	X	-	-	-
17	CLA	Q	5236	X	-	-	-
17	CLA	Q	5237	X	-	-	-
17	CLA	Q	5238	X	-	-	-
17	CLA	Q	5239	X	-	-	-
17	CLA	Q	5240	X	-	-	-
17	CLA	Q	5241	X	-	-	-
17	CLA	Q	5242	X	-	-	-
17	CLA	Q	8001	X	-	-	-
17	CLA	U	5229	X	-	-	-
17	CLA	U	5301	X	-	-	-
17	CLA	U	8003	X	-	-	-
17	CLA	U	8004	X	-	-	-
17	CLA	U	8005	X	-	-	-
17	CLA	U	8006	X	-	-	-
17	CLA	V	5233	X	-	-	-
17	CLA	V	5701	X	-	-	-
17	CLA	W	5801	X	-	-	-
17	CLA	Z	5101	X	-	-	-
17	CLA	Z	5302	X	-	-	-
17	CLA	Z	8008	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 13938 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 PLANT PHOTOSYSTEM I: SUBUNIT PSAA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	726	Total	C	0	0	726
			726	726			
1	P	726	Total	C	0	0	726
			726	726			

- Molecule 2 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAB.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	732	Total	C	0	0	732
			732	732			
2	Q	732	Total	C	0	0	732
			732	732			

- Molecule 3 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAC.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	80	Total	C	0	0	80
			80	80			
3	R	80	Total	C	0	0	80
			80	80			

- Molecule 4 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAD.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	154	Total	C	0	0	154
			154	154			
4	S	154	Total	C	0	0	154
			154	154			

- Molecule 5 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	64	Total C 64 64	0	0	64
5	T	64	Total C 64 64	0	0	64

- Molecule 6 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAF.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	154	Total C 154 154	0	0	154
6	U	154	Total C 154 154	0	0	154

- Molecule 7 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAG.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	74	Total C 74 74	0	0	74
7	V	74	Total C 74 74	0	0	74

- Molecule 8 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAH.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	H	52	Total C 52 52	0	0	52
8	W	52	Total C 52 52	0	0	52

- Molecule 9 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	I	30	Total C 30 30	0	0	30
9	Y	30	Total C 30 30	0	0	30

- Molecule 10 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAJ.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	41	Total C 41 41	0	0	41

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	Z	41	Total C 41 41	0	0	41

- Molecule 11 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAK.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	K	42	Total C 42 42	0	0	42
11	5	42	Total C 42 42	0	0	42

- Molecule 12 is a protein called PLANT PHOTOSYSTEM I: SUBUNIT PSAL.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	L	135	Total C 135 135	0	0	135
12	6	135	Total C 135 135	0	0	135

- Molecule 13 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	1	109	Total C 109 109	0	0	109
13	7	109	Total C 109 109	0	0	109

- Molecule 14 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	2	115	Total C 115 115	0	0	115
14	8	115	Total C 115 115	0	0	115

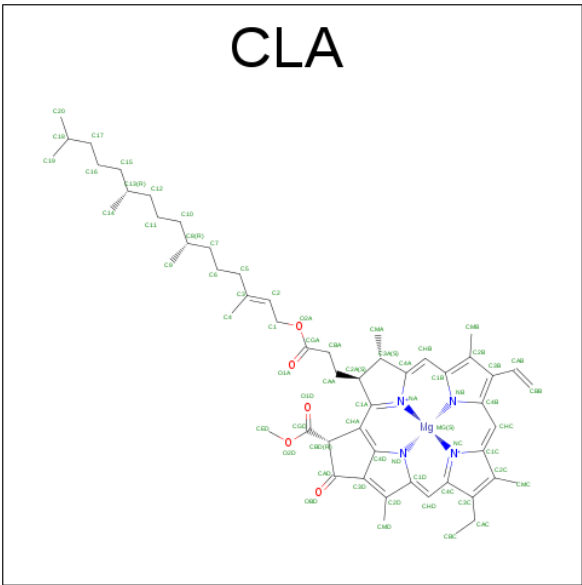
- Molecule 15 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA3.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
15	3	117	Total	C	0	0	117
			117	117			
15	9	117	Total	C	0	0	117
			117	117			

- Molecule 16 is a protein called PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUB-UNIT LHCA4.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
16	4	119	Total	C	0	0	119
			119	119			
16	0	119	Total	C	0	0	119
			119	119			

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	G	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	G	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	H	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	J	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	1	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	2	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	3	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	4	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	5	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	6	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	V	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	W	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Q	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	U	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	Z	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	P	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	7	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		

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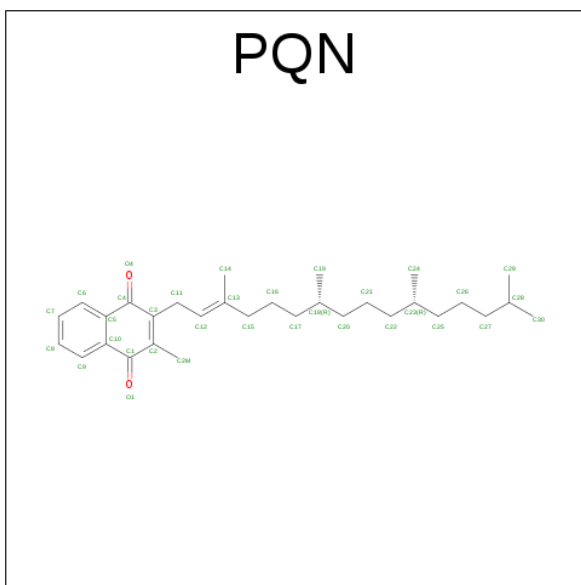
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	8	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	9	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

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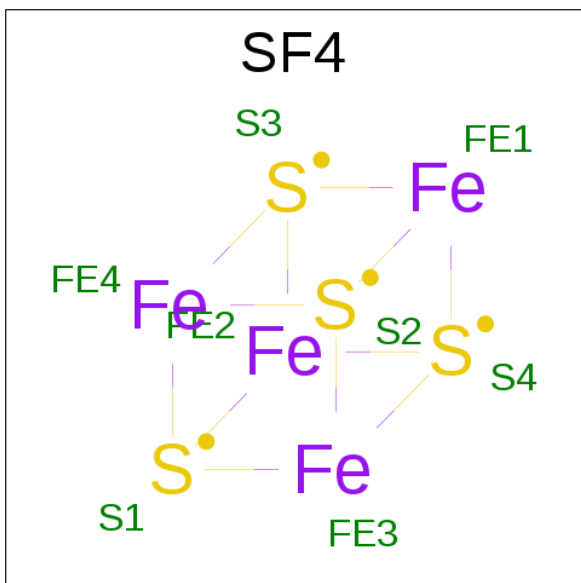
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		
17	0	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			13	11	2		
18	B	1	Total	C	O	0	0
			13	11	2		
18	P	1	Total	C	O	0	0
			13	11	2		
18	Q	1	Total	C	O	0	0
			13	11	2		

- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	C	1	Total 8	Fe 4	S 4	0	0
19	P	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0
19	R	1	Total 8	Fe 4	S 4	0	0

3 Residue-property plots

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.

Note EDS was not executed.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: PLANT PHOTOSYSTEM I: SUBUNIT PSAA

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain B:  100%



- Molecule 2: PLANT PHOTOSYSTEM I: SUBUNIT PSAB

Chain Q:  100%



- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: PLANT PHOTOSYSTEM I: SUBUNIT PSAC

Chain R:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PLANT PHOTOSYSTEM I: SUBUNIT PSAD

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: PLANT PHOTOSYSTEM I: SUBUNIT PSAE

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: PLANT PHOTOSYSTEM I: SUBUNIT PSAF

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: PLANT PHOTOSYSTEM I: SUBUNIT PSAG

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: PLANT PHOTOSYSTEM I: SUBUNIT PSAH

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: PLANT PHOTOSYSTEM I: SUBUNIT PSAI

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: PLANT PHOTOSYSTEM I: SUBUNIT PSAJ

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: PLANT PHOTOSYSTEM I: SUBUNIT PSAK

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: PLANT PHOTOSYSTEM I: SUBUNIT PSAL

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 1:  100%

There are no outlier residues recorded for this chain.

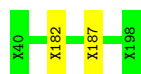
- Molecule 13: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA1

Chain 7:  100%

There are no outlier residues recorded for this chain.

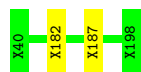
- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 2:  98%



- Molecule 14: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA2

Chain 8:  98%



- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA3

Chain 9:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: PLANT LIGHT HARVESTING COMPLEX I(LHCI): SUBUNIT LHCA4

Chain 0:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	182.28Å 190.38Å 220.25Å 90.00° 90.48° 90.00°	Depositor
Resolution (Å)	50.00 – 4.44	Depositor
% Data completeness (in resolution range)	99.6 (50.00-4.44)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.410 , 0.420	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13938	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

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: SF4, CLA, PQN

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	726	0	0	0	0
1	P	726	0	0	0	0
2	B	732	0	0	1	0
2	Q	732	0	0	1	0
3	C	80	0	0	0	0
3	R	80	0	0	0	0
4	D	154	0	0	0	0
4	S	154	0	0	0	0
5	E	64	0	0	0	0
5	T	64	0	0	0	0
6	F	154	0	0	0	0
6	U	154	0	0	0	0
7	G	74	0	0	0	0
7	V	74	0	0	0	0
8	H	52	0	0	0	0
8	W	52	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	30	0	0	0	0
9	Y	30	0	0	0	0
10	J	41	0	0	0	0
10	Z	41	0	0	0	0
11	5	42	0	0	0	0
11	K	42	0	0	0	0
12	6	135	0	0	0	0
12	L	135	0	0	0	0
13	1	109	0	0	0	0
13	7	109	0	0	0	0
14	2	115	0	0	1	0
14	8	115	0	0	1	0
15	3	117	0	0	0	0
15	9	117	0	0	0	0
16	0	119	0	0	0	0
16	4	119	0	0	0	0
17	0	400	0	48	0	0
17	1	325	0	39	0	0
17	2	375	0	45	0	0
17	3	350	0	42	0	0
17	4	400	0	48	0	0
17	5	75	0	9	0	0
17	6	100	0	12	0	0
17	7	325	0	39	0	0
17	8	375	0	45	0	0
17	9	350	0	42	0	0
17	A	1125	0	135	0	0
17	B	1125	0	135	0	0
17	F	150	0	18	0	0
17	G	50	0	6	0	0
17	H	25	0	3	0	0
17	J	75	0	9	0	0
17	K	75	0	9	0	0
17	L	100	0	12	0	0
17	P	1125	0	135	0	0
17	Q	1125	0	135	0	0
17	U	150	0	18	0	0
17	V	50	0	6	0	0
17	W	25	0	3	0	0
17	Z	75	0	9	0	0
18	A	13	0	7	0	0
18	B	13	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	P	13	0	7	0	0
18	Q	13	0	7	0	0
19	A	8	0	0	0	0
19	C	16	0	0	0	0
19	P	8	0	0	0	0
19	R	16	0	0	0	0
All	All	13938	0	1030	4	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 0.

All (4) 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)
14:8:182:UNK:CA	14:8:187:UNK:CA	2.92	0.48
14:2:182:UNK:CA	14:2:187:UNK:CA	2.92	0.47
2:B:5:UNK:CA	2:B:6:UNK:CA	2.97	0.42
2:Q:5:UNK:CA	2:Q:6:UNK:CA	2.97	0.42

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

344 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$
17	CLA	0	1011	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	0	1012	-	17,32,73	2.14	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	0	1013	-	17,32,73	2.11	4 (23%)	24,54,113	1.69	4 (16%)
17	CLA	0	1014	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	0	1015	-	17,32,73	2.13	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	0	1016	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	0	1017	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	0	1021	-	17,32,73	2.11	4 (23%)	24,54,113	1.68	4 (16%)
17	CLA	0	1022	-	17,32,73	2.13	4 (23%)	24,54,113	1.73	4 (16%)
17	CLA	0	1023	-	17,32,73	2.09	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	0	1025	-	17,32,73	2.11	4 (23%)	24,54,113	1.69	4 (16%)
17	CLA	0	1026	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	0	1031	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	0	1032	-	17,32,73	2.10	4 (23%)	24,54,113	1.73	4 (16%)
17	CLA	0	1033	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	0	8002	-	17,32,73	2.13	4 (23%)	24,54,113	1.73	4 (16%)
17	CLA	1	1011	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	1	1012	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	1	1013	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	1	1014	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	1	1015	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	1	1016	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	1	1017	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	1	1021	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	1	1022	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	1	1023	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	1	1025	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	1	1026	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	1	1031	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	1011	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	2	1012	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	2	1013	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	2	1014	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	2	1015	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	1016	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	2	1017	-	17,32,73	2.13	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	2	1021	-	17,32,73	2.10	4 (23%)	24,54,113	1.69	4 (16%)
17	CLA	2	1022	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	1023	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	1025	-	17,32,73	2.12	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	1026	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	2	1031	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	1033	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	2	4007	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	3	1011	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	3	1012	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	3	1014	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	3	1015	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	3	1016	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	3	1017	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	3	1021	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	3	1022	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	3	1025	-	17,32,73	2.09	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	3	1026	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	3	1031	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	3	1032	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	3	1033	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	3	1041	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	4	1011	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1012	-	17,32,73	2.15	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1013	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	4	1014	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	4	1015	-	17,32,73	2.13	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1016	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1017	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	4	1021	-	17,32,73	2.11	4 (23%)	24,54,113	1.68	4 (16%)
17	CLA	4	1022	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1023	-	17,32,73	2.10	4 (23%)	24,54,113	1.69	4 (16%)
17	CLA	4	1025	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	4	1026	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1031	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1032	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	4	1033	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	4	4002	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	5	5401	-	17,32,73	2.08	4 (23%)	24,54,113	1.54	4 (16%)
17	CLA	5	5403	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	5	5404	-	17,32,73	2.12	4 (23%)	24,54,113	1.73	4 (16%)
17	CLA	6	5501	-	17,32,73	2.10	4 (23%)	24,54,113	1.51	5 (20%)
17	CLA	6	5502	-	17,32,73	2.19	4 (23%)	24,54,113	1.60	3 (12%)
17	CLA	6	5503	-	17,32,73	1.99	4 (23%)	24,54,113	1.52	3 (12%)
17	CLA	6	5504	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	7	1011	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	7	1012	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	7	1013	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	7	1014	-	17,32,73	2.09	4 (23%)	24,54,113	1.69	4 (16%)
17	CLA	7	1015	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	7	1016	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	7	1017	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	7	1021	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	7	1022	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	7	1023	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	7	1025	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	7	1026	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	7	1031	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	8	1011	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	1012	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	8	1013	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	1014	-	17,32,73	2.09	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	8	1015	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	8	1016	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	8	1017	-	17,32,73	2.13	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	1021	-	17,32,73	2.10	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	8	1022	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	1023	-	17,32,73	2.12	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	8	1025	-	17,32,73	2.13	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	8	1026	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	1031	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	1033	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	8	8007	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	9	1011	-	17,32,73	2.13	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	9	1012	-	17,32,73	2.09	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	9	1014	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	9	1015	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	9	1016	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	9	1017	-	17,32,73	2.12	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	9	1021	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	9	1022	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	9	1025	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	9	1026	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	9	1031	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	9	1032	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	9	1033	-	17,32,73	2.10	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	9	1041	-	17,32,73	2.13	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	A	1011	-	17,32,73	1.92	4 (23%)	24,54,113	1.49	4 (16%)
17	CLA	A	1012	-	17,32,73	1.84	3 (17%)	24,54,113	1.80	5 (20%)
17	CLA	A	1013	-	17,32,73	2.15	4 (23%)	24,54,113	1.45	3 (12%)
17	CLA	A	1102	-	17,32,73	1.85	4 (23%)	24,54,113	1.58	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1103	-	17,32,73	1.92	4 (23%)	24,54,113	1.74	4 (16%)
17	CLA	A	1104	-	17,32,73	2.00	5 (29%)	24,54,113	1.74	4 (16%)
17	CLA	A	1105	-	17,32,73	1.98	4 (23%)	24,54,113	1.54	3 (12%)
17	CLA	A	1106	-	17,32,73	2.09	4 (23%)	24,54,113	1.63	4 (16%)
17	CLA	A	1107	-	17,32,73	1.82	4 (23%)	24,54,113	1.66	4 (16%)
17	CLA	A	1108	-	17,32,73	1.92	4 (23%)	24,54,113	2.11	6 (25%)
17	CLA	A	1109	-	17,32,73	2.08	4 (23%)	24,54,113	1.53	3 (12%)
17	CLA	A	1110	-	17,32,73	2.04	4 (23%)	24,54,113	1.75	5 (20%)
17	CLA	A	1111	-	17,32,73	2.07	4 (23%)	24,54,113	1.78	5 (20%)
17	CLA	A	1112	-	17,32,73	2.20	3 (17%)	24,54,113	1.59	4 (16%)
17	CLA	A	1113	-	17,32,73	1.93	4 (23%)	24,54,113	2.26	6 (25%)
17	CLA	A	1114	-	17,32,73	1.96	3 (17%)	24,54,113	1.63	4 (16%)
17	CLA	A	1115	-	17,32,73	2.12	3 (17%)	24,54,113	1.40	3 (12%)
17	CLA	A	1116	-	17,32,73	1.97	3 (17%)	24,54,113	1.68	4 (16%)
17	CLA	A	1117	-	17,32,73	1.76	4 (23%)	24,54,113	1.54	3 (12%)
17	CLA	A	1118	-	17,32,73	2.10	3 (17%)	24,54,113	1.80	4 (16%)
17	CLA	A	1119	-	17,32,73	2.02	3 (17%)	24,54,113	1.55	4 (16%)
17	CLA	A	1120	-	17,32,73	1.97	3 (17%)	24,54,113	1.67	4 (16%)
17	CLA	A	1121	-	17,32,73	2.02	4 (23%)	24,54,113	1.44	3 (12%)
17	CLA	A	1122	-	17,32,73	1.93	4 (23%)	24,54,113	1.62	4 (16%)
17	CLA	A	1123	-	17,32,73	2.02	3 (17%)	24,54,113	1.76	3 (12%)
17	CLA	A	1124	-	17,32,73	1.97	4 (23%)	24,54,113	1.46	4 (16%)
17	CLA	A	1125	-	17,32,73	2.08	3 (17%)	24,54,113	1.81	5 (20%)
17	CLA	A	1126	-	17,32,73	2.05	4 (23%)	24,54,113	1.54	3 (12%)
17	CLA	A	1127	-	17,32,73	1.70	4 (23%)	24,54,113	1.50	3 (12%)
17	CLA	A	1128	-	17,32,73	2.19	4 (23%)	24,54,113	1.55	5 (20%)
17	CLA	A	1129	-	17,32,73	2.07	3 (17%)	24,54,113	1.75	4 (16%)
17	CLA	A	1131	-	17,32,73	1.75	4 (23%)	24,54,113	1.59	4 (16%)
17	CLA	A	1132	-	17,32,73	1.90	4 (23%)	24,54,113	1.57	4 (16%)
17	CLA	A	1133	-	17,32,73	1.81	3 (17%)	24,54,113	1.62	5 (20%)
17	CLA	A	1134	-	17,32,73	2.01	4 (23%)	24,54,113	1.69	4 (16%)
17	CLA	A	1135	-	17,32,73	1.94	5 (29%)	24,54,113	1.68	2 (8%)
17	CLA	A	1136	-	17,32,73	2.24	5 (29%)	24,54,113	1.44	3 (12%)
17	CLA	A	1137	-	17,32,73	2.03	5 (29%)	24,54,113	2.16	6 (25%)
17	CLA	A	1138	-	17,32,73	2.11	3 (17%)	24,54,113	1.64	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	A	1139	-	17,32,73	1.86	4 (23%)	24,54,113	1.52	3 (12%)
17	CLA	A	1140	-	17,32,73	2.00	3 (17%)	24,54,113	1.65	4 (16%)
17	CLA	A	1402	-	17,32,73	2.03	4 (23%)	24,54,113	1.70	3 (12%)
17	CLA	A	1901	-	17,32,73	2.10	4 (23%)	24,54,113	2.44	6 (25%)
18	PQN	A	2001	-	14,14,34	4.39	13 (92%)	20,20,45	0.94	1 (5%)
19	SF4	A	3001	-	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	A	4009	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	A	4010	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	B	1021	-	17,32,73	2.02	4 (23%)	24,54,113	1.59	3 (12%)
17	CLA	B	1022	-	17,32,73	2.06	3 (17%)	24,54,113	1.77	4 (16%)
17	CLA	B	1023	-	17,32,73	2.41	5 (29%)	24,54,113	1.65	4 (16%)
17	CLA	B	1130	-	17,32,73	1.99	4 (23%)	24,54,113	1.66	3 (12%)
17	CLA	B	1201	-	17,32,73	1.99	4 (23%)	24,54,113	1.63	4 (16%)
17	CLA	B	1202	-	17,32,73	1.84	4 (23%)	24,54,113	1.59	1 (4%)
17	CLA	B	1203	-	17,32,73	1.95	4 (23%)	24,54,113	1.55	3 (12%)
17	CLA	B	1204	-	17,32,73	2.21	4 (23%)	24,54,113	1.77	4 (16%)
17	CLA	B	1205	-	17,32,73	2.15	4 (23%)	24,54,113	1.40	3 (12%)
17	CLA	B	1206	-	17,32,73	1.55	4 (23%)	24,54,113	1.72	5 (20%)
17	CLA	B	1207	-	17,32,73	2.16	4 (23%)	24,54,113	1.78	5 (20%)
17	CLA	B	1208	-	17,32,73	2.06	4 (23%)	24,54,113	1.55	4 (16%)
17	CLA	B	1209	-	17,32,73	2.01	3 (17%)	24,54,113	1.63	4 (16%)
17	CLA	B	1210	-	17,32,73	2.08	5 (29%)	24,54,113	1.64	4 (16%)
17	CLA	B	1211	-	17,32,73	1.92	4 (23%)	24,54,113	1.56	4 (16%)
17	CLA	B	1212	-	17,32,73	2.05	3 (17%)	24,54,113	1.58	4 (16%)
17	CLA	B	1213	-	17,32,73	2.00	3 (17%)	24,54,113	1.47	4 (16%)
17	CLA	B	1214	-	17,32,73	2.11	4 (23%)	24,54,113	1.64	4 (16%)
17	CLA	B	1215	-	17,32,73	1.85	4 (23%)	24,54,113	1.56	3 (12%)
17	CLA	B	1216	-	17,32,73	1.97	3 (17%)	24,54,113	1.52	4 (16%)
17	CLA	B	1217	-	17,32,73	1.94	3 (17%)	24,54,113	1.71	4 (16%)
17	CLA	B	1218	-	17,32,73	2.05	3 (17%)	24,54,113	1.73	4 (16%)
17	CLA	B	1219	-	17,32,73	2.14	4 (23%)	24,54,113	2.15	6 (25%)
17	CLA	B	1220	-	17,32,73	2.07	3 (17%)	24,54,113	1.58	4 (16%)
17	CLA	B	1221	-	17,32,73	2.16	4 (23%)	24,54,113	1.84	4 (16%)
17	CLA	B	1222	-	17,32,73	1.89	4 (23%)	24,54,113	1.57	3 (12%)
17	CLA	B	1223	-	17,32,73	1.99	3 (17%)	24,54,113	1.73	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	B	1224	-	17,32,73	1.98	4 (23%)	24,54,113	1.68	4 (16%)
17	CLA	B	1225	-	17,32,73	1.95	4 (23%)	24,54,113	1.38	3 (12%)
17	CLA	B	1226	-	17,32,73	1.78	4 (23%)	24,54,113	1.39	3 (12%)
17	CLA	B	1227	-	17,32,73	1.98	3 (17%)	24,54,113	1.72	5 (20%)
17	CLA	B	1228	-	17,32,73	2.15	3 (17%)	24,54,113	1.73	5 (20%)
17	CLA	B	1230	-	17,32,73	1.89	4 (23%)	24,54,113	1.54	3 (12%)
17	CLA	B	1231	-	17,32,73	2.19	3 (17%)	24,54,113	1.72	4 (16%)
17	CLA	B	1232	-	17,32,73	2.15	3 (17%)	24,54,113	1.68	5 (20%)
17	CLA	B	1234	-	17,32,73	2.00	3 (17%)	24,54,113	1.63	4 (16%)
17	CLA	B	1235	-	17,32,73	2.14	4 (23%)	24,54,113	1.61	5 (20%)
17	CLA	B	1236	-	17,32,73	1.97	4 (23%)	24,54,113	1.50	3 (12%)
17	CLA	B	1237	-	17,32,73	2.02	5 (29%)	24,54,113	1.64	5 (20%)
17	CLA	B	1238	-	17,32,73	1.86	5 (29%)	24,54,113	1.56	5 (20%)
17	CLA	B	1239	-	17,32,73	1.85	4 (23%)	24,54,113	1.60	2 (8%)
17	CLA	B	1240	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	B	1241	-	17,32,73	2.12	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	B	1242	-	17,32,73	2.12	4 (23%)	24,54,113	1.70	4 (16%)
18	PQN	B	2002	-	14,14,34	4.25	12 (85%)	20,20,45	0.99	1 (5%)
17	CLA	B	4001	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
19	SF4	C	3002	-	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	C	3003	-	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	F	1229	-	17,32,73	2.04	4 (23%)	24,54,113	1.64	3 (12%)
17	CLA	F	1301	-	17,32,73	2.09	3 (17%)	24,54,113	1.62	4 (16%)
17	CLA	F	4003	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	F	4004	-	17,32,73	2.11	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	F	4005	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	F	4006	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	G	1233	-	17,32,73	2.02	3 (17%)	24,54,113	1.67	4 (16%)
17	CLA	G	1701	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	H	1801	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	J	1101	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	J	1302	-	17,32,73	2.02	4 (23%)	24,54,113	2.40	6 (25%)
17	CLA	J	4008	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	K	1401	-	17,32,73	2.09	4 (23%)	24,54,113	1.55	4 (16%)
17	CLA	K	1403	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	K	1404	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	L	1501	-	17,32,73	2.10	4 (23%)	24,54,113	1.50	5 (20%)
17	CLA	L	1502	-	17,32,73	2.19	4 (23%)	24,54,113	1.58	3 (12%)
17	CLA	L	1503	-	17,32,73	1.99	4 (23%)	24,54,113	1.51	3 (12%)
17	CLA	L	1504	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	P	5011	-	17,32,73	1.93	4 (23%)	24,54,113	1.49	4 (16%)
17	CLA	P	5012	-	17,32,73	1.84	3 (17%)	24,54,113	1.80	5 (20%)
17	CLA	P	5013	-	17,32,73	2.16	4 (23%)	24,54,113	1.45	4 (16%)
17	CLA	P	5102	-	17,32,73	1.85	4 (23%)	24,54,113	1.58	3 (12%)
17	CLA	P	5103	-	17,32,73	1.92	4 (23%)	24,54,113	1.74	4 (16%)
17	CLA	P	5104	-	17,32,73	2.00	5 (29%)	24,54,113	1.74	5 (20%)
17	CLA	P	5105	-	17,32,73	1.99	4 (23%)	24,54,113	1.53	3 (12%)
17	CLA	P	5106	-	17,32,73	2.09	4 (23%)	24,54,113	1.63	4 (16%)
17	CLA	P	5107	-	17,32,73	1.83	4 (23%)	24,54,113	1.65	4 (16%)
17	CLA	P	5108	-	17,32,73	1.92	4 (23%)	24,54,113	2.11	6 (25%)
17	CLA	P	5109	-	17,32,73	2.07	4 (23%)	24,54,113	1.54	3 (12%)
17	CLA	P	5110	-	17,32,73	2.03	4 (23%)	24,54,113	1.76	5 (20%)
17	CLA	P	5111	-	17,32,73	2.08	4 (23%)	24,54,113	1.78	5 (20%)
17	CLA	P	5112	-	17,32,73	2.21	3 (17%)	24,54,113	1.58	4 (16%)
17	CLA	P	5113	-	17,32,73	1.94	4 (23%)	24,54,113	2.26	6 (25%)
17	CLA	P	5114	-	17,32,73	1.96	3 (17%)	24,54,113	1.62	4 (16%)
17	CLA	P	5115	-	17,32,73	2.12	3 (17%)	24,54,113	1.40	3 (12%)
17	CLA	P	5116	-	17,32,73	1.96	3 (17%)	24,54,113	1.68	4 (16%)
17	CLA	P	5117	-	17,32,73	1.75	4 (23%)	24,54,113	1.54	3 (12%)
17	CLA	P	5118	-	17,32,73	2.09	3 (17%)	24,54,113	1.80	4 (16%)
17	CLA	P	5119	-	17,32,73	2.02	3 (17%)	24,54,113	1.55	4 (16%)
17	CLA	P	5120	-	17,32,73	1.97	3 (17%)	24,54,113	1.67	4 (16%)
17	CLA	P	5121	-	17,32,73	2.02	4 (23%)	24,54,113	1.45	3 (12%)
17	CLA	P	5122	-	17,32,73	1.94	4 (23%)	24,54,113	1.62	4 (16%)
17	CLA	P	5123	-	17,32,73	2.02	3 (17%)	24,54,113	1.77	3 (12%)
17	CLA	P	5124	-	17,32,73	1.97	4 (23%)	24,54,113	1.47	4 (16%)
17	CLA	P	5125	-	17,32,73	2.09	3 (17%)	24,54,113	1.82	5 (20%)
17	CLA	P	5126	-	17,32,73	2.05	5 (29%)	24,54,113	1.55	3 (12%)
17	CLA	P	5127	-	17,32,73	1.70	4 (23%)	24,54,113	1.51	3 (12%)
17	CLA	P	5128	-	17,32,73	2.19	4 (23%)	24,54,113	1.56	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	P	5129	-	17,32,73	2.07	3 (17%)	24,54,113	1.75	4 (16%)
17	CLA	P	5131	-	17,32,73	1.74	4 (23%)	24,54,113	1.59	4 (16%)
17	CLA	P	5132	-	17,32,73	1.89	4 (23%)	24,54,113	1.57	4 (16%)
17	CLA	P	5133	-	17,32,73	1.81	3 (17%)	24,54,113	1.62	5 (20%)
17	CLA	P	5134	-	17,32,73	2.01	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	P	5135	-	17,32,73	1.94	5 (29%)	24,54,113	1.67	2 (8%)
17	CLA	P	5136	-	17,32,73	2.25	5 (29%)	24,54,113	1.44	3 (12%)
17	CLA	P	5137	-	17,32,73	2.04	5 (29%)	24,54,113	2.17	6 (25%)
17	CLA	P	5138	-	17,32,73	2.11	3 (17%)	24,54,113	1.64	4 (16%)
17	CLA	P	5139	-	17,32,73	1.87	4 (23%)	24,54,113	1.52	3 (12%)
17	CLA	P	5140	-	17,32,73	2.00	3 (17%)	24,54,113	1.65	4 (16%)
17	CLA	P	5402	-	17,32,73	2.03	4 (23%)	24,54,113	1.70	3 (12%)
17	CLA	P	5901	-	17,32,73	2.10	4 (23%)	24,54,113	2.43	6 (25%)
18	PQN	P	6001	-	14,14,34	4.38	13 (92%)	20,20,45	0.94	1 (5%)
19	SF4	P	7001	-	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	P	8009	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	P	8010	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	Q	5021	-	17,32,73	2.01	4 (23%)	24,54,113	1.58	3 (12%)
17	CLA	Q	5022	-	17,32,73	2.06	3 (17%)	24,54,113	1.77	4 (16%)
17	CLA	Q	5023	-	17,32,73	2.41	5 (29%)	24,54,113	1.66	5 (20%)
17	CLA	Q	5130	-	17,32,73	2.00	4 (23%)	24,54,113	1.66	3 (12%)
17	CLA	Q	5201	-	17,32,73	1.98	4 (23%)	24,54,113	1.63	4 (16%)
17	CLA	Q	5202	-	17,32,73	1.84	4 (23%)	24,54,113	1.59	1 (4%)
17	CLA	Q	5203	-	17,32,73	1.97	4 (23%)	24,54,113	1.56	3 (12%)
17	CLA	Q	5204	-	17,32,73	2.20	4 (23%)	24,54,113	1.77	4 (16%)
17	CLA	Q	5205	-	17,32,73	2.15	4 (23%)	24,54,113	1.40	3 (12%)
17	CLA	Q	5206	-	17,32,73	1.56	4 (23%)	24,54,113	1.72	5 (20%)
17	CLA	Q	5207	-	17,32,73	2.17	4 (23%)	24,54,113	1.79	5 (20%)
17	CLA	Q	5208	-	17,32,73	2.05	4 (23%)	24,54,113	1.55	4 (16%)
17	CLA	Q	5209	-	17,32,73	2.00	3 (17%)	24,54,113	1.63	4 (16%)
17	CLA	Q	5210	-	17,32,73	2.08	5 (29%)	24,54,113	1.63	4 (16%)
17	CLA	Q	5211	-	17,32,73	1.92	4 (23%)	24,54,113	1.57	4 (16%)
17	CLA	Q	5212	-	17,32,73	2.06	3 (17%)	24,54,113	1.60	4 (16%)
17	CLA	Q	5213	-	17,32,73	2.01	3 (17%)	24,54,113	1.47	4 (16%)
17	CLA	Q	5214	-	17,32,73	2.11	4 (23%)	24,54,113	1.64	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	Q	5215	-	17,32,73	1.85	4 (23%)	24,54,113	1.57	3 (12%)
17	CLA	Q	5216	-	17,32,73	1.97	3 (17%)	24,54,113	1.52	4 (16%)
17	CLA	Q	5217	-	17,32,73	1.94	3 (17%)	24,54,113	1.70	4 (16%)
17	CLA	Q	5218	-	17,32,73	2.05	3 (17%)	24,54,113	1.72	4 (16%)
17	CLA	Q	5219	-	17,32,73	2.14	4 (23%)	24,54,113	2.15	5 (20%)
17	CLA	Q	5220	-	17,32,73	2.08	4 (23%)	24,54,113	1.59	4 (16%)
17	CLA	Q	5221	-	17,32,73	2.15	4 (23%)	24,54,113	1.84	4 (16%)
17	CLA	Q	5222	-	17,32,73	1.90	4 (23%)	24,54,113	1.57	3 (12%)
17	CLA	Q	5223	-	17,32,73	2.00	3 (17%)	24,54,113	1.74	5 (20%)
17	CLA	Q	5224	-	17,32,73	1.98	4 (23%)	24,54,113	1.67	4 (16%)
17	CLA	Q	5225	-	17,32,73	1.95	4 (23%)	24,54,113	1.39	3 (12%)
17	CLA	Q	5226	-	17,32,73	1.78	4 (23%)	24,54,113	1.38	3 (12%)
17	CLA	Q	5227	-	17,32,73	1.98	3 (17%)	24,54,113	1.72	5 (20%)
17	CLA	Q	5228	-	17,32,73	2.17	3 (17%)	24,54,113	1.73	5 (20%)
17	CLA	Q	5230	-	17,32,73	1.89	4 (23%)	24,54,113	1.54	4 (16%)
17	CLA	Q	5231	-	17,32,73	2.18	3 (17%)	24,54,113	1.70	4 (16%)
17	CLA	Q	5232	-	17,32,73	2.14	3 (17%)	24,54,113	1.68	5 (20%)
17	CLA	Q	5234	-	17,32,73	2.00	3 (17%)	24,54,113	1.63	4 (16%)
17	CLA	Q	5235	-	17,32,73	2.14	4 (23%)	24,54,113	1.60	5 (20%)
17	CLA	Q	5236	-	17,32,73	1.97	4 (23%)	24,54,113	1.51	3 (12%)
17	CLA	Q	5237	-	17,32,73	2.02	5 (29%)	24,54,113	1.65	5 (20%)
17	CLA	Q	5238	-	17,32,73	1.86	5 (29%)	24,54,113	1.57	5 (20%)
17	CLA	Q	5239	-	17,32,73	1.84	4 (23%)	24,54,113	1.60	2 (8%)
17	CLA	Q	5240	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	Q	5241	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	Q	5242	-	17,32,73	2.11	4 (23%)	24,54,113	1.69	4 (16%)
18	PQN	Q	6002	-	14,14,34	4.25	12 (85%)	20,20,45	1.00	1 (5%)
17	CLA	Q	8001	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
19	SF4	R	7002	-	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	R	7003	-	0,12,12	0.00	-	0,24,24	0.00	-
17	CLA	U	5229	-	17,32,73	2.04	4 (23%)	24,54,113	1.66	3 (12%)
17	CLA	U	5301	-	17,32,73	2.08	3 (17%)	24,54,113	1.62	4 (16%)
17	CLA	U	8003	-	17,32,73	2.09	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	U	8004	-	17,32,73	2.11	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	U	8005	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CLA	U	8006	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	V	5233	-	17,32,73	2.02	3 (17%)	24,54,113	1.67	4 (16%)
17	CLA	V	5701	-	17,32,73	2.12	4 (23%)	24,54,113	1.72	4 (16%)
17	CLA	W	5801	-	17,32,73	2.11	4 (23%)	24,54,113	1.70	4 (16%)
17	CLA	Z	5101	-	17,32,73	2.10	4 (23%)	24,54,113	1.71	4 (16%)
17	CLA	Z	5302	-	17,32,73	2.02	4 (23%)	24,54,113	2.40	6 (25%)
17	CLA	Z	8008	-	17,32,73	2.12	4 (23%)	24,54,113	1.71	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	0	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1013	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1023	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1032	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	1033	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	0	8002	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1013	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1016	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	1	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1023	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	1	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1013	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1023	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	1033	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	2	4007	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1032	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	1033	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	3	1041	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1013	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1023	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1032	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	1033	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	4	4002	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	5	5401	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	5	5403	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	5	5404	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	6	5501	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	6	5502	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	6	5503	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	6	5504	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1013	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1022	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	7	1023	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	7	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1013	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1023	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	1033	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	8	8007	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1011	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1012	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1014	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1016	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1017	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1021	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1022	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1025	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1026	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1031	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1032	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1033	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	9	1041	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1011	-	2/2/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1012	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1013	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1102	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1103	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1104	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1105	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1106	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1107	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1108	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1109	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1110	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1111	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1112	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1113	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1114	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1115	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1116	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1117	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1118	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1119	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1120	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1121	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1122	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1123	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1124	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1125	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1126	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1127	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1128	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1129	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1131	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1132	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1133	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1134	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1135	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	1136	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1137	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1138	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1139	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1140	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1402	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	1901	-	3/3/7/25	0/0/66/135	0/0/8/9
18	PQN	A	2001	-	-	0/0/16/43	0/2/2/2
19	SF4	A	3001	-	-	0/0/48/48	0/6/5/5
17	CLA	A	4009	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	A	4010	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1021	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1022	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1023	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1130	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1201	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1202	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1203	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1204	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1205	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1206	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1207	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1208	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1209	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1210	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1211	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1212	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1213	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1214	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1215	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1216	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1217	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1218	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1219	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1220	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	1221	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1222	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1223	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1224	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1225	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1226	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1227	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1228	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1230	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1231	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1232	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1234	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1235	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1236	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1237	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1238	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1239	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1240	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1241	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	B	1242	-	3/3/7/25	0/0/66/135	0/0/8/9
18	PQN	B	2002	-	-	0/0/16/43	0/2/2/2
17	CLA	B	4001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	SF4	C	3002	-	-	0/0/48/48	0/6/5/5
19	SF4	C	3003	-	-	0/0/48/48	0/6/5/5
17	CLA	F	1229	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	F	1301	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	F	4003	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	F	4004	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	F	4005	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	F	4006	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	G	1233	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	G	1701	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	H	1801	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	J	1101	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	J	1302	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	J	4008	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	K	1401	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	K	1403	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	K	1404	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	L	1501	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	L	1502	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	L	1503	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	L	1504	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5011	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5012	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5013	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5102	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5103	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5104	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5105	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5106	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5107	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5108	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5109	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5110	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5111	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5112	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5113	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5114	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5115	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5116	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5117	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5118	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5119	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5120	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5121	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5122	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5123	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5124	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	P	5125	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5126	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5127	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5128	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5129	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5131	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5132	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5133	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5134	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5135	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5136	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5137	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5138	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5139	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5140	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5402	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	5901	-	3/3/7/25	0/0/66/135	0/0/8/9
18	PQN	P	6001	-	-	0/0/16/43	0/2/2/2
19	SF4	P	7001	-	-	0/0/48/48	0/6/5/5
17	CLA	P	8009	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	P	8010	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5021	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5022	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5023	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5130	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5201	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5202	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5203	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5204	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5205	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5206	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5207	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5208	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5209	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5210	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5211	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	Q	5212	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5213	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5214	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5215	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5216	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5217	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5218	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5219	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5220	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5221	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5222	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5223	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5224	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5225	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5226	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5227	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5228	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5230	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5231	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5232	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5234	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5235	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5236	-	1/1/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5237	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5238	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5239	-	2/2/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5240	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5241	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Q	5242	-	3/3/7/25	0/0/66/135	0/0/8/9
18	PQN	Q	6002	-	-	0/0/16/43	0/2/2/2
17	CLA	Q	8001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	SF4	R	7002	-	-	0/0/48/48	0/6/5/5
19	SF4	R	7003	-	-	0/0/48/48	0/6/5/5
17	CLA	U	5229	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	U	5301	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	U	8003	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	U	8004	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	U	8005	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	U	8006	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	V	5233	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	V	5701	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	W	5801	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Z	5101	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Z	5302	-	3/3/7/25	0/0/66/135	0/0/8/9
17	CLA	Z	8008	-	3/3/7/25	0/0/66/135	0/0/8/9

All (1344) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5228	CLA	C1B-CHB	-5.31	1.32	1.43
18	A	2001	PQN	C2M-C2	-5.30	1.36	1.50
18	P	6001	PQN	C2M-C2	-5.30	1.36	1.50
17	B	1228	CLA	C1B-CHB	-5.29	1.32	1.43
17	Q	5205	CLA	C1B-CHB	-5.28	1.32	1.43
17	B	1205	CLA	C1B-CHB	-5.28	1.32	1.43
17	P	5013	CLA	C1B-CHB	-5.20	1.33	1.43
17	A	1013	CLA	C1B-CHB	-5.18	1.33	1.43
17	A	1129	CLA	C1B-CHB	-5.16	1.33	1.43
17	P	5129	CLA	C1B-CHB	-5.15	1.33	1.43
17	A	1119	CLA	C1B-CHB	-5.14	1.33	1.43
17	P	5119	CLA	C1B-CHB	-5.13	1.33	1.43
17	Q	5023	CLA	C1B-CHB	-5.10	1.33	1.43
17	B	1023	CLA	C1B-CHB	-5.10	1.33	1.43
18	Q	6002	PQN	C2M-C2	-5.09	1.37	1.50
18	B	2002	PQN	C2M-C2	-5.09	1.37	1.50
17	Q	5204	CLA	C1B-CHB	-5.07	1.33	1.43
17	B	1204	CLA	C1B-CHB	-5.07	1.33	1.43
17	P	5124	CLA	C1B-CHB	-5.03	1.33	1.43
17	A	1124	CLA	C1B-CHB	-5.02	1.33	1.43
17	L	1502	CLA	C1B-CHB	-5.01	1.33	1.43
17	6	5502	CLA	C1B-CHB	-5.00	1.33	1.43
17	A	1138	CLA	C1B-CHB	-4.98	1.33	1.43
17	B	1021	CLA	C1B-CHB	-4.97	1.33	1.43
17	P	5138	CLA	C1B-CHB	-4.97	1.33	1.43
17	4	1012	CLA	C1B-CHB	-4.97	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1214	CLA	C1B-CHB	-4.96	1.33	1.43
17	Q	5021	CLA	C1B-CHB	-4.95	1.33	1.43
17	0	1012	CLA	C1B-CHB	-4.94	1.33	1.43
17	Q	5214	CLA	C1B-CHB	-4.94	1.33	1.43
17	B	1208	CLA	C1B-CHB	-4.93	1.33	1.43
17	9	1011	CLA	C1B-CHB	-4.93	1.33	1.43
17	Q	5208	CLA	C1B-CHB	-4.92	1.33	1.43
17	9	1017	CLA	C1B-CHB	-4.92	1.33	1.43
17	B	1221	CLA	C1B-CHB	-4.92	1.33	1.43
17	0	8002	CLA	C1B-CHB	-4.91	1.33	1.43
17	3	1011	CLA	C1B-CHB	-4.91	1.33	1.43
17	P	8009	CLA	C1B-CHB	-4.91	1.33	1.43
17	4	4002	CLA	C1B-CHB	-4.90	1.33	1.43
17	0	1015	CLA	C1B-CHB	-4.90	1.33	1.43
17	0	1031	CLA	C1B-CHB	-4.90	1.33	1.43
17	V	5701	CLA	C1B-CHB	-4.90	1.33	1.43
17	P	5115	CLA	C1B-CHB	-4.89	1.33	1.43
17	A	4009	CLA	C1B-CHB	-4.89	1.33	1.43
17	7	1012	CLA	C1B-CHB	-4.89	1.33	1.43
17	3	1017	CLA	C1B-CHB	-4.89	1.33	1.43
17	2	1015	CLA	C1B-CHB	-4.89	1.33	1.43
17	A	1106	CLA	C1B-CHB	-4.89	1.33	1.43
17	8	1025	CLA	C1B-CHB	-4.88	1.33	1.43
17	8	1011	CLA	C1B-CHB	-4.88	1.33	1.43
17	Q	5236	CLA	C1B-CHB	-4.88	1.33	1.43
17	4	1015	CLA	C1B-CHB	-4.88	1.33	1.43
17	1	1016	CLA	C1B-CHB	-4.88	1.33	1.43
17	Q	5221	CLA	C1B-CHB	-4.88	1.33	1.43
17	P	5106	CLA	C1B-CHB	-4.88	1.33	1.43
17	1	1026	CLA	C1B-CHB	-4.88	1.33	1.43
17	9	1041	CLA	C1B-CHB	-4.88	1.33	1.43
17	3	1014	CLA	C1B-CHB	-4.88	1.33	1.43
17	2	1025	CLA	C1B-CHB	-4.88	1.33	1.43
17	2	1011	CLA	C1B-CHB	-4.88	1.33	1.43
17	9	1032	CLA	C1B-CHB	-4.88	1.33	1.43
17	P	5112	CLA	C1B-CHB	-4.88	1.33	1.43
17	A	1115	CLA	C1B-CHB	-4.88	1.33	1.43
17	B	4001	CLA	C1B-CHB	-4.88	1.33	1.43
17	Q	8001	CLA	C1B-CHB	-4.88	1.33	1.43
17	0	1013	CLA	C1B-CHB	-4.88	1.33	1.43
17	G	1701	CLA	C1B-CHB	-4.87	1.33	1.43
17	8	1031	CLA	C1B-CHB	-4.87	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1041	CLA	C1B-CHB	-4.87	1.33	1.43
17	B	1236	CLA	C1B-CHB	-4.87	1.33	1.43
17	2	1031	CLA	C1B-CHB	-4.87	1.33	1.43
17	7	1016	CLA	C1B-CHB	-4.87	1.33	1.43
17	8	1015	CLA	C1B-CHB	-4.87	1.33	1.43
17	1	1025	CLA	C1B-CHB	-4.87	1.33	1.43
17	Q	5235	CLA	C1B-CHB	-4.87	1.33	1.43
17	B	1241	CLA	C1B-CHB	-4.87	1.33	1.43
17	8	1026	CLA	C1B-CHB	-4.87	1.33	1.43
17	J	4008	CLA	C1B-CHB	-4.87	1.33	1.43
17	Q	5240	CLA	C1B-CHB	-4.87	1.33	1.43
17	0	1025	CLA	C1B-CHB	-4.87	1.33	1.43
17	4	1031	CLA	C1B-CHB	-4.86	1.33	1.43
17	B	1235	CLA	C1B-CHB	-4.86	1.33	1.43
17	0	1016	CLA	C1B-CHB	-4.86	1.33	1.43
17	3	1032	CLA	C1B-CHB	-4.86	1.33	1.43
17	2	1033	CLA	C1B-CHB	-4.86	1.33	1.43
17	4	1025	CLA	C1B-CHB	-4.86	1.33	1.43
17	P	8010	CLA	C1B-CHB	-4.86	1.33	1.43
17	2	1026	CLA	C1B-CHB	-4.86	1.33	1.43
17	4	1011	CLA	C1B-CHB	-4.86	1.33	1.43
17	4	1016	CLA	C1B-CHB	-4.86	1.33	1.43
17	Z	8008	CLA	C1B-CHB	-4.86	1.33	1.43
17	B	1210	CLA	C1B-CHB	-4.86	1.33	1.43
17	8	1033	CLA	C1B-CHB	-4.86	1.33	1.43
17	4	1033	CLA	C1B-CHB	-4.86	1.33	1.43
17	4	1017	CLA	C1B-CHB	-4.86	1.33	1.43
17	5	5404	CLA	C1B-CHB	-4.86	1.33	1.43
17	3	1021	CLA	C1B-CHB	-4.86	1.33	1.43
17	4	1026	CLA	C1B-CHB	-4.86	1.33	1.43
17	0	1014	CLA	C1B-CHB	-4.86	1.33	1.43
17	8	1017	CLA	C1B-CHB	-4.86	1.33	1.43
17	3	1026	CLA	C1B-CHB	-4.86	1.33	1.43
17	A	4010	CLA	C1B-CHB	-4.86	1.33	1.43
17	2	1012	CLA	C1B-CHB	-4.86	1.33	1.43
17	B	1240	CLA	C1B-CHB	-4.86	1.33	1.43
17	U	8003	CLA	C1B-CHB	-4.86	1.33	1.43
17	0	1033	CLA	C1B-CHB	-4.86	1.33	1.43
17	7	1025	CLA	C1B-CHB	-4.85	1.33	1.43
17	8	1023	CLA	C1B-CHB	-4.85	1.33	1.43
17	A	1112	CLA	C1B-CHB	-4.85	1.33	1.43
17	F	4003	CLA	C1B-CHB	-4.85	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1021	CLA	C1B-CHB	-4.85	1.33	1.43
17	7	1026	CLA	C1B-CHB	-4.85	1.33	1.43
17	9	1026	CLA	C1B-CHB	-4.85	1.33	1.43
17	9	1014	CLA	C1B-CHB	-4.85	1.33	1.43
17	U	8004	CLA	C1B-CHB	-4.85	1.33	1.43
17	K	1404	CLA	C1B-CHB	-4.85	1.33	1.43
17	Q	5210	CLA	C1B-CHB	-4.85	1.33	1.43
17	9	1022	CLA	C1B-CHB	-4.85	1.33	1.43
17	F	4004	CLA	C1B-CHB	-4.85	1.33	1.43
17	L	1504	CLA	C1B-CHB	-4.85	1.33	1.43
17	3	1022	CLA	C1B-CHB	-4.85	1.33	1.43
17	2	1017	CLA	C1B-CHB	-4.85	1.33	1.43
17	U	8005	CLA	C1B-CHB	-4.85	1.33	1.43
17	9	1031	CLA	C1B-CHB	-4.85	1.33	1.43
17	Q	5241	CLA	C1B-CHB	-4.85	1.33	1.43
17	4	1022	CLA	C1B-CHB	-4.85	1.33	1.43
17	U	8006	CLA	C1B-CHB	-4.85	1.33	1.43
17	J	1101	CLA	C1B-CHB	-4.84	1.33	1.43
17	7	1023	CLA	C1B-CHB	-4.84	1.33	1.43
17	2	1023	CLA	C1B-CHB	-4.84	1.33	1.43
17	F	4006	CLA	C1B-CHB	-4.84	1.33	1.43
17	4	1014	CLA	C1B-CHB	-4.84	1.33	1.43
17	1	1023	CLA	C1B-CHB	-4.84	1.33	1.43
17	H	1801	CLA	C1B-CHB	-4.84	1.33	1.43
17	W	5801	CLA	C1B-CHB	-4.84	1.33	1.43
17	4	1013	CLA	C1B-CHB	-4.84	1.33	1.43
17	1	1012	CLA	C1B-CHB	-4.84	1.33	1.43
17	1	1022	CLA	C1B-CHB	-4.84	1.33	1.43
17	0	1022	CLA	C1B-CHB	-4.84	1.33	1.43
17	0	1011	CLA	C1B-CHB	-4.84	1.33	1.43
17	0	1026	CLA	C1B-CHB	-4.84	1.33	1.43
17	F	4005	CLA	C1B-CHB	-4.84	1.33	1.43
17	9	1025	CLA	C1B-CHB	-4.84	1.33	1.43
17	4	1021	CLA	C1B-CHB	-4.84	1.33	1.43
17	2	1013	CLA	C1B-CHB	-4.84	1.33	1.43
17	1	1011	CLA	C1B-CHB	-4.83	1.33	1.43
17	1	1021	CLA	C1B-CHB	-4.83	1.33	1.43
17	B	1242	CLA	C1B-CHB	-4.83	1.33	1.43
17	2	1016	CLA	C1B-CHB	-4.83	1.33	1.43
17	7	1021	CLA	C1B-CHB	-4.83	1.33	1.43
17	8	1022	CLA	C1B-CHB	-4.83	1.33	1.43
17	0	1017	CLA	C1B-CHB	-4.83	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	1017	CLA	C1B-CHB	-4.83	1.33	1.43
17	7	1013	CLA	C1B-CHB	-4.82	1.33	1.43
17	1	1014	CLA	C1B-CHB	-4.82	1.33	1.43
17	4	1023	CLA	C1B-CHB	-4.82	1.33	1.43
17	1	1013	CLA	C1B-CHB	-4.82	1.33	1.43
17	8	1012	CLA	C1B-CHB	-4.82	1.33	1.43
17	9	1016	CLA	C1B-CHB	-4.82	1.33	1.43
17	7	1022	CLA	C1B-CHB	-4.82	1.33	1.43
17	3	1031	CLA	C1B-CHB	-4.82	1.33	1.43
17	4	1032	CLA	C1B-CHB	-4.82	1.33	1.43
17	3	1016	CLA	C1B-CHB	-4.82	1.33	1.43
17	2	1014	CLA	C1B-CHB	-4.82	1.33	1.43
17	3	1025	CLA	C1B-CHB	-4.82	1.33	1.43
17	6	5504	CLA	C1B-CHB	-4.82	1.33	1.43
17	3	1015	CLA	C1B-CHB	-4.82	1.33	1.43
17	3	1033	CLA	C1B-CHB	-4.81	1.33	1.43
17	0	1023	CLA	C1B-CHB	-4.81	1.33	1.43
17	1	1031	CLA	C1B-CHB	-4.81	1.33	1.43
17	8	1013	CLA	C1B-CHB	-4.81	1.33	1.43
17	1	1017	CLA	C1B-CHB	-4.81	1.33	1.43
17	2	1021	CLA	C1B-CHB	-4.81	1.33	1.43
17	0	1021	CLA	C1B-CHB	-4.81	1.33	1.43
17	K	1403	CLA	C1B-CHB	-4.81	1.33	1.43
17	8	1016	CLA	C1B-CHB	-4.81	1.33	1.43
17	8	1021	CLA	C1B-CHB	-4.81	1.33	1.43
17	Z	5101	CLA	C1B-CHB	-4.81	1.33	1.43
17	Q	5242	CLA	C1B-CHB	-4.81	1.33	1.43
17	7	1011	CLA	C1B-CHB	-4.81	1.33	1.43
17	9	1033	CLA	C1B-CHB	-4.80	1.33	1.43
17	8	8007	CLA	C1B-CHB	-4.80	1.33	1.43
17	2	1022	CLA	C1B-CHB	-4.80	1.33	1.43
17	1	1015	CLA	C1B-CHB	-4.80	1.33	1.43
17	5	5403	CLA	C1B-CHB	-4.80	1.33	1.43
17	7	1014	CLA	C1B-CHB	-4.80	1.33	1.43
17	3	1012	CLA	C1B-CHB	-4.80	1.33	1.43
17	9	1015	CLA	C1B-CHB	-4.80	1.33	1.43
17	9	1012	CLA	C1B-CHB	-4.79	1.33	1.43
17	B	1227	CLA	C1B-CHB	-4.79	1.33	1.43
17	8	1014	CLA	C1B-CHB	-4.79	1.33	1.43
17	A	1103	CLA	C1B-CHB	-4.79	1.33	1.43
17	0	1032	CLA	C1B-CHB	-4.78	1.33	1.43
17	7	1031	CLA	C1B-CHB	-4.78	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5103	CLA	C1B-CHB	-4.78	1.33	1.43
17	2	4007	CLA	C1B-CHB	-4.77	1.33	1.43
17	7	1015	CLA	C1B-CHB	-4.77	1.33	1.43
17	P	5136	CLA	C1B-CHB	-4.76	1.34	1.43
17	B	1232	CLA	C1B-CHB	-4.76	1.34	1.43
17	B	1231	CLA	C1B-CHB	-4.76	1.34	1.43
17	Q	5227	CLA	C1B-CHB	-4.76	1.34	1.43
17	Q	5232	CLA	C1B-CHB	-4.76	1.34	1.43
17	A	1132	CLA	C1B-CHB	-4.76	1.34	1.43
17	P	5132	CLA	C1B-CHB	-4.74	1.34	1.43
17	A	1136	CLA	C1B-CHB	-4.74	1.34	1.43
17	Q	5231	CLA	C1B-CHB	-4.74	1.34	1.43
17	P	5122	CLA	C1B-CHB	-4.72	1.34	1.43
17	Q	5211	CLA	C1B-CHB	-4.72	1.34	1.43
17	P	5111	CLA	C1B-CHB	-4.71	1.34	1.43
17	A	1111	CLA	C1B-CHB	-4.71	1.34	1.43
17	Q	5216	CLA	C1B-CHB	-4.70	1.34	1.43
17	A	1122	CLA	C1B-CHB	-4.70	1.34	1.43
17	B	1216	CLA	C1B-CHB	-4.69	1.34	1.43
17	B	1211	CLA	C1B-CHB	-4.69	1.34	1.43
17	K	1401	CLA	C1B-CHB	-4.68	1.34	1.43
17	P	5109	CLA	C1B-CHB	-4.68	1.34	1.43
17	A	1109	CLA	C1B-CHB	-4.67	1.34	1.43
17	P	5126	CLA	C1B-CHB	-4.66	1.34	1.43
17	5	5401	CLA	C1B-CHB	-4.66	1.34	1.43
17	A	1126	CLA	C1B-CHB	-4.64	1.34	1.43
17	Q	5212	CLA	C1B-CHB	-4.63	1.34	1.43
17	A	1901	CLA	C1B-CHB	-4.61	1.34	1.43
17	A	1114	CLA	C1B-CHB	-4.59	1.34	1.43
17	B	1212	CLA	C1B-CHB	-4.59	1.34	1.43
17	P	5901	CLA	C1B-CHB	-4.59	1.34	1.43
17	P	5114	CLA	C1B-CHB	-4.58	1.34	1.43
17	Q	5022	CLA	C1B-CHB	-4.56	1.34	1.43
17	B	1237	CLA	C1B-CHB	-4.55	1.34	1.43
17	B	1022	CLA	C1B-CHB	-4.54	1.34	1.43
17	U	5229	CLA	C1B-CHB	-4.53	1.34	1.43
17	Q	5237	CLA	C1B-CHB	-4.52	1.34	1.43
17	F	1229	CLA	C1B-CHB	-4.50	1.34	1.43
17	Q	5225	CLA	C1B-CHB	-4.50	1.34	1.43
17	P	5121	CLA	C1B-CHB	-4.48	1.34	1.43
17	A	1121	CLA	C1B-CHB	-4.47	1.34	1.43
17	P	5120	CLA	C1B-CHB	-4.47	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1225	CLA	C1B-CHB	-4.46	1.34	1.43
17	A	1120	CLA	C1B-CHB	-4.46	1.34	1.43
17	A	1108	CLA	C1B-CHB	-4.45	1.34	1.43
17	P	5107	CLA	C1B-CHB	-4.45	1.34	1.43
17	B	1213	CLA	C1B-CHB	-4.45	1.34	1.43
17	A	1110	CLA	C1B-CHB	-4.44	1.34	1.43
17	P	5110	CLA	C1B-CHB	-4.44	1.34	1.43
17	A	1107	CLA	C1B-CHB	-4.44	1.34	1.43
17	Q	5213	CLA	C1B-CHB	-4.44	1.34	1.43
17	P	5108	CLA	C1B-CHB	-4.43	1.34	1.43
17	B	1201	CLA	C1B-CHB	-4.40	1.34	1.43
17	B	1207	CLA	C1B-CHB	-4.40	1.34	1.43
17	Q	5220	CLA	C1B-CHB	-4.40	1.34	1.43
17	Q	5207	CLA	C1B-CHB	-4.40	1.34	1.43
17	B	1220	CLA	C1B-CHB	-4.39	1.34	1.43
17	A	1117	CLA	C1B-CHB	-4.37	1.34	1.43
17	F	1301	CLA	C1B-CHB	-4.37	1.34	1.43
17	P	5117	CLA	C1B-CHB	-4.37	1.34	1.43
17	U	5301	CLA	C1B-CHB	-4.37	1.34	1.43
17	Q	5201	CLA	C1B-CHB	-4.36	1.34	1.43
17	B	1219	CLA	C1B-CHB	-4.35	1.34	1.43
17	Q	5215	CLA	C1B-CHB	-4.34	1.34	1.43
17	Q	5219	CLA	C1B-CHB	-4.33	1.34	1.43
17	A	1116	CLA	C1B-CHB	-4.32	1.34	1.43
17	P	5011	CLA	C1B-CHB	-4.32	1.34	1.43
17	B	1238	CLA	C1B-CHB	-4.32	1.34	1.43
17	B	1215	CLA	C1B-CHB	-4.32	1.34	1.43
17	P	5116	CLA	C1B-CHB	-4.31	1.34	1.43
17	Q	5238	CLA	C1B-CHB	-4.31	1.34	1.43
17	A	1128	CLA	C1B-CHB	-4.30	1.34	1.43
17	P	5140	CLA	C1B-CHB	-4.29	1.34	1.43
17	A	1011	CLA	C1B-CHB	-4.29	1.34	1.43
17	P	5128	CLA	C1B-CHB	-4.28	1.35	1.43
17	A	1140	CLA	C1B-CHB	-4.27	1.35	1.43
17	B	1239	CLA	C1B-CHB	-4.27	1.35	1.43
17	A	1402	CLA	C1B-CHB	-4.26	1.35	1.43
17	P	5402	CLA	C1B-CHB	-4.26	1.35	1.43
17	Q	5239	CLA	C1B-CHB	-4.24	1.35	1.43
17	L	1503	CLA	C1B-CHB	-4.24	1.35	1.43
17	6	5501	CLA	C1B-CHB	-4.22	1.35	1.43
17	G	1233	CLA	C1B-CHB	-4.22	1.35	1.43
17	L	1501	CLA	C1B-CHB	-4.21	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	6	5503	CLA	C1B-CHB	-4.21	1.35	1.43
17	V	5233	CLA	C1B-CHB	-4.20	1.35	1.43
17	P	5134	CLA	C1B-CHB	-4.19	1.35	1.43
17	A	1123	CLA	C1B-CHB	-4.19	1.35	1.43
17	A	1134	CLA	C1B-CHB	-4.18	1.35	1.43
17	P	5104	CLA	C1B-CHB	-4.18	1.35	1.43
17	P	5123	CLA	C1B-CHB	-4.17	1.35	1.43
17	A	1104	CLA	C1B-CHB	-4.17	1.35	1.43
17	B	1218	CLA	C1B-CHB	-4.16	1.35	1.43
17	A	1105	CLA	C1B-CHB	-4.15	1.35	1.43
17	P	5105	CLA	C1B-CHB	-4.15	1.35	1.43
17	P	5118	CLA	C1B-CHB	-4.15	1.35	1.43
17	P	5102	CLA	C1B-CHB	-4.14	1.35	1.43
17	Z	5302	CLA	C1B-CHB	-4.14	1.35	1.43
17	A	1118	CLA	C1B-CHB	-4.14	1.35	1.43
17	A	1102	CLA	C1B-CHB	-4.14	1.35	1.43
17	J	1302	CLA	C1B-CHB	-4.12	1.35	1.43
17	Q	5218	CLA	C1B-CHB	-4.12	1.35	1.43
17	P	5133	CLA	C1B-CHB	-4.11	1.35	1.43
17	A	1133	CLA	C1B-CHB	-4.11	1.35	1.43
17	P	5139	CLA	C1B-CHB	-4.09	1.35	1.43
17	Q	5217	CLA	C1B-CHB	-4.09	1.35	1.43
17	Q	5222	CLA	C1B-CHB	-4.08	1.35	1.43
17	B	1222	CLA	C1B-CHB	-4.07	1.35	1.43
17	B	1217	CLA	C1B-CHB	-4.07	1.35	1.43
17	P	5137	CLA	C1B-CHB	-4.07	1.35	1.43
17	A	1137	CLA	C1B-CHB	-4.07	1.35	1.43
17	Q	5224	CLA	C1B-CHB	-4.07	1.35	1.43
17	A	1139	CLA	C1B-CHB	-4.06	1.35	1.43
17	B	1224	CLA	C1B-CHB	-4.06	1.35	1.43
17	P	5125	CLA	C1B-CHB	-4.04	1.35	1.43
17	A	1125	CLA	C1B-CHB	-4.04	1.35	1.43
17	B	1234	CLA	C1B-CHB	-4.00	1.35	1.43
17	Q	5234	CLA	C1B-CHB	-3.99	1.35	1.43
17	A	1012	CLA	C1B-CHB	-3.97	1.35	1.43
17	Q	5206	CLA	C1B-CHB	-3.96	1.35	1.43
17	B	1206	CLA	C1B-CHB	-3.95	1.35	1.43
17	B	1209	CLA	C1B-CHB	-3.94	1.35	1.43
17	P	5113	CLA	C1B-CHB	-3.94	1.35	1.43
17	A	1113	CLA	C1B-CHB	-3.92	1.35	1.43
17	P	5012	CLA	C1B-CHB	-3.92	1.35	1.43
17	B	1203	CLA	C1B-CHB	-3.90	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5209	CLA	C1B-CHB	-3.90	1.35	1.43
17	Q	5203	CLA	C1B-CHB	-3.89	1.35	1.43
17	Q	5223	CLA	C1B-CHB	-3.83	1.35	1.43
17	B	1223	CLA	C1B-CHB	-3.81	1.35	1.43
17	B	1202	CLA	C1B-CHB	-3.80	1.35	1.43
17	Q	5202	CLA	C1B-CHB	-3.77	1.36	1.43
17	A	1127	CLA	C1B-CHB	-3.72	1.36	1.43
17	P	5127	CLA	C1B-CHB	-3.70	1.36	1.43
17	B	1230	CLA	C1B-CHB	-3.70	1.36	1.43
17	Q	5230	CLA	C1B-CHB	-3.69	1.36	1.43
17	Q	5130	CLA	C1B-CHB	-3.57	1.36	1.43
17	A	1131	CLA	C1B-CHB	-3.54	1.36	1.43
17	B	1130	CLA	C1B-CHB	-3.54	1.36	1.43
17	P	5131	CLA	C1B-CHB	-3.50	1.36	1.43
17	Q	5207	CLA	C4B-CHC	-3.31	1.36	1.43
17	B	1207	CLA	C4B-CHC	-3.27	1.37	1.43
17	A	1135	CLA	C1B-CHB	-3.21	1.37	1.43
17	P	5135	CLA	C1B-CHB	-3.21	1.37	1.43
17	B	1226	CLA	C1B-CHB	-3.07	1.37	1.43
17	Q	5226	CLA	C1B-CHB	-3.07	1.37	1.43
17	A	1135	CLA	C4B-CHC	-3.03	1.37	1.43
17	P	5135	CLA	C4B-CHC	-3.03	1.37	1.43
17	A	1131	CLA	C4B-CHC	-2.92	1.37	1.43
17	P	5131	CLA	C4B-CHC	-2.90	1.37	1.43
18	A	2001	PQN	C2-C1	-2.88	1.44	1.48
18	P	6001	PQN	C2-C1	-2.83	1.44	1.48
17	B	1225	CLA	C4B-CHC	-2.75	1.38	1.43
17	B	1239	CLA	C4B-CHC	-2.74	1.38	1.43
17	Q	5239	CLA	C4B-CHC	-2.73	1.38	1.43
17	Q	5225	CLA	C4B-CHC	-2.73	1.38	1.43
17	B	1204	CLA	C4B-CHC	-2.72	1.38	1.43
17	B	1201	CLA	C4B-CHC	-2.71	1.38	1.43
17	Q	5204	CLA	C4B-CHC	-2.71	1.38	1.43
17	P	5132	CLA	C4B-CHC	-2.69	1.38	1.43
17	Q	5201	CLA	C4B-CHC	-2.68	1.38	1.43
17	P	5121	CLA	C4B-CHC	-2.67	1.38	1.43
17	A	1121	CLA	C4B-CHC	-2.66	1.38	1.43
17	A	1132	CLA	C4B-CHC	-2.65	1.38	1.43
17	B	1208	CLA	C4B-CHC	-2.64	1.38	1.43
17	Q	5208	CLA	C4B-CHC	-2.63	1.38	1.43
17	Q	5237	CLA	C4B-CHC	-2.63	1.38	1.43
17	B	1237	CLA	C4B-CHC	-2.63	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	1139	CLA	C4B-CHC	-2.62	1.38	1.43
17	P	5136	CLA	C4B-CHC	-2.60	1.38	1.43
17	P	5139	CLA	C4B-CHC	-2.59	1.38	1.43
17	A	1136	CLA	C4B-CHC	-2.58	1.38	1.43
17	B	1230	CLA	C4B-CHC	-2.56	1.38	1.43
18	A	2001	PQN	C10-C1	-2.55	1.43	1.48
18	Q	6002	PQN	C5-C4	-2.55	1.43	1.48
18	B	2002	PQN	C5-C4	-2.54	1.43	1.48
17	Q	5230	CLA	C4B-CHC	-2.54	1.38	1.43
18	P	6001	PQN	C10-C1	-2.54	1.43	1.48
17	B	1215	CLA	C4B-CHC	-2.54	1.38	1.43
17	Q	5203	CLA	C4B-CHC	-2.53	1.38	1.43
17	Q	5215	CLA	C4B-CHC	-2.52	1.38	1.43
17	P	5117	CLA	C4B-CHC	-2.52	1.38	1.43
17	B	1203	CLA	C4B-CHC	-2.51	1.38	1.43
17	Q	5202	CLA	C4B-CHC	-2.50	1.38	1.43
17	A	1117	CLA	C4B-CHC	-2.49	1.38	1.43
17	A	1122	CLA	C4B-CHC	-2.47	1.38	1.43
17	P	5122	CLA	C4B-CHC	-2.46	1.38	1.43
17	B	1202	CLA	C4B-CHC	-2.46	1.38	1.43
17	B	1226	CLA	C4B-CHC	-2.45	1.38	1.43
17	A	1108	CLA	C4B-CHC	-2.45	1.38	1.43
17	Q	5226	CLA	C4B-CHC	-2.45	1.38	1.43
17	P	5108	CLA	C4B-CHC	-2.45	1.38	1.43
17	Q	5205	CLA	C4B-CHC	-2.45	1.38	1.43
17	B	1205	CLA	C4B-CHC	-2.44	1.38	1.43
18	P	6001	PQN	C5-C4	-2.42	1.44	1.48
18	A	2001	PQN	C5-C4	-2.41	1.44	1.48
17	A	1013	CLA	C4B-CHC	-2.39	1.38	1.43
17	P	5013	CLA	C4B-CHC	-2.39	1.38	1.43
17	Q	5211	CLA	C4B-CHC	-2.39	1.38	1.43
17	B	1211	CLA	C4B-CHC	-2.38	1.38	1.43
17	A	1109	CLA	C4B-CHC	-2.37	1.38	1.43
17	A	1102	CLA	C4B-CHC	-2.37	1.38	1.43
17	P	5111	CLA	C4B-CHC	-2.37	1.38	1.43
17	P	5109	CLA	C4B-CHC	-2.37	1.38	1.43
17	Q	5222	CLA	C4B-CHC	-2.36	1.38	1.43
17	P	5102	CLA	C4B-CHC	-2.36	1.38	1.43
17	Q	5214	CLA	C4B-CHC	-2.36	1.38	1.43
17	6	5502	CLA	C4B-CHC	-2.35	1.38	1.43
17	A	1111	CLA	C4B-CHC	-2.34	1.38	1.43
17	B	1222	CLA	C4B-CHC	-2.34	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	1502	CLA	C4B-CHC	-2.33	1.38	1.43
17	B	1214	CLA	C4B-CHC	-2.33	1.38	1.43
18	B	2002	PQN	C2-C1	-2.31	1.44	1.48
18	Q	6002	PQN	C2-C1	-2.31	1.44	1.48
17	A	1901	CLA	C1C-NC	-2.31	1.33	1.37
17	P	5901	CLA	C1C-NC	-2.29	1.33	1.37
17	P	5104	CLA	C4B-CHC	-2.29	1.39	1.43
17	6	5503	CLA	C4B-CHC	-2.29	1.39	1.43
17	L	1503	CLA	C4B-CHC	-2.29	1.39	1.43
17	A	1128	CLA	C4B-CHC	-2.28	1.39	1.43
17	B	1238	CLA	C4B-CHC	-2.26	1.39	1.43
17	U	8005	CLA	C4B-CHC	-2.26	1.39	1.43
17	P	5128	CLA	C4B-CHC	-2.26	1.39	1.43
17	A	1104	CLA	C4B-CHC	-2.26	1.39	1.43
17	8	1025	CLA	C4B-CHC	-2.25	1.39	1.43
17	B	1236	CLA	C4B-CHC	-2.25	1.39	1.43
17	A	1113	CLA	C4B-CHC	-2.24	1.39	1.43
17	9	1021	CLA	C4B-CHC	-2.24	1.39	1.43
17	Q	5238	CLA	C4B-CHC	-2.23	1.39	1.43
17	A	1134	CLA	C4B-CHC	-2.23	1.39	1.43
17	7	1015	CLA	C4B-CHC	-2.23	1.39	1.43
17	P	5113	CLA	C4B-CHC	-2.23	1.39	1.43
17	0	1025	CLA	C4B-CHC	-2.22	1.39	1.43
17	2	1025	CLA	C4B-CHC	-2.22	1.39	1.43
17	P	5402	CLA	C4B-CHC	-2.22	1.39	1.43
17	0	1022	CLA	C4B-CHC	-2.22	1.39	1.43
17	4	1022	CLA	C4B-CHC	-2.22	1.39	1.43
17	8	1023	CLA	C4B-CHC	-2.22	1.39	1.43
17	4	1012	CLA	C4B-CHC	-2.21	1.39	1.43
17	F	4005	CLA	C4B-CHC	-2.21	1.39	1.43
17	1	1011	CLA	C4B-CHC	-2.21	1.39	1.43
17	P	5134	CLA	C4B-CHC	-2.21	1.39	1.43
17	Q	5236	CLA	C4B-CHC	-2.21	1.39	1.43
17	9	1022	CLA	C4B-CHC	-2.21	1.39	1.43
17	P	8010	CLA	C4B-CHC	-2.21	1.39	1.43
17	3	1021	CLA	C4B-CHC	-2.21	1.39	1.43
17	P	5137	CLA	C4B-CHC	-2.21	1.39	1.43
17	3	1022	CLA	C4B-CHC	-2.21	1.39	1.43
17	B	1242	CLA	C4B-CHC	-2.20	1.39	1.43
17	U	8004	CLA	C4B-CHC	-2.20	1.39	1.43
17	A	1402	CLA	C4B-CHC	-2.20	1.39	1.43
17	A	1137	CLA	C4B-CHC	-2.20	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1025	CLA	C4B-CHC	-2.20	1.39	1.43
17	A	1126	CLA	C4B-CHC	-2.20	1.39	1.43
17	7	1023	CLA	C4B-CHC	-2.20	1.39	1.43
17	P	5126	CLA	C4B-CHC	-2.20	1.39	1.43
17	0	1012	CLA	C4B-CHC	-2.20	1.39	1.43
17	8	1022	CLA	C4B-CHC	-2.20	1.39	1.43
17	9	1041	CLA	C4B-CHC	-2.20	1.39	1.43
17	A	4010	CLA	C4B-CHC	-2.20	1.39	1.43
17	3	1025	CLA	C4B-CHC	-2.19	1.39	1.43
17	4	1011	CLA	C4B-CHC	-2.19	1.39	1.43
17	4	1015	CLA	C4B-CHC	-2.19	1.39	1.43
17	4	1025	CLA	C4B-CHC	-2.19	1.39	1.43
17	1	1015	CLA	C4B-CHC	-2.19	1.39	1.43
17	P	5105	CLA	C4B-CHC	-2.19	1.39	1.43
17	0	1015	CLA	C4B-CHC	-2.19	1.39	1.43
17	Q	5210	CLA	C4B-CHC	-2.19	1.39	1.43
17	8	1013	CLA	C4B-CHC	-2.19	1.39	1.43
17	0	8002	CLA	C4B-CHC	-2.19	1.39	1.43
17	A	1124	CLA	C4B-CHC	-2.19	1.39	1.43
17	8	1017	CLA	C4B-CHC	-2.19	1.39	1.43
17	7	1021	CLA	C4B-CHC	-2.19	1.39	1.43
17	5	5401	CLA	C4B-CHC	-2.19	1.39	1.43
17	A	1110	CLA	C4B-CHC	-2.19	1.39	1.43
17	G	1701	CLA	C4B-CHC	-2.19	1.39	1.43
17	8	1031	CLA	C4B-CHC	-2.19	1.39	1.43
17	P	5124	CLA	C4B-CHC	-2.19	1.39	1.43
17	0	1011	CLA	C4B-CHC	-2.19	1.39	1.43
17	1	1021	CLA	C4B-CHC	-2.19	1.39	1.43
17	1	1023	CLA	C4B-CHC	-2.18	1.39	1.43
17	2	1022	CLA	C4B-CHC	-2.18	1.39	1.43
17	K	1403	CLA	C4B-CHC	-2.18	1.39	1.43
17	Q	5206	CLA	C4B-CHC	-2.18	1.39	1.43
17	0	1023	CLA	C4B-CHC	-2.18	1.39	1.43
17	8	8007	CLA	C4B-CHC	-2.18	1.39	1.43
17	2	1012	CLA	C4B-CHC	-2.18	1.39	1.43
17	H	1801	CLA	C4B-CHC	-2.18	1.39	1.43
17	B	1206	CLA	C4B-CHC	-2.18	1.39	1.43
17	2	1026	CLA	C4B-CHC	-2.18	1.39	1.43
17	3	1011	CLA	C4B-CHC	-2.18	1.39	1.43
17	A	4009	CLA	C4B-CHC	-2.18	1.39	1.43
17	7	1011	CLA	C4B-CHC	-2.18	1.39	1.43
17	Q	5240	CLA	C4B-CHC	-2.18	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	4007	CLA	C4B-CHC	-2.18	1.39	1.43
17	A	1103	CLA	C4B-CHC	-2.18	1.39	1.43
17	F	4004	CLA	C4B-CHC	-2.18	1.39	1.43
17	3	1017	CLA	C4B-CHC	-2.18	1.39	1.43
17	2	1023	CLA	C4B-CHC	-2.18	1.39	1.43
17	7	1026	CLA	C4B-CHC	-2.18	1.39	1.43
17	W	5801	CLA	C4B-CHC	-2.18	1.39	1.43
17	2	1013	CLA	C4B-CHC	-2.18	1.39	1.43
17	1	1013	CLA	C4B-CHC	-2.18	1.39	1.43
17	3	1031	CLA	C4B-CHC	-2.18	1.39	1.43
17	P	5110	CLA	C4B-CHC	-2.18	1.39	1.43
17	1	1026	CLA	C4B-CHC	-2.18	1.39	1.43
17	8	1014	CLA	C4B-CHC	-2.18	1.39	1.43
17	P	5103	CLA	C4B-CHC	-2.18	1.39	1.43
17	2	1031	CLA	C4B-CHC	-2.17	1.39	1.43
17	8	1012	CLA	C4B-CHC	-2.17	1.39	1.43
17	1	1025	CLA	C4B-CHC	-2.17	1.39	1.43
17	B	1210	CLA	C4B-CHC	-2.17	1.39	1.43
17	K	1401	CLA	C4B-CHC	-2.17	1.39	1.43
17	0	1032	CLA	C4B-CHC	-2.17	1.39	1.43
17	J	1101	CLA	C4B-CHC	-2.17	1.39	1.43
17	7	1013	CLA	C4B-CHC	-2.17	1.39	1.43
17	5	5404	CLA	C4B-CHC	-2.17	1.39	1.43
17	4	1031	CLA	C4B-CHC	-2.17	1.39	1.43
17	3	1041	CLA	C4B-CHC	-2.17	1.39	1.43
17	4	1026	CLA	C4B-CHC	-2.17	1.39	1.43
17	K	1404	CLA	C4B-CHC	-2.17	1.39	1.43
17	7	1025	CLA	C4B-CHC	-2.17	1.39	1.43
17	0	1033	CLA	C4B-CHC	-2.17	1.39	1.43
17	J	4008	CLA	C4B-CHC	-2.17	1.39	1.43
17	5	5403	CLA	C4B-CHC	-2.17	1.39	1.43
17	9	1011	CLA	C4B-CHC	-2.17	1.39	1.43
17	8	1033	CLA	C4B-CHC	-2.17	1.39	1.43
17	A	1137	CLA	C1C-NC	-2.17	1.34	1.37
17	Q	5242	CLA	C4B-CHC	-2.17	1.39	1.43
17	9	1015	CLA	C4B-CHC	-2.17	1.39	1.43
17	1	1016	CLA	C4B-CHC	-2.17	1.39	1.43
17	2	1014	CLA	C4B-CHC	-2.17	1.39	1.43
17	7	1016	CLA	C4B-CHC	-2.17	1.39	1.43
17	B	1240	CLA	C4B-CHC	-2.17	1.39	1.43
17	1	1031	CLA	C4B-CHC	-2.17	1.39	1.43
17	9	1016	CLA	C4B-CHC	-2.17	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	9	1017	CLA	C4B-CHC	-2.17	1.39	1.43
17	4	1033	CLA	C4B-CHC	-2.17	1.39	1.43
17	2	1017	CLA	C4B-CHC	-2.16	1.39	1.43
17	7	1022	CLA	C4B-CHC	-2.16	1.39	1.43
17	7	1031	CLA	C4B-CHC	-2.16	1.39	1.43
17	A	1105	CLA	C4B-CHC	-2.16	1.39	1.43
17	B	4001	CLA	C4B-CHC	-2.16	1.39	1.43
17	0	1021	CLA	C4B-CHC	-2.16	1.39	1.43
17	V	5701	CLA	C4B-CHC	-2.16	1.39	1.43
17	Z	5101	CLA	C4B-CHC	-2.16	1.39	1.43
17	3	1012	CLA	C4B-CHC	-2.16	1.39	1.43
17	4	1032	CLA	C4B-CHC	-2.16	1.39	1.43
17	F	4003	CLA	C4B-CHC	-2.16	1.39	1.43
17	1	1022	CLA	C4B-CHC	-2.16	1.39	1.43
17	9	1031	CLA	C4B-CHC	-2.16	1.39	1.43
17	4	4002	CLA	C4B-CHC	-2.16	1.39	1.43
17	0	1017	CLA	C4B-CHC	-2.16	1.39	1.43
17	4	1023	CLA	C4B-CHC	-2.16	1.39	1.43
17	Q	5241	CLA	C4B-CHC	-2.16	1.39	1.43
17	F	4006	CLA	C4B-CHC	-2.16	1.39	1.43
17	9	1012	CLA	C4B-CHC	-2.16	1.39	1.43
17	2	1033	CLA	C4B-CHC	-2.16	1.39	1.43
17	3	1033	CLA	C4B-CHC	-2.16	1.39	1.43
17	P	8009	CLA	C4B-CHC	-2.16	1.39	1.43
17	1	1012	CLA	C4B-CHC	-2.16	1.39	1.43
17	4	1014	CLA	C4B-CHC	-2.16	1.39	1.43
17	U	8003	CLA	C4B-CHC	-2.16	1.39	1.43
17	3	1015	CLA	C4B-CHC	-2.15	1.39	1.43
17	4	1016	CLA	C4B-CHC	-2.15	1.39	1.43
17	0	1016	CLA	C4B-CHC	-2.15	1.39	1.43
17	9	1032	CLA	C4B-CHC	-2.15	1.39	1.43
17	3	1026	CLA	C4B-CHC	-2.15	1.39	1.43
17	0	1031	CLA	C4B-CHC	-2.15	1.39	1.43
17	3	1016	CLA	C4B-CHC	-2.15	1.39	1.43
17	L	1504	CLA	C4B-CHC	-2.15	1.39	1.43
17	8	1026	CLA	C4B-CHC	-2.15	1.39	1.43
17	B	1130	CLA	C4B-CHC	-2.15	1.39	1.43
17	0	1026	CLA	C4B-CHC	-2.15	1.39	1.43
17	U	8006	CLA	C4B-CHC	-2.15	1.39	1.43
17	Z	8008	CLA	C4B-CHC	-2.15	1.39	1.43
17	2	1011	CLA	C4B-CHC	-2.15	1.39	1.43
17	Q	5130	CLA	C4B-CHC	-2.15	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	8001	CLA	C4B-CHC	-2.14	1.39	1.43
17	B	1241	CLA	C4B-CHC	-2.14	1.39	1.43
17	6	5504	CLA	C4B-CHC	-2.14	1.39	1.43
17	8	1011	CLA	C4B-CHC	-2.14	1.39	1.43
17	2	1021	CLA	C4B-CHC	-2.14	1.39	1.43
17	8	1021	CLA	C4B-CHC	-2.14	1.39	1.43
17	8	1015	CLA	C4B-CHC	-2.14	1.39	1.43
17	9	1014	CLA	C4B-CHC	-2.13	1.39	1.43
17	2	1015	CLA	C4B-CHC	-2.13	1.39	1.43
17	P	5137	CLA	C1C-NC	-2.13	1.34	1.37
17	1	1014	CLA	C4B-CHC	-2.13	1.39	1.43
17	4	1021	CLA	C4B-CHC	-2.13	1.39	1.43
17	0	1013	CLA	C4B-CHC	-2.13	1.39	1.43
17	2	1016	CLA	C4B-CHC	-2.13	1.39	1.43
17	8	1016	CLA	C4B-CHC	-2.13	1.39	1.43
17	0	1014	CLA	C4B-CHC	-2.13	1.39	1.43
17	3	1014	CLA	C4B-CHC	-2.13	1.39	1.43
17	1	1017	CLA	C4B-CHC	-2.12	1.39	1.43
17	4	1013	CLA	C4B-CHC	-2.12	1.39	1.43
17	7	1012	CLA	C4B-CHC	-2.12	1.39	1.43
17	9	1033	CLA	C4B-CHC	-2.12	1.39	1.43
17	4	1017	CLA	C4B-CHC	-2.12	1.39	1.43
17	9	1026	CLA	C4B-CHC	-2.11	1.39	1.43
17	3	1032	CLA	C4B-CHC	-2.11	1.39	1.43
17	7	1014	CLA	C4B-CHC	-2.11	1.39	1.43
17	7	1017	CLA	C4B-CHC	-2.10	1.39	1.43
18	Q	6002	PQN	C10-C1	-2.09	1.44	1.48
17	U	5229	CLA	C4B-CHC	-2.08	1.39	1.43
17	B	1219	CLA	C1C-NC	-2.07	1.34	1.37
18	B	2002	PQN	C10-C1	-2.05	1.44	1.48
17	F	1229	CLA	C4B-CHC	-2.05	1.39	1.43
17	A	1011	CLA	C4B-CHC	-2.05	1.39	1.43
17	Q	5219	CLA	C1C-NC	-2.03	1.34	1.37
17	P	5011	CLA	C4B-CHC	-2.03	1.39	1.43
17	P	5107	CLA	C4B-CHC	-2.01	1.39	1.43
17	A	1127	CLA	C4B-CHC	-2.01	1.39	1.43
17	P	5126	CLA	C1C-NC	-2.01	1.34	1.37
17	P	5127	CLA	C4B-CHC	-2.00	1.39	1.43
17	A	1107	CLA	C4B-CHC	-2.00	1.39	1.43
17	Q	5220	CLA	C3C-C4C	2.00	1.47	1.43
17	A	1106	CLA	C2C-C1C	2.03	1.47	1.43
17	P	5106	CLA	C2C-C1C	2.03	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	1302	CLA	C2C-C1C	2.04	1.47	1.43
17	Z	5302	CLA	C2C-C1C	2.04	1.47	1.43
17	B	1235	CLA	CHC-C1C	2.05	1.45	1.39
17	A	1104	CLA	C3C-C4C	2.05	1.47	1.43
17	Q	5235	CLA	CHC-C1C	2.05	1.45	1.39
17	P	5104	CLA	C3C-C4C	2.06	1.47	1.43
17	B	1210	CLA	C3C-C4C	2.06	1.47	1.43
17	Q	5210	CLA	C3C-C4C	2.06	1.47	1.43
17	A	1136	CLA	C3C-C4C	2.07	1.47	1.43
17	Q	5021	CLA	C2C-C1C	2.09	1.47	1.43
17	P	5136	CLA	C3C-C4C	2.09	1.47	1.43
17	B	1021	CLA	C2C-C1C	2.10	1.47	1.43
17	Q	5224	CLA	C2C-C1C	2.10	1.47	1.43
17	B	1224	CLA	C2C-C1C	2.13	1.47	1.43
17	B	1238	CLA	C3C-C4C	2.13	1.47	1.43
17	Q	5221	CLA	C2C-C1C	2.14	1.47	1.43
17	B	1221	CLA	C2C-C1C	2.14	1.47	1.43
17	P	5135	CLA	C3C-C4C	2.15	1.47	1.43
17	Q	5238	CLA	C3C-C4C	2.15	1.47	1.43
17	A	1135	CLA	C3C-C4C	2.19	1.48	1.43
17	B	1023	CLA	C3C-C4C	2.24	1.48	1.43
17	Q	5023	CLA	C3C-C4C	2.27	1.48	1.43
17	B	1023	CLA	C2C-C1C	2.28	1.48	1.43
17	Q	5023	CLA	C2C-C1C	2.28	1.48	1.43
18	P	6001	PQN	C7-C6	2.29	1.43	1.38
18	Q	6002	PQN	C8-C7	2.31	1.43	1.38
18	A	2001	PQN	C7-C6	2.32	1.43	1.38
17	Q	5237	CLA	C3C-C4C	2.33	1.48	1.43
17	B	1237	CLA	C3C-C4C	2.33	1.48	1.43
18	B	2002	PQN	C8-C7	2.33	1.43	1.38
17	P	5119	CLA	C2B-C1B	2.39	1.44	1.40
18	P	6001	PQN	C9-C10	2.39	1.43	1.39
17	A	1119	CLA	C2B-C1B	2.40	1.44	1.40
18	A	2001	PQN	C9-C10	2.41	1.43	1.39
18	Q	6002	PQN	C8-C9	2.41	1.43	1.38
18	B	2002	PQN	C8-C9	2.41	1.43	1.38
18	A	2001	PQN	C8-C7	2.43	1.43	1.38
17	L	1501	CLA	C2C-C1C	2.44	1.48	1.43
18	P	6001	PQN	C8-C7	2.44	1.44	1.38
17	6	5501	CLA	C2C-C1C	2.45	1.48	1.43
18	A	2001	PQN	C8-C9	2.46	1.43	1.38
18	P	6001	PQN	C8-C9	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	6002	PQN	C9-C10	2.52	1.43	1.39
18	B	2002	PQN	C9-C10	2.56	1.43	1.39
17	Q	5206	CLA	C3B-C4B	2.57	1.44	1.40
17	B	1206	CLA	C3B-C4B	2.59	1.44	1.40
17	A	1117	CLA	C2B-C1B	2.68	1.44	1.40
17	P	5117	CLA	C2B-C1B	2.68	1.44	1.40
17	Q	5211	CLA	C2B-C1B	2.69	1.44	1.40
17	B	1211	CLA	C2B-C1B	2.71	1.44	1.40
17	Q	5022	CLA	C2B-C1B	2.74	1.44	1.40
17	B	1022	CLA	C2B-C1B	2.74	1.44	1.40
17	A	1131	CLA	C3B-C4B	2.75	1.44	1.40
17	P	5131	CLA	C3B-C4B	2.77	1.44	1.40
17	Q	5238	CLA	C3B-C4B	2.85	1.45	1.40
17	A	1107	CLA	C2B-C1B	2.87	1.45	1.40
17	B	1238	CLA	C3B-C4B	2.87	1.45	1.40
17	P	5107	CLA	C2B-C1B	2.93	1.45	1.40
17	Q	5237	CLA	C2B-C1B	2.96	1.45	1.40
17	B	1237	CLA	C2B-C1B	2.97	1.45	1.40
17	Q	5216	CLA	C2B-C1B	2.98	1.45	1.40
17	B	1216	CLA	C2B-C1B	2.99	1.45	1.40
18	A	2001	PQN	C10-C5	3.02	1.45	1.40
18	P	6001	PQN	C10-C5	3.03	1.45	1.40
17	B	1206	CLA	C2B-C1B	3.03	1.45	1.40
17	B	1225	CLA	C2B-C1B	3.05	1.45	1.40
18	A	2001	PQN	C6-C5	3.05	1.44	1.39
17	Q	5206	CLA	C2B-C1B	3.05	1.45	1.40
17	P	5129	CLA	C2B-C1B	3.05	1.45	1.40
18	P	6001	PQN	C6-C5	3.06	1.44	1.39
17	A	1129	CLA	C2B-C1B	3.08	1.45	1.40
17	Q	5225	CLA	C2B-C1B	3.09	1.45	1.40
17	Q	5232	CLA	C2B-C1B	3.11	1.45	1.40
17	P	5124	CLA	C2B-C1B	3.11	1.45	1.40
17	A	1124	CLA	C2B-C1B	3.13	1.45	1.40
17	P	5102	CLA	C2B-C1B	3.13	1.45	1.40
17	P	5108	CLA	C2B-C1B	3.14	1.45	1.40
17	A	1102	CLA	C2B-C1B	3.15	1.45	1.40
17	B	1232	CLA	C2B-C1B	3.15	1.45	1.40
17	A	1120	CLA	C2B-C1B	3.15	1.45	1.40
18	Q	6002	PQN	C6-C5	3.16	1.44	1.39
17	P	5120	CLA	C2B-C1B	3.16	1.45	1.40
17	A	1108	CLA	C2B-C1B	3.16	1.45	1.40
18	B	2002	PQN	C6-C5	3.17	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	U	5229	CLA	C2B-C1B	3.19	1.45	1.40
17	Q	5239	CLA	C3B-C4B	3.19	1.45	1.40
17	B	1214	CLA	C2B-C1B	3.20	1.45	1.40
17	F	1229	CLA	C2B-C1B	3.21	1.45	1.40
17	B	1239	CLA	C3B-C4B	3.22	1.45	1.40
17	P	5011	CLA	C3B-C4B	3.24	1.45	1.40
17	A	1011	CLA	C3B-C4B	3.25	1.45	1.40
17	A	1122	CLA	C2B-C1B	3.25	1.45	1.40
17	P	5132	CLA	C3B-C4B	3.25	1.45	1.40
17	B	1224	CLA	C2B-C1B	3.25	1.45	1.40
17	Q	5214	CLA	C2B-C1B	3.26	1.45	1.40
17	A	1132	CLA	C3B-C4B	3.26	1.45	1.40
17	6	5503	CLA	C2B-C1B	3.26	1.45	1.40
17	L	1503	CLA	C2B-C1B	3.26	1.45	1.40
17	Q	5212	CLA	C2B-C1B	3.26	1.45	1.40
17	P	5122	CLA	C2B-C1B	3.26	1.45	1.40
17	Q	5224	CLA	C2B-C1B	3.27	1.45	1.40
17	A	1901	CLA	C2B-C1B	3.28	1.45	1.40
17	B	1212	CLA	C2B-C1B	3.28	1.45	1.40
17	A	1012	CLA	C2B-C1B	3.28	1.45	1.40
17	P	5012	CLA	C2B-C1B	3.29	1.45	1.40
17	P	5901	CLA	C2B-C1B	3.30	1.45	1.40
17	P	5106	CLA	C2B-C1B	3.33	1.45	1.40
17	B	1227	CLA	C2B-C1B	3.33	1.45	1.40
17	A	1106	CLA	C2B-C1B	3.34	1.45	1.40
17	Q	5227	CLA	C2B-C1B	3.34	1.45	1.40
17	P	5132	CLA	C2B-C1B	3.34	1.45	1.40
17	A	1114	CLA	C2B-C1B	3.37	1.45	1.40
17	F	4005	CLA	C2B-C1B	3.38	1.45	1.40
17	9	1022	CLA	C2B-C1B	3.39	1.45	1.40
17	A	1132	CLA	C2B-C1B	3.39	1.45	1.40
17	1	1022	CLA	C2B-C1B	3.39	1.45	1.40
17	P	5114	CLA	C2B-C1B	3.39	1.45	1.40
17	Q	5201	CLA	C2B-C1B	3.39	1.45	1.40
17	9	1016	CLA	C2B-C1B	3.39	1.45	1.40
17	8	1014	CLA	C2B-C1B	3.39	1.45	1.40
17	3	1016	CLA	C2B-C1B	3.40	1.45	1.40
17	0	1023	CLA	C2B-C1B	3.40	1.45	1.40
17	7	1021	CLA	C2B-C1B	3.40	1.45	1.40
17	2	1014	CLA	C2B-C1B	3.40	1.45	1.40
17	3	1022	CLA	C2B-C1B	3.40	1.45	1.40
17	7	1016	CLA	C2B-C1B	3.41	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5236	CLA	C2B-C1B	3.41	1.45	1.40
17	Q	5240	CLA	C2B-C1B	3.41	1.45	1.40
17	P	8010	CLA	C2B-C1B	3.41	1.45	1.40
17	P	8009	CLA	C2B-C1B	3.41	1.45	1.40
17	A	1127	CLA	C3B-C4B	3.41	1.45	1.40
17	2	1015	CLA	C2B-C1B	3.41	1.45	1.40
17	U	8005	CLA	C2B-C1B	3.41	1.45	1.40
17	4	1023	CLA	C2B-C1B	3.42	1.45	1.40
17	B	1201	CLA	C2B-C1B	3.42	1.45	1.40
17	U	8003	CLA	C2B-C1B	3.42	1.45	1.40
17	7	1022	CLA	C2B-C1B	3.42	1.45	1.40
17	3	1025	CLA	C2B-C1B	3.42	1.45	1.40
17	1	1021	CLA	C2B-C1B	3.42	1.45	1.40
17	3	1026	CLA	C2B-C1B	3.43	1.46	1.40
17	B	1236	CLA	C2B-C1B	3.43	1.46	1.40
17	8	1015	CLA	C2B-C1B	3.43	1.46	1.40
17	8	1012	CLA	C2B-C1B	3.43	1.46	1.40
17	B	1228	CLA	C2B-C1B	3.43	1.46	1.40
17	P	5127	CLA	C3B-C4B	3.43	1.46	1.40
17	B	1239	CLA	C2B-C1B	3.43	1.46	1.40
17	0	1025	CLA	C2B-C1B	3.43	1.46	1.40
17	8	1031	CLA	C2B-C1B	3.43	1.46	1.40
17	A	1133	CLA	C2B-C1B	3.44	1.46	1.40
17	8	1025	CLA	C2B-C1B	3.44	1.46	1.40
17	1	1015	CLA	C2B-C1B	3.44	1.46	1.40
17	B	1240	CLA	C2B-C1B	3.44	1.46	1.40
17	1	1012	CLA	C2B-C1B	3.44	1.46	1.40
17	0	1014	CLA	C2B-C1B	3.44	1.46	1.40
17	4	1016	CLA	C2B-C1B	3.44	1.46	1.40
17	9	1041	CLA	C2B-C1B	3.44	1.46	1.40
17	3	1041	CLA	C2B-C1B	3.44	1.46	1.40
17	3	1015	CLA	C2B-C1B	3.44	1.46	1.40
17	7	1013	CLA	C2B-C1B	3.44	1.46	1.40
17	4	1031	CLA	C2B-C1B	3.44	1.46	1.40
17	7	1015	CLA	C2B-C1B	3.44	1.46	1.40
17	Z	5302	CLA	C2B-C1B	3.44	1.46	1.40
17	3	1021	CLA	C2B-C1B	3.44	1.46	1.40
17	F	4004	CLA	C2B-C1B	3.45	1.46	1.40
17	9	1021	CLA	C2B-C1B	3.45	1.46	1.40
17	6	5504	CLA	C2B-C1B	3.45	1.46	1.40
17	0	1016	CLA	C2B-C1B	3.45	1.46	1.40
17	2	1025	CLA	C2B-C1B	3.45	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	1302	CLA	C2B-C1B	3.45	1.46	1.40
17	9	1015	CLA	C2B-C1B	3.45	1.46	1.40
17	0	1026	CLA	C2B-C1B	3.45	1.46	1.40
17	4	1032	CLA	C2B-C1B	3.45	1.46	1.40
17	4	1025	CLA	C2B-C1B	3.45	1.46	1.40
17	2	1031	CLA	C2B-C1B	3.45	1.46	1.40
17	Q	5239	CLA	C2B-C1B	3.45	1.46	1.40
17	2	1016	CLA	C2B-C1B	3.45	1.46	1.40
17	0	1031	CLA	C2B-C1B	3.45	1.46	1.40
17	2	1021	CLA	C2B-C1B	3.45	1.46	1.40
17	0	1032	CLA	C2B-C1B	3.45	1.46	1.40
17	U	8006	CLA	C2B-C1B	3.45	1.46	1.40
17	Q	5242	CLA	C2B-C1B	3.45	1.46	1.40
17	2	1023	CLA	C2B-C1B	3.45	1.46	1.40
17	1	1016	CLA	C2B-C1B	3.45	1.46	1.40
17	9	1025	CLA	C2B-C1B	3.45	1.46	1.40
17	1	1026	CLA	C2B-C1B	3.45	1.46	1.40
17	9	1026	CLA	C2B-C1B	3.45	1.46	1.40
17	2	1012	CLA	C2B-C1B	3.45	1.46	1.40
17	9	1011	CLA	C2B-C1B	3.45	1.46	1.40
17	Z	5101	CLA	C2B-C1B	3.45	1.46	1.40
17	7	1026	CLA	C2B-C1B	3.45	1.46	1.40
17	4	1026	CLA	C2B-C1B	3.45	1.46	1.40
17	7	1025	CLA	C2B-C1B	3.45	1.46	1.40
17	8	1013	CLA	C2B-C1B	3.46	1.46	1.40
17	8	1016	CLA	C2B-C1B	3.46	1.46	1.40
17	1	1013	CLA	C2B-C1B	3.46	1.46	1.40
17	9	1012	CLA	C2B-C1B	3.46	1.46	1.40
17	F	4003	CLA	C2B-C1B	3.46	1.46	1.40
17	2	1013	CLA	C2B-C1B	3.46	1.46	1.40
17	A	4010	CLA	C2B-C1B	3.46	1.46	1.40
17	A	4009	CLA	C2B-C1B	3.46	1.46	1.40
17	3	1011	CLA	C2B-C1B	3.46	1.46	1.40
17	U	8004	CLA	C2B-C1B	3.46	1.46	1.40
17	J	4008	CLA	C2B-C1B	3.46	1.46	1.40
17	8	1023	CLA	C2B-C1B	3.46	1.46	1.40
17	8	1021	CLA	C2B-C1B	3.46	1.46	1.40
17	4	1014	CLA	C2B-C1B	3.46	1.46	1.40
17	0	1017	CLA	C2B-C1B	3.46	1.46	1.40
17	1	1025	CLA	C2B-C1B	3.46	1.46	1.40
17	3	1031	CLA	C2B-C1B	3.46	1.46	1.40
17	0	1011	CLA	C2B-C1B	3.46	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5133	CLA	C2B-C1B	3.46	1.46	1.40
17	7	1011	CLA	C2B-C1B	3.47	1.46	1.40
17	2	1022	CLA	C2B-C1B	3.47	1.46	1.40
17	4	1017	CLA	C2B-C1B	3.47	1.46	1.40
17	J	1101	CLA	C2B-C1B	3.47	1.46	1.40
17	2	1033	CLA	C2B-C1B	3.47	1.46	1.40
17	3	1033	CLA	C2B-C1B	3.47	1.46	1.40
17	Q	5221	CLA	C2B-C1B	3.47	1.46	1.40
17	L	1504	CLA	C2B-C1B	3.47	1.46	1.40
17	9	1017	CLA	C2B-C1B	3.47	1.46	1.40
17	B	1242	CLA	C2B-C1B	3.47	1.46	1.40
17	Z	8008	CLA	C2B-C1B	3.47	1.46	1.40
17	Q	5208	CLA	C2B-C1B	3.47	1.46	1.40
17	7	1031	CLA	C2B-C1B	3.47	1.46	1.40
17	8	1022	CLA	C2B-C1B	3.47	1.46	1.40
17	1	1017	CLA	C2B-C1B	3.48	1.46	1.40
17	9	1031	CLA	C2B-C1B	3.48	1.46	1.40
17	4	1011	CLA	C2B-C1B	3.48	1.46	1.40
17	1	1031	CLA	C2B-C1B	3.48	1.46	1.40
17	8	1033	CLA	C2B-C1B	3.48	1.46	1.40
18	B	2002	PQN	C10-C5	3.48	1.46	1.40
17	8	1011	CLA	C2B-C1B	3.48	1.46	1.40
17	3	1012	CLA	C2B-C1B	3.48	1.46	1.40
17	2	1011	CLA	C2B-C1B	3.48	1.46	1.40
17	7	1023	CLA	C2B-C1B	3.48	1.46	1.40
17	B	1235	CLA	C2B-C1B	3.49	1.46	1.40
17	0	1033	CLA	C2B-C1B	3.49	1.46	1.40
17	Q	5228	CLA	C2B-C1B	3.49	1.46	1.40
17	H	1801	CLA	C2B-C1B	3.49	1.46	1.40
17	B	1241	CLA	C2B-C1B	3.49	1.46	1.40
17	2	1026	CLA	C2B-C1B	3.49	1.46	1.40
17	7	1014	CLA	C2B-C1B	3.49	1.46	1.40
17	Q	5213	CLA	C2B-C1B	3.49	1.46	1.40
17	3	1017	CLA	C2B-C1B	3.49	1.46	1.40
17	0	8002	CLA	C2B-C1B	3.49	1.46	1.40
17	B	1221	CLA	C2B-C1B	3.49	1.46	1.40
17	K	1404	CLA	C2B-C1B	3.50	1.46	1.40
17	7	1012	CLA	C2B-C1B	3.50	1.46	1.40
17	8	8007	CLA	C2B-C1B	3.50	1.46	1.40
17	4	1015	CLA	C2B-C1B	3.50	1.46	1.40
17	1	1011	CLA	C2B-C1B	3.50	1.46	1.40
17	4	1021	CLA	C2B-C1B	3.50	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	7	1017	CLA	C2B-C1B	3.50	1.46	1.40
17	F	4006	CLA	C2B-C1B	3.50	1.46	1.40
17	K	1403	CLA	C2B-C1B	3.50	1.46	1.40
17	4	1022	CLA	C2B-C1B	3.50	1.46	1.40
17	4	1033	CLA	C2B-C1B	3.50	1.46	1.40
17	G	1701	CLA	C2B-C1B	3.50	1.46	1.40
17	B	1213	CLA	C2B-C1B	3.50	1.46	1.40
17	Q	5241	CLA	C2B-C1B	3.50	1.46	1.40
17	B	4001	CLA	C2B-C1B	3.50	1.46	1.40
17	1	1023	CLA	C2B-C1B	3.50	1.46	1.40
17	P	5116	CLA	C2B-C1B	3.50	1.46	1.40
17	3	1014	CLA	C2B-C1B	3.50	1.46	1.40
17	5	5404	CLA	C2B-C1B	3.50	1.46	1.40
17	Q	8001	CLA	C2B-C1B	3.50	1.46	1.40
17	2	4007	CLA	C2B-C1B	3.51	1.46	1.40
17	4	1013	CLA	C2B-C1B	3.51	1.46	1.40
17	0	1013	CLA	C2B-C1B	3.51	1.46	1.40
17	Q	5235	CLA	C2B-C1B	3.51	1.46	1.40
17	9	1033	CLA	C2B-C1B	3.51	1.46	1.40
17	9	1014	CLA	C2B-C1B	3.51	1.46	1.40
17	W	5801	CLA	C2B-C1B	3.52	1.46	1.40
17	2	1017	CLA	C2B-C1B	3.52	1.46	1.40
18	Q	6002	PQN	C10-C5	3.52	1.46	1.40
17	8	1026	CLA	C2B-C1B	3.52	1.46	1.40
17	Q	5215	CLA	C2B-C1B	3.52	1.46	1.40
17	8	1017	CLA	C2B-C1B	3.52	1.46	1.40
17	9	1032	CLA	C2B-C1B	3.52	1.46	1.40
17	4	4002	CLA	C2B-C1B	3.52	1.46	1.40
17	1	1014	CLA	C2B-C1B	3.53	1.46	1.40
17	A	1116	CLA	C2B-C1B	3.53	1.46	1.40
17	0	1015	CLA	C2B-C1B	3.53	1.46	1.40
17	P	5127	CLA	C2B-C1B	3.53	1.46	1.40
17	5	5403	CLA	C2B-C1B	3.53	1.46	1.40
17	3	1032	CLA	C2B-C1B	3.53	1.46	1.40
17	B	1208	CLA	C2B-C1B	3.53	1.46	1.40
17	0	1021	CLA	C2B-C1B	3.53	1.46	1.40
17	0	1022	CLA	C2B-C1B	3.53	1.46	1.40
17	A	1127	CLA	C2B-C1B	3.54	1.46	1.40
17	V	5701	CLA	C2B-C1B	3.54	1.46	1.40
17	A	1121	CLA	C2B-C1B	3.54	1.46	1.40
17	0	1012	CLA	C2B-C1B	3.54	1.46	1.40
17	B	1215	CLA	C2B-C1B	3.55	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5121	CLA	C2B-C1B	3.55	1.46	1.40
17	A	1135	CLA	C3B-C4B	3.55	1.46	1.40
17	P	5103	CLA	C2B-C1B	3.56	1.46	1.40
17	B	1220	CLA	C2B-C1B	3.56	1.46	1.40
17	Q	5220	CLA	C2B-C1B	3.57	1.46	1.40
17	A	1140	CLA	C2B-C1B	3.57	1.46	1.40
17	A	1103	CLA	C2B-C1B	3.58	1.46	1.40
17	P	5135	CLA	C3B-C4B	3.58	1.46	1.40
17	P	5140	CLA	C2B-C1B	3.59	1.46	1.40
17	P	5139	CLA	C2B-C1B	3.59	1.46	1.40
17	4	1012	CLA	C2B-C1B	3.61	1.46	1.40
17	B	1021	CLA	C2B-C1B	3.61	1.46	1.40
17	A	1139	CLA	C2B-C1B	3.61	1.46	1.40
17	P	5123	CLA	C2B-C1B	3.62	1.46	1.40
17	Q	5215	CLA	C3B-C4B	3.63	1.46	1.40
17	A	1123	CLA	C2B-C1B	3.63	1.46	1.40
17	B	1215	CLA	C3B-C4B	3.64	1.46	1.40
17	Q	5021	CLA	C2B-C1B	3.65	1.46	1.40
17	P	5139	CLA	C3B-C4B	3.68	1.46	1.40
17	B	1202	CLA	C3B-C4B	3.68	1.46	1.40
17	P	5115	CLA	C2B-C1B	3.68	1.46	1.40
17	Q	5226	CLA	C3B-C4B	3.68	1.46	1.40
17	A	1139	CLA	C3B-C4B	3.68	1.46	1.40
17	A	1115	CLA	C2B-C1B	3.68	1.46	1.40
17	A	1128	CLA	C2B-C1B	3.69	1.46	1.40
17	B	1226	CLA	C3B-C4B	3.71	1.46	1.40
17	P	5128	CLA	C2B-C1B	3.71	1.46	1.40
17	Q	5202	CLA	C3B-C4B	3.72	1.46	1.40
17	Q	5234	CLA	C2B-C1B	3.72	1.46	1.40
17	B	1023	CLA	C2B-C1B	3.72	1.46	1.40
17	A	1126	CLA	C2B-C1B	3.72	1.46	1.40
17	B	1234	CLA	C2B-C1B	3.73	1.46	1.40
17	Q	5023	CLA	C2B-C1B	3.73	1.46	1.40
17	Q	5218	CLA	C2B-C1B	3.73	1.46	1.40
17	A	1103	CLA	C3B-C4B	3.74	1.46	1.40
17	P	5126	CLA	C2B-C1B	3.74	1.46	1.40
17	A	1131	CLA	C2B-C1B	3.74	1.46	1.40
17	B	1218	CLA	C2B-C1B	3.74	1.46	1.40
17	P	5131	CLA	C2B-C1B	3.75	1.46	1.40
17	A	1113	CLA	C2B-C1B	3.76	1.46	1.40
17	5	5401	CLA	C2B-C1B	3.76	1.46	1.40
17	K	1401	CLA	C2B-C1B	3.76	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5103	CLA	C3B-C4B	3.77	1.46	1.40
17	A	1112	CLA	C2B-C1B	3.77	1.46	1.40
17	Q	5222	CLA	C2B-C1B	3.77	1.46	1.40
17	B	1222	CLA	C2B-C1B	3.77	1.46	1.40
17	B	1226	CLA	C2B-C1B	3.78	1.46	1.40
17	B	1238	CLA	C2B-C1B	3.79	1.46	1.40
17	Q	5230	CLA	C2B-C1B	3.80	1.46	1.40
17	A	1122	CLA	C3B-C4B	3.80	1.46	1.40
17	B	1230	CLA	C2B-C1B	3.80	1.46	1.40
17	P	5113	CLA	C2B-C1B	3.81	1.46	1.40
17	P	5112	CLA	C2B-C1B	3.81	1.46	1.40
17	A	1117	CLA	C3B-C4B	3.82	1.46	1.40
17	Q	5238	CLA	C2B-C1B	3.82	1.46	1.40
17	P	5117	CLA	C3B-C4B	3.82	1.46	1.40
17	P	5122	CLA	C3B-C4B	3.82	1.46	1.40
17	B	1217	CLA	C2B-C1B	3.82	1.46	1.40
17	Q	5226	CLA	C2B-C1B	3.83	1.46	1.40
17	Q	5217	CLA	C2B-C1B	3.83	1.46	1.40
17	P	5104	CLA	C2B-C1B	3.83	1.46	1.40
17	P	5138	CLA	C2B-C1B	3.84	1.46	1.40
17	A	1138	CLA	C2B-C1B	3.85	1.46	1.40
17	A	1104	CLA	C2B-C1B	3.86	1.46	1.40
17	A	1013	CLA	C2B-C1B	3.87	1.46	1.40
17	P	5013	CLA	C2B-C1B	3.87	1.46	1.40
17	A	1110	CLA	C2B-C1B	3.89	1.46	1.40
17	P	5105	CLA	C2B-C1B	3.90	1.46	1.40
17	P	5110	CLA	C2B-C1B	3.90	1.46	1.40
17	L	1501	CLA	C2B-C1B	3.90	1.46	1.40
17	B	1210	CLA	C2B-C1B	3.90	1.46	1.40
17	Q	5204	CLA	C2B-C1B	3.91	1.46	1.40
17	A	1105	CLA	C2B-C1B	3.91	1.46	1.40
17	Q	5210	CLA	C2B-C1B	3.92	1.46	1.40
17	P	5109	CLA	C2B-C1B	3.92	1.46	1.40
17	A	1134	CLA	C2B-C1B	3.92	1.46	1.40
17	P	5134	CLA	C2B-C1B	3.93	1.46	1.40
17	B	1204	CLA	C2B-C1B	3.93	1.46	1.40
17	Q	5209	CLA	C2B-C1B	3.94	1.46	1.40
17	A	1109	CLA	C2B-C1B	3.94	1.46	1.40
17	6	5501	CLA	C2B-C1B	3.95	1.46	1.40
17	6	5502	CLA	C2B-C1B	3.95	1.46	1.40
17	B	1202	CLA	C2B-C1B	3.95	1.46	1.40
17	G	1233	CLA	C2B-C1B	3.96	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5202	CLA	C2B-C1B	3.97	1.46	1.40
17	L	1502	CLA	C2B-C1B	3.97	1.46	1.40
17	B	1209	CLA	C2B-C1B	3.98	1.46	1.40
17	V	5233	CLA	C2B-C1B	3.98	1.46	1.40
17	Q	5236	CLA	C3B-C4B	4.00	1.47	1.40
17	P	5118	CLA	C2B-C1B	4.02	1.47	1.40
17	B	1236	CLA	C3B-C4B	4.04	1.47	1.40
17	Q	5219	CLA	C2B-C1B	4.05	1.47	1.40
17	A	1118	CLA	C2B-C1B	4.05	1.47	1.40
17	A	1137	CLA	C2B-C1B	4.07	1.47	1.40
17	A	1136	CLA	C2B-C1B	4.09	1.47	1.40
17	B	1219	CLA	C2B-C1B	4.10	1.47	1.40
17	A	1125	CLA	C2B-C1B	4.10	1.47	1.40
17	P	5137	CLA	C2B-C1B	4.11	1.47	1.40
17	B	1222	CLA	C3B-C4B	4.11	1.47	1.40
17	Q	5211	CLA	C3B-C4B	4.11	1.47	1.40
17	Q	5205	CLA	C2B-C1B	4.12	1.47	1.40
17	P	5136	CLA	C2B-C1B	4.12	1.47	1.40
17	P	5125	CLA	C2B-C1B	4.12	1.47	1.40
17	A	1113	CLA	C3B-C4B	4.12	1.47	1.40
17	A	1133	CLA	C3B-C4B	4.12	1.47	1.40
17	Q	5021	CLA	C3B-C4B	4.13	1.47	1.40
17	P	5133	CLA	C3B-C4B	4.13	1.47	1.40
17	B	1021	CLA	C3B-C4B	4.13	1.47	1.40
17	A	1108	CLA	C3B-C4B	4.13	1.47	1.40
17	P	5113	CLA	C3B-C4B	4.13	1.47	1.40
17	Q	5222	CLA	C3B-C4B	4.14	1.47	1.40
17	P	5102	CLA	C3B-C4B	4.14	1.47	1.40
17	B	1205	CLA	C2B-C1B	4.15	1.47	1.40
17	A	1102	CLA	C3B-C4B	4.15	1.47	1.40
17	B	1211	CLA	C3B-C4B	4.15	1.47	1.40
17	P	5124	CLA	C3B-C4B	4.15	1.47	1.40
17	P	5108	CLA	C3B-C4B	4.16	1.47	1.40
17	Q	5223	CLA	C2B-C1B	4.16	1.47	1.40
17	B	1225	CLA	C3B-C4B	4.17	1.47	1.40
17	B	1223	CLA	C2B-C1B	4.17	1.47	1.40
17	A	1111	CLA	C2B-C1B	4.17	1.47	1.40
17	Q	5225	CLA	C3B-C4B	4.17	1.47	1.40
17	A	1124	CLA	C3B-C4B	4.18	1.47	1.40
17	A	1107	CLA	C3B-C4B	4.19	1.47	1.40
17	P	5402	CLA	C2B-C1B	4.20	1.47	1.40
17	A	1402	CLA	C2B-C1B	4.21	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5111	CLA	C2B-C1B	4.21	1.47	1.40
17	P	5107	CLA	C3B-C4B	4.23	1.47	1.40
17	A	1012	CLA	C3B-C4B	4.24	1.47	1.40
17	A	1137	CLA	C3B-C4B	4.24	1.47	1.40
17	P	5137	CLA	C3B-C4B	4.25	1.47	1.40
17	P	5012	CLA	C3B-C4B	4.25	1.47	1.40
17	B	1203	CLA	C3B-C4B	4.26	1.47	1.40
17	U	5301	CLA	C2B-C1B	4.28	1.47	1.40
17	Q	5237	CLA	C3B-C4B	4.30	1.47	1.40
17	F	1301	CLA	C2B-C1B	4.30	1.47	1.40
17	B	1237	CLA	C3B-C4B	4.31	1.47	1.40
17	B	1203	CLA	C2B-C1B	4.31	1.47	1.40
17	Q	5203	CLA	C3B-C4B	4.32	1.47	1.40
17	Q	5231	CLA	C2B-C1B	4.34	1.47	1.40
17	Q	5203	CLA	C2B-C1B	4.36	1.47	1.40
17	A	1111	CLA	C3B-C4B	4.37	1.47	1.40
17	P	5111	CLA	C3B-C4B	4.38	1.47	1.40
17	B	1207	CLA	C3B-C4B	4.38	1.47	1.40
17	Q	5230	CLA	C3B-C4B	4.38	1.47	1.40
17	B	1231	CLA	C2B-C1B	4.39	1.47	1.40
17	P	5126	CLA	C3B-C4B	4.40	1.47	1.40
17	A	1011	CLA	C2B-C1B	4.40	1.47	1.40
17	Q	5207	CLA	C3B-C4B	4.40	1.47	1.40
17	B	1230	CLA	C3B-C4B	4.41	1.47	1.40
17	A	1126	CLA	C3B-C4B	4.41	1.47	1.40
17	B	1130	CLA	C3B-C4B	4.43	1.47	1.40
17	B	1227	CLA	C3B-C4B	4.44	1.47	1.40
17	Q	5130	CLA	C3B-C4B	4.46	1.47	1.40
17	P	5011	CLA	C2B-C1B	4.46	1.47	1.40
17	Q	5227	CLA	C3B-C4B	4.49	1.47	1.40
17	Q	5210	CLA	C3B-C4B	4.49	1.47	1.40
17	B	1210	CLA	C3B-C4B	4.50	1.47	1.40
17	Q	5208	CLA	C3B-C4B	4.52	1.47	1.40
17	B	1208	CLA	C3B-C4B	4.53	1.47	1.40
17	A	1105	CLA	C3B-C4B	4.54	1.47	1.40
17	A	1114	CLA	C3B-C4B	4.56	1.47	1.40
17	A	1109	CLA	C3B-C4B	4.56	1.47	1.40
17	P	5114	CLA	C3B-C4B	4.57	1.47	1.40
17	A	1013	CLA	C3B-C4B	4.57	1.47	1.40
17	P	5109	CLA	C3B-C4B	4.57	1.47	1.40
17	P	5105	CLA	C3B-C4B	4.58	1.47	1.40
17	Q	5205	CLA	C3B-C4B	4.61	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	1205	CLA	C3B-C4B	4.62	1.48	1.40
17	A	1104	CLA	C3B-C4B	4.62	1.48	1.40
17	P	5013	CLA	C3B-C4B	4.62	1.48	1.40
17	B	1217	CLA	C3B-C4B	4.63	1.48	1.40
17	L	1503	CLA	C3B-C4B	4.63	1.48	1.40
17	B	1216	CLA	C3B-C4B	4.64	1.48	1.40
17	Q	5216	CLA	C3B-C4B	4.64	1.48	1.40
17	Q	5201	CLA	C3B-C4B	4.65	1.48	1.40
17	Q	5217	CLA	C3B-C4B	4.65	1.48	1.40
17	Z	5302	CLA	C3B-C4B	4.65	1.48	1.40
17	J	1302	CLA	C3B-C4B	4.66	1.48	1.40
17	B	1201	CLA	C3B-C4B	4.67	1.48	1.40
17	P	5104	CLA	C3B-C4B	4.67	1.48	1.40
17	6	5503	CLA	C3B-C4B	4.67	1.48	1.40
17	A	1402	CLA	C3B-C4B	4.69	1.48	1.40
17	P	5402	CLA	C3B-C4B	4.73	1.48	1.40
17	A	1135	CLA	C2B-C1B	4.73	1.48	1.40
17	P	5135	CLA	C2B-C1B	4.74	1.48	1.40
17	P	5110	CLA	C3B-C4B	4.76	1.48	1.40
17	5	5401	CLA	C3B-C4B	4.76	1.48	1.40
17	L	1502	CLA	C3B-C4B	4.76	1.48	1.40
17	6	5502	CLA	C3B-C4B	4.77	1.48	1.40
17	K	1401	CLA	C3B-C4B	4.78	1.48	1.40
17	B	1130	CLA	C2B-C1B	4.78	1.48	1.40
17	P	5121	CLA	C3B-C4B	4.78	1.48	1.40
17	Q	5130	CLA	C2B-C1B	4.79	1.48	1.40
17	Q	5207	CLA	C2B-C1B	4.79	1.48	1.40
17	B	1207	CLA	C2B-C1B	4.80	1.48	1.40
17	A	1121	CLA	C3B-C4B	4.80	1.48	1.40
17	A	1110	CLA	C3B-C4B	4.80	1.48	1.40
17	P	5106	CLA	C3B-C4B	4.81	1.48	1.40
17	B	1223	CLA	C3B-C4B	4.81	1.48	1.40
17	V	5233	CLA	C3B-C4B	4.81	1.48	1.40
17	A	1106	CLA	C3B-C4B	4.81	1.48	1.40
17	G	1233	CLA	C3B-C4B	4.81	1.48	1.40
17	Q	5223	CLA	C3B-C4B	4.81	1.48	1.40
17	P	5116	CLA	C3B-C4B	4.82	1.48	1.40
17	A	1134	CLA	C3B-C4B	4.83	1.48	1.40
17	A	1116	CLA	C3B-C4B	4.83	1.48	1.40
17	P	5134	CLA	C3B-C4B	4.84	1.48	1.40
17	Q	5209	CLA	C3B-C4B	4.90	1.48	1.40
17	B	1209	CLA	C3B-C4B	4.90	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	5120	CLA	C3B-C4B	4.91	1.48	1.40
17	A	1120	CLA	C3B-C4B	4.92	1.48	1.40
17	A	1138	CLA	C3B-C4B	4.93	1.48	1.40
17	Q	5231	CLA	C3B-C4B	4.94	1.48	1.40
17	P	5138	CLA	C3B-C4B	4.94	1.48	1.40
17	B	1231	CLA	C3B-C4B	4.95	1.48	1.40
17	A	1119	CLA	C3B-C4B	4.95	1.48	1.40
17	L	1501	CLA	C3B-C4B	4.97	1.48	1.40
17	P	5119	CLA	C3B-C4B	4.97	1.48	1.40
17	6	5501	CLA	C3B-C4B	4.97	1.48	1.40
17	Q	5234	CLA	C3B-C4B	4.98	1.48	1.40
17	A	1129	CLA	C3B-C4B	4.98	1.48	1.40
17	U	5301	CLA	C3B-C4B	4.99	1.48	1.40
17	A	1123	CLA	C3B-C4B	5.00	1.48	1.40
17	P	5123	CLA	C3B-C4B	5.00	1.48	1.40
17	B	1234	CLA	C3B-C4B	5.00	1.48	1.40
17	B	1204	CLA	C3B-C4B	5.01	1.48	1.40
17	Q	5204	CLA	C3B-C4B	5.01	1.48	1.40
17	B	1220	CLA	C3B-C4B	5.02	1.48	1.40
17	B	1213	CLA	C3B-C4B	5.02	1.48	1.40
17	B	1214	CLA	C3B-C4B	5.02	1.48	1.40
17	A	1901	CLA	C3B-C4B	5.03	1.48	1.40
17	F	1229	CLA	C3B-C4B	5.03	1.48	1.40
17	Q	5214	CLA	C3B-C4B	5.04	1.48	1.40
17	F	1301	CLA	C3B-C4B	5.04	1.48	1.40
17	P	5129	CLA	C3B-C4B	5.04	1.48	1.40
17	U	8003	CLA	C3B-C4B	5.04	1.48	1.40
17	P	5901	CLA	C3B-C4B	5.04	1.48	1.40
17	Q	5220	CLA	C3B-C4B	5.05	1.48	1.40
17	P	5140	CLA	C3B-C4B	5.05	1.48	1.40
17	Q	5213	CLA	C3B-C4B	5.06	1.48	1.40
17	U	5229	CLA	C3B-C4B	5.06	1.48	1.40
17	F	4003	CLA	C3B-C4B	5.07	1.48	1.40
17	9	1025	CLA	C3B-C4B	5.07	1.48	1.40
17	B	1228	CLA	C3B-C4B	5.07	1.48	1.40
17	7	1026	CLA	C3B-C4B	5.08	1.48	1.40
17	1	1026	CLA	C3B-C4B	5.09	1.48	1.40
17	A	1140	CLA	C3B-C4B	5.09	1.48	1.40
17	Q	5228	CLA	C3B-C4B	5.10	1.48	1.40
17	4	1017	CLA	C3B-C4B	5.10	1.48	1.40
17	9	1012	CLA	C3B-C4B	5.10	1.48	1.40
17	B	1218	CLA	C3B-C4B	5.11	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	8001	CLA	C3B-C4B	5.11	1.48	1.40
17	0	1023	CLA	C3B-C4B	5.11	1.48	1.40
17	3	1025	CLA	C3B-C4B	5.12	1.48	1.40
17	Q	5218	CLA	C3B-C4B	5.12	1.48	1.40
17	Q	5219	CLA	C3B-C4B	5.12	1.48	1.40
17	1	1031	CLA	C3B-C4B	5.12	1.48	1.40
17	B	1219	CLA	C3B-C4B	5.12	1.48	1.40
17	Q	5235	CLA	C3B-C4B	5.12	1.48	1.40
17	8	1026	CLA	C3B-C4B	5.12	1.48	1.40
17	9	1014	CLA	C3B-C4B	5.13	1.48	1.40
17	7	1014	CLA	C3B-C4B	5.13	1.48	1.40
17	2	1014	CLA	C3B-C4B	5.13	1.48	1.40
17	1	1014	CLA	C3B-C4B	5.13	1.48	1.40
17	0	1017	CLA	C3B-C4B	5.13	1.48	1.40
17	2	1021	CLA	C3B-C4B	5.14	1.48	1.40
17	8	1014	CLA	C3B-C4B	5.14	1.48	1.40
17	2	1026	CLA	C3B-C4B	5.14	1.48	1.40
17	3	1031	CLA	C3B-C4B	5.14	1.48	1.40
17	L	1504	CLA	C3B-C4B	5.14	1.48	1.40
17	7	1015	CLA	C3B-C4B	5.14	1.48	1.40
17	2	1016	CLA	C3B-C4B	5.14	1.48	1.40
17	U	8006	CLA	C3B-C4B	5.15	1.48	1.40
17	3	1014	CLA	C3B-C4B	5.15	1.48	1.40
17	B	4001	CLA	C3B-C4B	5.15	1.48	1.40
17	3	1012	CLA	C3B-C4B	5.15	1.48	1.40
17	0	1013	CLA	C3B-C4B	5.15	1.48	1.40
17	A	4009	CLA	C3B-C4B	5.15	1.48	1.40
17	4	1014	CLA	C3B-C4B	5.15	1.48	1.40
17	4	4002	CLA	C3B-C4B	5.15	1.48	1.40
17	4	1023	CLA	C3B-C4B	5.15	1.48	1.40
17	9	1031	CLA	C3B-C4B	5.15	1.48	1.40
17	8	1012	CLA	C3B-C4B	5.15	1.48	1.40
17	0	1021	CLA	C3B-C4B	5.15	1.48	1.40
17	3	1017	CLA	C3B-C4B	5.15	1.48	1.40
17	P	8009	CLA	C3B-C4B	5.15	1.48	1.40
17	1	1015	CLA	C3B-C4B	5.15	1.48	1.40
17	F	4006	CLA	C3B-C4B	5.16	1.48	1.40
17	9	1017	CLA	C3B-C4B	5.16	1.48	1.40
17	7	1031	CLA	C3B-C4B	5.16	1.48	1.40
17	2	1012	CLA	C3B-C4B	5.16	1.48	1.40
17	B	1240	CLA	C3B-C4B	5.16	1.48	1.40
17	7	1012	CLA	C3B-C4B	5.16	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	1033	CLA	C3B-C4B	5.16	1.48	1.40
17	8	1021	CLA	C3B-C4B	5.16	1.49	1.40
17	4	1025	CLA	C3B-C4B	5.16	1.49	1.40
17	Q	5240	CLA	C3B-C4B	5.16	1.49	1.40
17	4	1021	CLA	C3B-C4B	5.16	1.49	1.40
17	2	1023	CLA	C3B-C4B	5.16	1.49	1.40
17	4	1013	CLA	C3B-C4B	5.16	1.49	1.40
17	G	1701	CLA	C3B-C4B	5.16	1.49	1.40
17	1	1025	CLA	C3B-C4B	5.16	1.49	1.40
17	0	1014	CLA	C3B-C4B	5.16	1.49	1.40
17	2	1015	CLA	C3B-C4B	5.16	1.49	1.40
17	8	1016	CLA	C3B-C4B	5.16	1.49	1.40
17	B	1235	CLA	C3B-C4B	5.17	1.49	1.40
17	V	5701	CLA	C3B-C4B	5.17	1.49	1.40
17	9	1021	CLA	C3B-C4B	5.17	1.49	1.40
17	8	1031	CLA	C3B-C4B	5.17	1.49	1.40
17	7	1021	CLA	C3B-C4B	5.17	1.49	1.40
17	1	1012	CLA	C3B-C4B	5.17	1.49	1.40
17	8	1015	CLA	C3B-C4B	5.17	1.49	1.40
17	9	1015	CLA	C3B-C4B	5.17	1.49	1.40
17	7	1022	CLA	C3B-C4B	5.17	1.49	1.40
17	9	1033	CLA	C3B-C4B	5.17	1.49	1.40
17	Q	5241	CLA	C3B-C4B	5.17	1.49	1.40
17	8	1023	CLA	C3B-C4B	5.17	1.49	1.40
17	Z	5101	CLA	C3B-C4B	5.17	1.49	1.40
17	7	1023	CLA	C3B-C4B	5.17	1.49	1.40
17	0	1025	CLA	C3B-C4B	5.17	1.49	1.40
17	6	5504	CLA	C3B-C4B	5.17	1.49	1.40
17	0	1012	CLA	C3B-C4B	5.17	1.49	1.40
17	8	1013	CLA	C3B-C4B	5.17	1.49	1.40
17	0	1033	CLA	C3B-C4B	5.17	1.49	1.40
17	1	1022	CLA	C3B-C4B	5.17	1.49	1.40
17	1	1021	CLA	C3B-C4B	5.17	1.49	1.40
17	1	1013	CLA	C3B-C4B	5.17	1.49	1.40
17	2	1011	CLA	C3B-C4B	5.17	1.49	1.40
17	1	1016	CLA	C3B-C4B	5.17	1.49	1.40
17	2	1031	CLA	C3B-C4B	5.17	1.49	1.40
17	J	1101	CLA	C3B-C4B	5.17	1.49	1.40
17	W	5801	CLA	C3B-C4B	5.17	1.49	1.40
17	3	1015	CLA	C3B-C4B	5.17	1.49	1.40
17	4	1012	CLA	C3B-C4B	5.18	1.49	1.40
17	J	4008	CLA	C3B-C4B	5.18	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	8	8007	CLA	C3B-C4B	5.18	1.49	1.40
17	7	1025	CLA	C3B-C4B	5.18	1.49	1.40
17	U	8004	CLA	C3B-C4B	5.18	1.49	1.40
17	7	1016	CLA	C3B-C4B	5.18	1.49	1.40
17	2	1013	CLA	C3B-C4B	5.18	1.49	1.40
17	2	4007	CLA	C3B-C4B	5.18	1.49	1.40
17	7	1013	CLA	C3B-C4B	5.18	1.49	1.40
17	2	1033	CLA	C3B-C4B	5.18	1.49	1.40
17	0	8002	CLA	C3B-C4B	5.18	1.49	1.40
17	5	5403	CLA	C3B-C4B	5.18	1.49	1.40
17	A	4010	CLA	C3B-C4B	5.18	1.49	1.40
17	H	1801	CLA	C3B-C4B	5.19	1.49	1.40
17	9	1016	CLA	C3B-C4B	5.19	1.49	1.40
17	K	1403	CLA	C3B-C4B	5.19	1.49	1.40
17	3	1022	CLA	C3B-C4B	5.19	1.49	1.40
17	9	1022	CLA	C3B-C4B	5.19	1.49	1.40
17	B	1241	CLA	C3B-C4B	5.19	1.49	1.40
17	F	4004	CLA	C3B-C4B	5.19	1.49	1.40
17	3	1011	CLA	C3B-C4B	5.19	1.49	1.40
17	8	1011	CLA	C3B-C4B	5.19	1.49	1.40
17	3	1026	CLA	C3B-C4B	5.19	1.49	1.40
17	3	1032	CLA	C3B-C4B	5.19	1.49	1.40
17	3	1016	CLA	C3B-C4B	5.19	1.49	1.40
17	0	1011	CLA	C3B-C4B	5.19	1.49	1.40
17	3	1021	CLA	C3B-C4B	5.20	1.49	1.40
17	1	1017	CLA	C3B-C4B	5.20	1.49	1.40
17	2	1025	CLA	C3B-C4B	5.20	1.49	1.40
17	0	1031	CLA	C3B-C4B	5.20	1.49	1.40
17	4	1032	CLA	C3B-C4B	5.20	1.49	1.40
17	3	1041	CLA	C3B-C4B	5.20	1.49	1.40
17	0	1032	CLA	C3B-C4B	5.20	1.49	1.40
17	Z	8008	CLA	C3B-C4B	5.20	1.49	1.40
17	7	1017	CLA	C3B-C4B	5.20	1.49	1.40
17	B	1242	CLA	C3B-C4B	5.20	1.49	1.40
17	9	1032	CLA	C3B-C4B	5.20	1.49	1.40
17	9	1026	CLA	C3B-C4B	5.21	1.49	1.40
17	P	8010	CLA	C3B-C4B	5.21	1.49	1.40
17	4	1033	CLA	C3B-C4B	5.21	1.49	1.40
17	0	1026	CLA	C3B-C4B	5.21	1.49	1.40
17	1	1011	CLA	C3B-C4B	5.21	1.49	1.40
17	9	1041	CLA	C3B-C4B	5.21	1.49	1.40
17	4	1016	CLA	C3B-C4B	5.21	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	4005	CLA	C3B-C4B	5.21	1.49	1.40
17	9	1011	CLA	C3B-C4B	5.21	1.49	1.40
17	7	1011	CLA	C3B-C4B	5.22	1.49	1.40
17	4	1031	CLA	C3B-C4B	5.22	1.49	1.40
17	8	1033	CLA	C3B-C4B	5.22	1.49	1.40
17	Q	5242	CLA	C3B-C4B	5.22	1.49	1.40
17	Q	5221	CLA	C3B-C4B	5.22	1.49	1.40
17	4	1022	CLA	C3B-C4B	5.22	1.49	1.40
17	K	1404	CLA	C3B-C4B	5.22	1.49	1.40
17	4	1011	CLA	C3B-C4B	5.22	1.49	1.40
17	5	5404	CLA	C3B-C4B	5.22	1.49	1.40
17	0	1015	CLA	C3B-C4B	5.22	1.49	1.40
17	1	1023	CLA	C3B-C4B	5.22	1.49	1.40
17	8	1022	CLA	C3B-C4B	5.23	1.49	1.40
17	B	1224	CLA	C3B-C4B	5.23	1.49	1.40
17	Q	5224	CLA	C3B-C4B	5.23	1.49	1.40
17	2	1022	CLA	C3B-C4B	5.23	1.49	1.40
17	A	1125	CLA	C3B-C4B	5.23	1.49	1.40
17	4	1026	CLA	C3B-C4B	5.23	1.49	1.40
17	8	1017	CLA	C3B-C4B	5.23	1.49	1.40
17	4	1015	CLA	C3B-C4B	5.24	1.49	1.40
17	B	1221	CLA	C3B-C4B	5.24	1.49	1.40
17	0	1022	CLA	C3B-C4B	5.24	1.49	1.40
17	U	8005	CLA	C3B-C4B	5.24	1.49	1.40
17	8	1025	CLA	C3B-C4B	5.25	1.49	1.40
17	P	5125	CLA	C3B-C4B	5.25	1.49	1.40
17	0	1016	CLA	C3B-C4B	5.25	1.49	1.40
17	2	1017	CLA	C3B-C4B	5.27	1.49	1.40
17	A	1118	CLA	C3B-C4B	5.28	1.49	1.40
17	P	5118	CLA	C3B-C4B	5.29	1.49	1.40
17	B	1022	CLA	C3B-C4B	5.29	1.49	1.40
17	Q	5022	CLA	C3B-C4B	5.29	1.49	1.40
17	A	1112	CLA	C3B-C4B	5.32	1.49	1.40
17	A	1115	CLA	C3B-C4B	5.33	1.49	1.40
17	P	5112	CLA	C3B-C4B	5.33	1.49	1.40
17	P	5115	CLA	C3B-C4B	5.33	1.49	1.40
17	A	1136	CLA	C3B-C4B	5.35	1.49	1.40
17	P	5136	CLA	C3B-C4B	5.35	1.49	1.40
17	B	1212	CLA	C3B-C4B	5.37	1.49	1.40
17	Q	5212	CLA	C3B-C4B	5.39	1.49	1.40
17	A	1128	CLA	C3B-C4B	5.63	1.49	1.40
17	P	5128	CLA	C3B-C4B	5.64	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	5232	CLA	C3B-C4B	5.67	1.49	1.40
17	B	1232	CLA	C3B-C4B	5.70	1.49	1.40
18	P	6001	PQN	C3-C2	5.77	1.46	1.35
18	A	2001	PQN	C3-C2	5.79	1.46	1.35
18	B	2002	PQN	C3-C2	5.80	1.46	1.35
18	Q	6002	PQN	C3-C2	5.82	1.46	1.35
17	Q	5023	CLA	C3B-C4B	6.10	1.50	1.40
17	B	1023	CLA	C3B-C4B	6.13	1.50	1.40
18	B	2002	PQN	O4-C4	8.09	1.42	1.24
18	Q	6002	PQN	O4-C4	8.10	1.42	1.24
18	B	2002	PQN	O1-C1	8.21	1.41	1.23
18	Q	6002	PQN	O1-C1	8.24	1.41	1.23
18	P	6001	PQN	O4-C4	8.39	1.42	1.24
18	A	2001	PQN	O4-C4	8.39	1.42	1.24
18	P	6001	PQN	O1-C1	8.65	1.42	1.23
18	A	2001	PQN	O1-C1	8.68	1.42	1.23

All (1332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	1302	CLA	C3B-C4B-NB	-4.32	106.32	110.11
17	Z	5302	CLA	C3B-C4B-NB	-4.32	106.32	110.11
17	P	5901	CLA	C3B-C4B-NB	-3.94	106.65	110.11
17	A	1901	CLA	C3B-C4B-NB	-3.92	106.67	110.11
17	Q	5221	CLA	C3B-C4B-NB	-3.85	106.73	110.11
17	B	1221	CLA	C3B-C4B-NB	-3.82	106.76	110.11
17	B	1022	CLA	C3B-C4B-NB	-3.82	106.76	110.11
17	Q	5022	CLA	C3B-C4B-NB	-3.82	106.76	110.11
17	P	5123	CLA	C3B-C4B-NB	-3.48	107.06	110.11
17	8	1025	CLA	C3B-C4B-NB	-3.46	107.07	110.11
17	1	1011	CLA	C3B-C4B-NB	-3.46	107.07	110.11
17	A	1123	CLA	C3B-C4B-NB	-3.45	107.08	110.11
17	8	8007	CLA	C3B-C4B-NB	-3.44	107.09	110.11
17	4	1011	CLA	C3B-C4B-NB	-3.43	107.09	110.11
17	7	1025	CLA	C3B-C4B-NB	-3.43	107.10	110.11
17	9	1015	CLA	C3B-C4B-NB	-3.43	107.10	110.11
17	U	8005	CLA	C3B-C4B-NB	-3.42	107.10	110.11
17	8	1013	CLA	C3B-C4B-NB	-3.42	107.10	110.11
17	9	1022	CLA	C3B-C4B-NB	-3.42	107.10	110.11
17	2	1025	CLA	C3B-C4B-NB	-3.42	107.10	110.11
17	8	1023	CLA	C3B-C4B-NB	-3.42	107.11	110.11
17	2	4007	CLA	C3B-C4B-NB	-3.42	107.11	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	0	1011	CLA	C3B-C4B-NB	-3.41	107.11	110.11
17	2	1011	CLA	C3B-C4B-NB	-3.41	107.11	110.11
17	7	1011	CLA	C3B-C4B-NB	-3.41	107.11	110.11
17	4	1012	CLA	C3B-C4B-NB	-3.41	107.11	110.11
17	2	1013	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	4	1015	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	3	1022	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	9	1011	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	P	5125	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	8	1033	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	P	8010	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	0	1015	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	1	1025	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	8	1012	CLA	C3B-C4B-NB	-3.41	107.12	110.11
17	G	1701	CLA	C3B-C4B-NB	-3.40	107.12	110.11
17	3	1015	CLA	C3B-C4B-NB	-3.40	107.12	110.11
17	3	1012	CLA	C3B-C4B-NB	-3.40	107.12	110.11
17	9	1012	CLA	C3B-C4B-NB	-3.40	107.12	110.11
17	7	1023	CLA	C3B-C4B-NB	-3.40	107.13	110.11
17	1	1023	CLA	C3B-C4B-NB	-3.40	107.13	110.11
17	0	1022	CLA	C3B-C4B-NB	-3.40	107.13	110.11
17	K	1403	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	3	1011	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	F	4005	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	9	1032	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	7	1015	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	3	1032	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	A	4010	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	4	1031	CLA	C3B-C4B-NB	-3.39	107.13	110.11
17	7	1013	CLA	C3B-C4B-NB	-3.39	107.14	110.11
17	0	1012	CLA	C3B-C4B-NB	-3.39	107.14	110.11
17	5	5403	CLA	C3B-C4B-NB	-3.39	107.14	110.11
17	4	1026	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	3	1026	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	2	1012	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	3	1033	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	4	1022	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	H	1801	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	0	1026	CLA	C3B-C4B-NB	-3.38	107.14	110.11
17	8	1021	CLA	C3B-C4B-NB	-3.38	107.15	110.11
17	9	1031	CLA	C3B-C4B-NB	-3.38	107.15	110.11
17	2	1017	CLA	C3B-C4B-NB	-3.37	107.15	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	1016	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	1	1022	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	3	1031	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	8	1011	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	1	1012	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	3	1025	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	2	1023	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	9	1041	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	1	1015	CLA	C3B-C4B-NB	-3.37	107.15	110.11
17	U	8004	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	K	1404	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	J	1101	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	W	5801	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	1	1013	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	V	5701	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	8	1017	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	0	1033	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	A	1125	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	2	1021	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	2	1033	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	Q	8001	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	9	1021	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	7	1031	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	5	5404	CLA	C3B-C4B-NB	-3.36	107.16	110.11
17	9	1026	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	0	1031	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	9	1025	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	7	1012	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	8	1022	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	U	8003	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	4	1033	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	1	1031	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	B	4001	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	F	4003	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	7	1017	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	4	1014	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	B	1242	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	0	1016	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	0	1014	CLA	C3B-C4B-NB	-3.35	107.17	110.11
17	2	1016	CLA	C3B-C4B-NB	-3.34	107.17	110.11
17	A	4009	CLA	C3B-C4B-NB	-3.34	107.17	110.11
17	1	1017	CLA	C3B-C4B-NB	-3.34	107.17	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	1041	CLA	C3B-C4B-NB	-3.34	107.17	110.11
17	3	1021	CLA	C3B-C4B-NB	-3.34	107.18	110.11
17	0	1032	CLA	C3B-C4B-NB	-3.34	107.18	110.11
17	P	5108	CLA	C3B-C4B-NB	-3.34	107.18	110.11
17	0	1017	CLA	C3B-C4B-NB	-3.34	107.18	110.11
17	7	1022	CLA	C3B-C4B-NB	-3.34	107.18	110.11
17	F	4004	CLA	C3B-C4B-NB	-3.33	107.18	110.11
17	Q	5241	CLA	C3B-C4B-NB	-3.33	107.18	110.11
17	0	8002	CLA	C3B-C4B-NB	-3.33	107.18	110.11
17	4	1032	CLA	C3B-C4B-NB	-3.33	107.18	110.11
17	J	4008	CLA	C3B-C4B-NB	-3.33	107.18	110.11
17	Q	5240	CLA	C3B-C4B-NB	-3.33	107.18	110.11
17	2	1014	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	4	4002	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	6	5504	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	4	1023	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	Z	5101	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	9	1016	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	4	1016	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	A	1108	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	1	1021	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	1	1016	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	4	1013	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	7	1016	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	0	1023	CLA	C3B-C4B-NB	-3.33	107.19	110.11
17	7	1026	CLA	C3B-C4B-NB	-3.32	107.19	110.11
17	L	1504	CLA	C3B-C4B-NB	-3.32	107.19	110.11
17	3	1016	CLA	C3B-C4B-NB	-3.32	107.20	110.11
17	4	1017	CLA	C3B-C4B-NB	-3.32	107.20	110.11
17	B	1240	CLA	C3B-C4B-NB	-3.32	107.20	110.11
17	2	1022	CLA	C3B-C4B-NB	-3.31	107.20	110.11
17	7	1021	CLA	C3B-C4B-NB	-3.31	107.20	110.11
17	B	1241	CLA	C3B-C4B-NB	-3.31	107.20	110.11
17	8	1014	CLA	C3B-C4B-NB	-3.31	107.20	110.11
17	P	8009	CLA	C3B-C4B-NB	-3.31	107.20	110.11
17	Q	5242	CLA	C3B-C4B-NB	-3.31	107.20	110.11
17	9	1033	CLA	C3B-C4B-NB	-3.31	107.21	110.11
17	9	1017	CLA	C3B-C4B-NB	-3.30	107.21	110.11
17	0	1013	CLA	C3B-C4B-NB	-3.30	107.21	110.11
17	F	4006	CLA	C3B-C4B-NB	-3.30	107.21	110.11
17	U	8006	CLA	C3B-C4B-NB	-3.30	107.21	110.11
17	4	1025	CLA	C3B-C4B-NB	-3.30	107.21	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	1026	CLA	C3B-C4B-NB	-3.30	107.21	110.11
17	1	1014	CLA	C3B-C4B-NB	-3.30	107.22	110.11
17	2	1026	CLA	C3B-C4B-NB	-3.29	107.22	110.11
17	3	1017	CLA	C3B-C4B-NB	-3.29	107.22	110.11
17	Z	8008	CLA	C3B-C4B-NB	-3.29	107.22	110.11
17	9	1014	CLA	C3B-C4B-NB	-3.29	107.22	110.11
17	2	1031	CLA	C3B-C4B-NB	-3.29	107.22	110.11
17	0	1025	CLA	C3B-C4B-NB	-3.29	107.22	110.11
17	A	1137	CLA	C3B-C4B-NB	-3.28	107.23	110.11
17	3	1014	CLA	C3B-C4B-NB	-3.28	107.23	110.11
17	P	5137	CLA	C3B-C4B-NB	-3.28	107.23	110.11
17	8	1031	CLA	C3B-C4B-NB	-3.27	107.24	110.11
17	2	1015	CLA	C3B-C4B-NB	-3.27	107.24	110.11
17	0	1021	CLA	C3B-C4B-NB	-3.26	107.24	110.11
17	4	1021	CLA	C3B-C4B-NB	-3.26	107.25	110.11
17	8	1026	CLA	C3B-C4B-NB	-3.25	107.25	110.11
17	8	1015	CLA	C3B-C4B-NB	-3.24	107.27	110.11
17	7	1014	CLA	C3B-C4B-NB	-3.24	107.27	110.11
17	Q	5219	CLA	C3C-C4C-NC	-3.19	106.70	109.99
17	P	5137	CLA	C3C-C4C-NC	-3.18	106.71	109.99
17	B	1219	CLA	C3C-C4C-NC	-3.18	106.71	109.99
17	A	1137	CLA	C3C-C4C-NC	-3.17	106.72	109.99
17	B	1224	CLA	C3B-C4B-NB	-3.15	107.35	110.11
17	B	1234	CLA	C3B-C4B-NB	-3.13	107.36	110.11
17	Q	5224	CLA	C3B-C4B-NB	-3.12	107.37	110.11
17	A	1012	CLA	C3B-C4B-NB	-3.11	107.38	110.11
17	Q	5234	CLA	C3B-C4B-NB	-3.09	107.39	110.11
17	P	5012	CLA	C3B-C4B-NB	-3.09	107.40	110.11
17	P	5129	CLA	C3B-C4B-NB	-3.05	107.43	110.11
17	U	5229	CLA	C3B-C4B-NB	-3.05	107.43	110.11
17	A	1129	CLA	C3B-C4B-NB	-3.04	107.44	110.11
17	F	1229	CLA	C3B-C4B-NB	-3.01	107.47	110.11
17	P	5113	CLA	C3C-C4C-NC	-3.00	106.90	109.99
17	A	1113	CLA	C3B-C4B-NB	-2.96	107.51	110.11
17	A	1113	CLA	C3C-C4C-NC	-2.96	106.93	109.99
17	P	5113	CLA	C3B-C4B-NB	-2.96	107.51	110.11
17	Q	5227	CLA	C3B-C4B-NB	-2.94	107.53	110.11
17	B	1227	CLA	C3B-C4B-NB	-2.94	107.53	110.11
17	B	1228	CLA	C3B-C4B-NB	-2.83	107.62	110.11
17	Q	5228	CLA	C3B-C4B-NB	-2.81	107.64	110.11
17	P	5116	CLA	C3B-C4B-NB	-2.81	107.64	110.11
17	A	1901	CLA	C3C-C4C-NC	-2.80	107.10	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1116	CLA	C3B-C4B-NB	-2.79	107.66	110.11
17	P	5901	CLA	C3C-C4C-NC	-2.78	107.12	109.99
17	B	1023	CLA	C3B-C4B-NB	-2.76	107.68	110.11
17	Q	5023	CLA	C3B-C4B-NB	-2.76	107.69	110.11
17	P	5402	CLA	C3B-C4B-NB	-2.71	107.73	110.11
17	Z	5302	CLA	C3C-C4C-NC	-2.70	107.20	109.99
17	J	1302	CLA	C3C-C4C-NC	-2.70	107.20	109.99
17	Q	5232	CLA	C3B-C4B-NB	-2.70	107.74	110.11
17	A	1402	CLA	C3B-C4B-NB	-2.67	107.76	110.11
17	B	1232	CLA	C3B-C4B-NB	-2.67	107.76	110.11
17	Q	5219	CLA	C3B-C4B-NB	-2.67	107.77	110.11
17	Q	5204	CLA	C3B-C4B-NB	-2.66	107.77	110.11
17	B	1204	CLA	C3B-C4B-NB	-2.65	107.78	110.11
17	P	5132	CLA	C3B-C4B-NB	-2.65	107.79	110.11
17	Q	5218	CLA	C3B-C4B-NB	-2.63	107.80	110.11
17	J	1302	CLA	C2B-C1B-NB	-2.63	107.80	110.11
17	A	1132	CLA	C3B-C4B-NB	-2.63	107.80	110.11
17	B	1219	CLA	C3B-C4B-NB	-2.62	107.81	110.11
17	Q	5223	CLA	C3B-C4B-NB	-2.62	107.81	110.11
17	P	5120	CLA	C3B-C4B-NB	-2.61	107.82	110.11
17	Z	5302	CLA	C2B-C1B-NB	-2.60	107.83	110.11
17	B	1218	CLA	C3B-C4B-NB	-2.60	107.83	110.11
17	Q	5207	CLA	C2B-C1B-NB	-2.59	107.83	110.11
17	Q	5238	CLA	C2B-C1B-NB	-2.59	107.84	110.11
17	B	1238	CLA	C2B-C1B-NB	-2.59	107.84	110.11
17	Q	5206	CLA	C2B-C1B-NB	-2.58	107.85	110.11
18	B	2002	PQN	C2-C3-C4	-2.57	119.57	123.17
18	Q	6002	PQN	C2-C3-C4	-2.57	119.58	123.17
17	A	1120	CLA	C3B-C4B-NB	-2.57	107.86	110.11
17	A	1107	CLA	C3B-C4B-NB	-2.56	107.86	110.11
17	B	1223	CLA	C3B-C4B-NB	-2.56	107.86	110.11
17	A	1108	CLA	C2B-C1B-NB	-2.56	107.86	110.11
17	B	1207	CLA	C2B-C1B-NB	-2.56	107.86	110.11
17	P	5107	CLA	C3B-C4B-NB	-2.55	107.87	110.11
17	Q	5210	CLA	C3B-C4B-NB	-2.55	107.87	110.11
17	P	5108	CLA	C2B-C1B-NB	-2.55	107.87	110.11
17	Q	5207	CLA	C3D-C2D-C1D	-2.55	104.11	106.30
17	B	1210	CLA	C3B-C4B-NB	-2.54	107.88	110.11
17	B	1207	CLA	C3D-C2D-C1D	-2.53	104.12	106.30
17	B	1206	CLA	C2B-C1B-NB	-2.53	107.89	110.11
17	P	5110	CLA	C3B-C4B-NB	-2.51	107.90	110.11
17	P	5140	CLA	C3B-C4B-NB	-2.51	107.90	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1110	CLA	C3B-C4B-NB	-2.50	107.91	110.11
17	B	1227	CLA	C3C-C4C-NC	-2.50	107.41	109.99
17	P	5118	CLA	C3B-C4B-NB	-2.49	107.92	110.11
18	P	6001	PQN	C2-C3-C4	-2.49	119.68	123.17
17	Q	5227	CLA	C3C-C4C-NC	-2.49	107.42	109.99
18	A	2001	PQN	C2-C3-C4	-2.49	119.69	123.17
17	P	5108	CLA	C3C-C4C-NC	-2.48	107.43	109.99
17	A	1118	CLA	C3B-C4B-NB	-2.48	107.93	110.11
17	B	1235	CLA	C3B-C4B-NB	-2.48	107.94	110.11
17	A	1140	CLA	C3B-C4B-NB	-2.47	107.94	110.11
17	A	1108	CLA	C3C-C4C-NC	-2.47	107.44	109.99
17	Q	5203	CLA	C3B-C4B-NB	-2.45	107.96	110.11
17	B	1203	CLA	C3B-C4B-NB	-2.44	107.97	110.11
17	A	1113	CLA	C2B-C1B-NB	-2.44	107.97	110.11
17	Q	5207	CLA	C3B-C4B-NB	-2.43	107.97	110.11
17	P	5113	CLA	C2B-C1B-NB	-2.43	107.97	110.11
17	Q	5235	CLA	C3B-C4B-NB	-2.42	107.98	110.11
17	P	5137	CLA	C2B-C1B-NB	-2.40	108.00	110.11
17	P	5128	CLA	C3B-C4B-NB	-2.39	108.01	110.11
17	B	1207	CLA	C3B-C4B-NB	-2.39	108.01	110.11
17	Q	5216	CLA	C3B-C4B-NB	-2.38	108.02	110.11
17	A	1111	CLA	C3B-C4B-NB	-2.38	108.02	110.11
17	P	5111	CLA	C3B-C4B-NB	-2.36	108.03	110.11
17	B	1216	CLA	C3B-C4B-NB	-2.36	108.03	110.11
17	A	1134	CLA	C3B-C4B-NB	-2.36	108.03	110.11
17	A	1137	CLA	C2B-C1B-NB	-2.36	108.03	110.11
17	A	1128	CLA	C3B-C4B-NB	-2.35	108.05	110.11
17	6	5503	CLA	C3B-C4B-NB	-2.34	108.06	110.11
17	L	1503	CLA	C3B-C4B-NB	-2.33	108.06	110.11
17	P	5134	CLA	C3B-C4B-NB	-2.31	108.08	110.11
17	B	1237	CLA	C3D-C2D-C1D	-2.30	104.32	106.30
17	Q	5237	CLA	C3D-C2D-C1D	-2.29	104.33	106.30
17	6	5502	CLA	C3C-C4C-NC	-2.28	107.64	109.99
17	Q	5212	CLA	C3B-C4B-NB	-2.27	108.11	110.11
17	A	1103	CLA	C3B-C4B-NB	-2.26	108.12	110.11
17	P	5103	CLA	C3B-C4B-NB	-2.26	108.12	110.11
17	L	1502	CLA	C3C-C4C-NC	-2.25	107.67	109.99
17	B	1212	CLA	C3B-C4B-NB	-2.25	108.14	110.11
17	Q	5220	CLA	C3B-C4B-NB	-2.23	108.15	110.11
17	B	1213	CLA	C3B-C4B-NB	-2.22	108.16	110.11
17	P	5104	CLA	C3B-C4B-NB	-2.22	108.16	110.11
17	P	5119	CLA	C3B-C4B-NB	-2.21	108.17	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1112	CLA	C3B-C4B-NB	-2.21	108.17	110.11
17	P	5132	CLA	C3D-C2D-C1D	-2.21	104.40	106.30
17	A	1104	CLA	C3B-C4B-NB	-2.21	108.17	110.11
17	P	5114	CLA	C3B-C4B-NB	-2.21	108.17	110.11
17	A	1138	CLA	C3B-C4B-NB	-2.21	108.17	110.11
17	A	1119	CLA	C3B-C4B-NB	-2.20	108.17	110.11
17	Q	5213	CLA	C3B-C4B-NB	-2.20	108.18	110.11
17	P	5112	CLA	C3B-C4B-NB	-2.20	108.18	110.11
17	Q	5238	CLA	C3C-C4C-NC	-2.20	107.72	109.99
17	P	5138	CLA	C3B-C4B-NB	-2.20	108.18	110.11
17	B	1231	CLA	C3C-C4C-NC	-2.19	107.73	109.99
17	B	1220	CLA	C3B-C4B-NB	-2.18	108.19	110.11
17	A	1012	CLA	C3D-C2D-C1D	-2.18	104.43	106.30
17	B	1204	CLA	C3C-C4C-NC	-2.17	107.75	109.99
17	P	5012	CLA	C3D-C2D-C1D	-2.17	104.43	106.30
17	B	1238	CLA	C3C-C4C-NC	-2.17	107.75	109.99
17	A	1122	CLA	C3B-C4B-NB	-2.17	108.21	110.11
17	L	1501	CLA	C3D-C2D-C1D	-2.17	104.44	106.30
17	Q	5231	CLA	C3C-C4C-NC	-2.17	107.75	109.99
17	F	1301	CLA	C3B-C4B-NB	-2.17	108.21	110.11
17	Q	5204	CLA	C3C-C4C-NC	-2.16	107.76	109.99
17	5	5401	CLA	C3B-C4B-NB	-2.16	108.21	110.11
17	B	1217	CLA	C3B-C4B-NB	-2.16	108.21	110.11
17	A	1132	CLA	C3D-C2D-C1D	-2.16	104.44	106.30
17	Q	5209	CLA	C3B-C4B-NB	-2.16	108.21	110.11
17	B	1209	CLA	C3B-C4B-NB	-2.16	108.22	110.11
17	P	5122	CLA	C3B-C4B-NB	-2.15	108.22	110.11
17	B	1235	CLA	C3C-C4C-NC	-2.15	107.77	109.99
17	A	1114	CLA	C3B-C4B-NB	-2.15	108.22	110.11
17	A	1136	CLA	C3C-C4C-NC	-2.15	107.77	109.99
17	6	5501	CLA	C3D-C2D-C1D	-2.15	104.45	106.30
17	Q	5214	CLA	C3B-C4B-NB	-2.14	108.22	110.11
17	A	1133	CLA	C3B-C4B-NB	-2.14	108.23	110.11
17	P	5133	CLA	C3B-C4B-NB	-2.14	108.23	110.11
17	P	5136	CLA	C3C-C4C-NC	-2.14	107.78	109.99
17	U	5301	CLA	C3B-C4B-NB	-2.14	108.23	110.11
17	A	1124	CLA	C3D-C2D-C1D	-2.14	104.46	106.30
17	B	1237	CLA	C3B-C4B-NB	-2.13	108.24	110.11
17	B	1201	CLA	C3D-C2D-C1D	-2.13	104.47	106.30
17	B	1228	CLA	C3D-C2D-C1D	-2.13	104.47	106.30
17	Q	5235	CLA	C3C-C4C-NC	-2.13	107.79	109.99
17	P	5011	CLA	C2B-C1B-NB	-2.13	108.24	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	5223	CLA	C2B-C1B-NB	-2.13	108.24	110.11
17	B	1214	CLA	C3B-C4B-NB	-2.13	108.24	110.11
17	P	5106	CLA	C3B-C4B-NB	-2.13	108.24	110.11
17	Q	5217	CLA	C3B-C4B-NB	-2.13	108.24	110.11
17	K	1401	CLA	C3B-C4B-NB	-2.13	108.24	110.11
17	Q	5201	CLA	C3D-C2D-C1D	-2.13	104.47	106.30
17	P	5125	CLA	C3D-C2D-C1D	-2.12	104.47	106.30
17	P	5111	CLA	C3D-C2D-C1D	-2.11	104.48	106.30
17	P	5133	CLA	C3C-C4C-NC	-2.11	107.81	109.99
17	A	1106	CLA	C3B-C4B-NB	-2.11	108.25	110.11
17	Q	5237	CLA	C3B-C4B-NB	-2.11	108.25	110.11
17	A	1011	CLA	C2B-C1B-NB	-2.11	108.25	110.11
17	B	1223	CLA	C2B-C1B-NB	-2.11	108.26	110.11
17	P	5124	CLA	C3D-C2D-C1D	-2.11	104.49	106.30
17	Q	5228	CLA	C3D-C2D-C1D	-2.11	104.49	106.30
17	B	1211	CLA	C3B-C4B-NB	-2.10	108.26	110.11
17	P	5110	CLA	C3C-C4C-NC	-2.09	107.83	109.99
17	A	1125	CLA	C3D-C2D-C1D	-2.09	104.50	106.30
17	A	1111	CLA	C3D-C2D-C1D	-2.09	104.50	106.30
17	A	1133	CLA	C3C-C4C-NC	-2.08	107.84	109.99
17	A	1110	CLA	C3C-C4C-NC	-2.07	107.85	109.99
17	Q	5211	CLA	C3B-C4B-NB	-2.06	108.30	110.11
17	B	1210	CLA	C3D-C2D-C1D	-2.05	104.53	106.30
17	B	1208	CLA	C3B-C4B-NB	-2.05	108.31	110.11
17	Q	5223	CLA	C3D-C2D-C1D	-2.05	104.54	106.30
17	A	1131	CLA	C3C-C4C-NC	-2.05	107.88	109.99
17	P	5013	CLA	C3D-C2D-C1D	-2.04	104.55	106.30
17	V	5233	CLA	C3B-C4B-NB	-2.04	108.32	110.11
17	P	5131	CLA	C3C-C4C-NC	-2.04	107.89	109.99
17	B	1219	CLA	C2B-C1B-NB	-2.04	108.32	110.11
17	Q	5230	CLA	C3D-C2D-C1D	-2.03	104.56	106.30
17	G	1233	CLA	C3B-C4B-NB	-2.03	108.33	110.11
17	Q	5208	CLA	C3B-C4B-NB	-2.02	108.33	110.11
17	6	5501	CLA	C3B-C4B-NB	-2.02	108.33	110.11
17	Q	5237	CLA	C3C-C4C-NC	-2.02	107.91	109.99
17	B	1237	CLA	C3C-C4C-NC	-2.01	107.91	109.99
17	Q	5238	CLA	C3D-C2D-C1D	-2.01	104.57	106.30
17	Q	5210	CLA	C3D-C2D-C1D	-2.01	104.57	106.30
17	Q	5023	CLA	C3C-C4C-NC	-2.01	107.91	109.99
17	L	1501	CLA	C3B-C4B-NB	-2.01	108.34	110.11
17	B	1238	CLA	C3D-C2D-C1D	-2.01	104.57	106.30
17	P	5104	CLA	C1C-NC-C4C	2.00	108.52	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	5231	CLA	C2A-C1A-CHA	2.01	126.07	122.63
17	P	5011	CLA	C2D-C1D-ND	2.02	111.89	110.14
17	B	1231	CLA	C2A-C1A-CHA	2.02	126.08	122.63
17	Q	5023	CLA	C2A-C1A-CHA	2.03	126.09	122.63
17	Q	5226	CLA	C1C-NC-C4C	2.04	108.55	106.23
17	B	1023	CLA	C2A-C1A-CHA	2.04	126.11	122.63
17	P	5124	CLA	C2A-C1A-CHA	2.04	126.12	122.63
17	B	1230	CLA	C2A-C1A-CHA	2.05	126.12	122.63
17	B	1206	CLA	C1C-NC-C4C	2.05	108.56	106.23
17	A	1124	CLA	C2A-C1A-CHA	2.05	126.13	122.63
17	B	1205	CLA	C2A-C1A-CHA	2.05	126.13	122.63
17	Q	5230	CLA	C2A-C1A-CHA	2.05	126.13	122.63
17	B	1205	CLA	C1C-NC-C4C	2.05	108.57	106.23
17	A	1127	CLA	C1C-NC-C4C	2.06	108.58	106.23
17	P	5127	CLA	C1C-NC-C4C	2.06	108.58	106.23
17	Q	5205	CLA	C2A-C1A-CHA	2.06	126.16	122.63
17	A	1011	CLA	C2D-C1D-ND	2.07	111.94	110.14
17	Q	5206	CLA	C1C-NC-C4C	2.07	108.60	106.23
17	F	1301	CLA	C1C-NC-C4C	2.08	108.60	106.23
17	A	1011	CLA	C1C-NC-C4C	2.08	108.60	106.23
17	P	5011	CLA	C1C-NC-C4C	2.08	108.60	106.23
17	A	1115	CLA	C2A-C1A-CHA	2.08	126.18	122.63
17	P	5115	CLA	C2A-C1A-CHA	2.08	126.18	122.63
17	Q	5205	CLA	C1C-NC-C4C	2.08	108.61	106.23
17	B	1226	CLA	C1C-NC-C4C	2.08	108.61	106.23
17	U	5301	CLA	C1C-NC-C4C	2.08	108.61	106.23
17	B	1130	CLA	C1C-NC-C4C	2.09	108.61	106.23
17	P	5103	CLA	C2A-C1A-CHA	2.09	126.20	122.63
17	A	1103	CLA	C2A-C1A-CHA	2.10	126.22	122.63
17	A	1103	CLA	C1C-NC-C4C	2.11	108.64	106.23
17	Q	5130	CLA	C1C-NC-C4C	2.12	108.65	106.23
17	4	1023	CLA	C1C-NC-C4C	2.12	108.65	106.23
17	P	5103	CLA	C1C-NC-C4C	2.12	108.65	106.23
17	A	1119	CLA	C2A-C1A-CHA	2.13	126.27	122.63
17	8	1022	CLA	C1C-NC-C4C	2.13	108.66	106.23
17	0	1023	CLA	C1C-NC-C4C	2.14	108.67	106.23
17	B	1212	CLA	C1C-NC-C4C	2.15	108.68	106.23
17	P	5119	CLA	C2A-C1A-CHA	2.15	126.30	122.63
17	2	1022	CLA	C1C-NC-C4C	2.15	108.69	106.23
17	8	1025	CLA	C1C-NC-C4C	2.16	108.69	106.23
17	A	1115	CLA	C1C-NC-C4C	2.16	108.70	106.23
17	0	1021	CLA	C1C-NC-C4C	2.16	108.70	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	5115	CLA	C1C-NC-C4C	2.17	108.71	106.23
17	2	1031	CLA	C1C-NC-C4C	2.17	108.71	106.23
17	B	1242	CLA	C1C-NC-C4C	2.17	108.71	106.23
17	Q	5203	CLA	C2A-C1A-CHA	2.17	126.34	122.63
17	2	1025	CLA	C1C-NC-C4C	2.18	108.71	106.23
17	8	1031	CLA	C1C-NC-C4C	2.18	108.71	106.23
17	7	1031	CLA	C1C-NC-C4C	2.18	108.72	106.23
17	B	1203	CLA	C2A-C1A-CHA	2.18	126.36	122.63
17	3	1016	CLA	C1C-NC-C4C	2.18	108.72	106.23
17	0	1015	CLA	C1C-NC-C4C	2.18	108.72	106.23
17	9	1033	CLA	C1C-NC-C4C	2.18	108.72	106.23
17	2	4007	CLA	C1C-NC-C4C	2.19	108.72	106.23
17	8	1033	CLA	C1C-NC-C4C	2.19	108.72	106.23
17	P	5139	CLA	C1C-NC-C4C	2.19	108.72	106.23
17	Q	5212	CLA	C1C-NC-C4C	2.19	108.72	106.23
17	Q	5242	CLA	C1C-NC-C4C	2.19	108.72	106.23
17	B	1235	CLA	C2A-C1A-CHA	2.19	126.36	122.63
17	9	1016	CLA	C1C-NC-C4C	2.19	108.73	106.23
17	3	1014	CLA	C1C-NC-C4C	2.19	108.73	106.23
17	4	1021	CLA	C1C-NC-C4C	2.19	108.73	106.23
17	1	1022	CLA	C1C-NC-C4C	2.19	108.73	106.23
17	2	1014	CLA	C1C-NC-C4C	2.19	108.73	106.23
17	0	8002	CLA	C1C-NC-C4C	2.19	108.73	106.23
17	3	1026	CLA	C1C-NC-C4C	2.20	108.73	106.23
17	5	5403	CLA	C1C-NC-C4C	2.20	108.73	106.23
17	Q	5235	CLA	C2A-C1A-CHA	2.20	126.38	122.63
17	1	1031	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	2	1033	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	7	1016	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	K	1403	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	A	1139	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	4	1025	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	8	1023	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	1	1016	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	4	1022	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	8	1011	CLA	C1C-NC-C4C	2.20	108.74	106.23
17	2	1023	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	2	1017	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	7	1022	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	9	1012	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	W	5801	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	8	1021	CLA	C1C-NC-C4C	2.21	108.75	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	1021	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	7	1025	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	8	1026	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	4	1015	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	0	1017	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	7	1011	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	P	5105	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	3	1015	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	H	1801	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	1	1013	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	1	1021	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	7	1021	CLA	C1C-NC-C4C	2.21	108.75	106.23
17	Z	5101	CLA	C1C-NC-C4C	2.21	108.76	106.23
17	4	1031	CLA	C1C-NC-C4C	2.21	108.76	106.23
17	8	1014	CLA	C1C-NC-C4C	2.21	108.76	106.23
17	3	1012	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	0	1011	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	7	1015	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	0	1026	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	9	1017	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	8	8007	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	4	4002	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	0	1031	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	1	1025	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	F	4003	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	3	1017	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	P	5140	CLA	C2A-C1A-CHA	2.22	126.42	122.63
17	0	1022	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	9	1041	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	8	1013	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	9	1014	CLA	C1C-NC-C4C	2.22	108.76	106.23
17	9	1026	CLA	C1C-NC-C4C	2.22	108.77	106.23
17	0	1025	CLA	C1C-NC-C4C	2.22	108.77	106.23
17	1	1023	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	4	1014	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	4	1017	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	3	1021	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	U	8006	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	2	1015	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	A	1105	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	A	1140	CLA	C2A-C1A-CHA	2.23	126.43	122.63
17	2	1013	CLA	C1C-NC-C4C	2.23	108.77	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	1026	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	3	1025	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	8	1016	CLA	C1C-NC-C4C	2.23	108.77	106.23
17	7	1014	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	7	1012	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	4	1033	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	0	1016	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	J	1101	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	5	5404	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	Q	5232	CLA	C3B-C2B-C1B	2.23	108.20	106.29
17	4	1011	CLA	C1C-NC-C4C	2.23	108.78	106.23
17	P	5131	CLA	C2A-C1A-CHA	2.24	126.45	122.63
17	9	1015	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	3	1011	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	B	1232	CLA	C3B-C2B-C1B	2.24	108.20	106.29
17	B	1240	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	9	1031	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	7	1023	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	1	1015	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	6	5504	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	J	4008	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	9	1011	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	9	1022	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	Q	5240	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	9	1025	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	9	1021	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	8	1017	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	7	1013	CLA	C1C-NC-C4C	2.24	108.78	106.23
17	Q	5224	CLA	C2A-C1A-CHA	2.24	126.46	122.63
17	A	1131	CLA	C2A-C1A-CHA	2.24	126.46	122.63
17	8	1015	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	U	8003	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	1	1012	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	3	1033	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	1	1011	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	Q	5225	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	0	1013	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	7	1017	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	Q	8001	CLA	C1C-NC-C4C	2.24	108.79	106.23
17	B	1225	CLA	C1C-NC-C4C	2.25	108.79	106.23
17	2	1026	CLA	C1C-NC-C4C	2.25	108.79	106.23
17	0	1014	CLA	C1C-NC-C4C	2.25	108.79	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	4006	CLA	C1C-NC-C4C	2.25	108.79	106.23
17	Q	5234	CLA	C1C-NC-C4C	2.25	108.79	106.23
17	K	1404	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	0	1033	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	P	8009	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	A	4009	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	L	1504	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	B	4001	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	3	1032	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	B	1234	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	1	1014	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	3	1022	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	4	1026	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	G	1701	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	3	1031	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	4	1013	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	A	4010	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	3	1041	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	F	4004	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	2	1011	CLA	C1C-NC-C4C	2.25	108.80	106.23
17	2	1016	CLA	C1C-NC-C4C	2.26	108.80	106.23
17	Z	8008	CLA	C1C-NC-C4C	2.26	108.80	106.23
17	4	1016	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	U	8004	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	B	1224	CLA	C2A-C1A-CHA	2.26	126.49	122.63
17	U	8005	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	4	1032	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	9	1032	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	1	1017	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	B	1241	CLA	C1C-NC-C4C	2.26	108.81	106.23
17	P	8010	CLA	C1C-NC-C4C	2.27	108.82	106.23
17	2	1012	CLA	C1C-NC-C4C	2.27	108.82	106.23
17	7	1026	CLA	C1C-NC-C4C	2.27	108.82	106.23
17	F	4005	CLA	C1C-NC-C4C	2.27	108.82	106.23
17	B	1226	CLA	C2A-C1A-CHA	2.27	126.51	122.63
17	Q	5241	CLA	C1C-NC-C4C	2.27	108.82	106.23
17	A	1013	CLA	C2A-C1A-CHA	2.28	126.52	122.63
17	0	1032	CLA	C1C-NC-C4C	2.28	108.83	106.23
17	Q	5226	CLA	C2A-C1A-CHA	2.29	126.54	122.63
17	V	5701	CLA	C1C-NC-C4C	2.29	108.84	106.23
17	P	5107	CLA	C1C-NC-C4C	2.30	108.85	106.23
17	P	5013	CLA	C2A-C1A-CHA	2.31	126.57	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	1012	CLA	C1C-NC-C4C	2.31	108.87	106.23
17	P	5117	CLA	C1C-NC-C4C	2.32	108.88	106.23
17	A	1107	CLA	C1C-NC-C4C	2.32	108.88	106.23
17	B	1238	CLA	C1C-NC-C4C	2.33	108.89	106.23
17	A	1109	CLA	C1C-NC-C4C	2.34	108.90	106.23
17	B	1239	CLA	C1C-NC-C4C	2.35	108.91	106.23
17	4	1012	CLA	C1C-NC-C4C	2.35	108.91	106.23
17	P	5109	CLA	C1C-NC-C4C	2.35	108.91	106.23
17	0	1012	CLA	C1C-NC-C4C	2.35	108.92	106.23
17	Q	5224	CLA	C1C-NC-C4C	2.36	108.92	106.23
17	A	1117	CLA	C1C-NC-C4C	2.36	108.92	106.23
17	Q	5021	CLA	C1C-NC-C4C	2.36	108.92	106.23
17	A	1125	CLA	C1C-NC-C4C	2.36	108.92	106.23
17	Q	5238	CLA	C1C-NC-C4C	2.36	108.92	106.23
17	A	1124	CLA	C1C-NC-C4C	2.36	108.93	106.23
17	P	5125	CLA	C1C-NC-C4C	2.37	108.93	106.23
17	B	1215	CLA	C2A-C1A-CHA	2.37	126.68	122.63
17	A	1128	CLA	C2A-C1A-CHA	2.37	126.68	122.63
17	B	1206	CLA	C3B-C2B-C1B	2.37	108.32	106.29
17	Q	5215	CLA	C2A-C1A-CHA	2.38	126.69	122.63
17	Q	5206	CLA	C3B-C2B-C1B	2.38	108.32	106.29
17	P	5124	CLA	C1C-NC-C4C	2.38	108.94	106.23
17	P	5128	CLA	C2A-C1A-CHA	2.38	126.69	122.63
17	Q	5201	CLA	C2A-C1A-CHA	2.39	126.70	122.63
17	B	1021	CLA	C1C-NC-C4C	2.39	108.95	106.23
17	Q	5239	CLA	C1C-NC-C4C	2.39	108.96	106.23
17	P	5128	CLA	C1C-NC-C4C	2.39	108.96	106.23
17	Q	5236	CLA	C2A-C1A-CHA	2.39	126.72	122.63
17	B	1201	CLA	C2A-C1A-CHA	2.40	126.72	122.63
17	B	1224	CLA	C1C-NC-C4C	2.40	108.96	106.23
17	P	5137	CLA	C2A-C1A-CHA	2.40	126.72	122.63
17	A	1128	CLA	C1C-NC-C4C	2.40	108.97	106.23
17	B	1236	CLA	C2A-C1A-CHA	2.40	126.73	122.63
17	A	1133	CLA	C2A-C1A-CHA	2.40	126.73	122.63
17	P	5131	CLA	C1C-NC-C4C	2.40	108.97	106.23
17	P	5133	CLA	C2A-C1A-CHA	2.40	126.73	122.63
17	A	1137	CLA	C2A-C1A-CHA	2.41	126.74	122.63
17	6	5501	CLA	C1C-NC-C4C	2.41	108.98	106.23
17	L	1501	CLA	C1C-NC-C4C	2.41	108.98	106.23
17	Q	5213	CLA	C1C-NC-C4C	2.42	108.99	106.23
17	Q	5209	CLA	C2A-C1A-CHA	2.43	126.77	122.63
17	B	1213	CLA	C1C-NC-C4C	2.43	109.00	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1131	CLA	C1C-NC-C4C	2.43	109.00	106.23
17	B	1219	CLA	C2A-C1A-CHA	2.43	126.78	122.63
17	Q	5219	CLA	C2A-C1A-CHA	2.44	126.79	122.63
17	P	5901	CLA	CHD-C4C-NC	2.44	127.37	124.50
17	B	1209	CLA	C2A-C1A-CHA	2.44	126.80	122.63
17	A	1013	CLA	C1C-NC-C4C	2.44	109.02	106.23
17	B	1222	CLA	C1C-NC-C4C	2.46	109.03	106.23
17	P	5132	CLA	C1C-NC-C4C	2.46	109.03	106.23
17	Q	5222	CLA	C1C-NC-C4C	2.46	109.04	106.23
17	A	1111	CLA	C1C-NC-C4C	2.46	109.04	106.23
17	Q	5216	CLA	C1C-NC-C4C	2.47	109.04	106.23
17	B	1021	CLA	C2A-C1A-CHA	2.47	126.85	122.63
17	P	5013	CLA	C1C-NC-C4C	2.47	109.05	106.23
17	Q	5021	CLA	C2A-C1A-CHA	2.47	126.85	122.63
17	P	5111	CLA	C1C-NC-C4C	2.47	109.05	106.23
17	B	1216	CLA	C1C-NC-C4C	2.47	109.05	106.23
17	5	5401	CLA	C1C-NC-C4C	2.48	109.05	106.23
17	B	1230	CLA	C1C-NC-C4C	2.48	109.06	106.23
17	A	1132	CLA	C1C-NC-C4C	2.48	109.06	106.23
17	K	1401	CLA	C1C-NC-C4C	2.48	109.06	106.23
17	A	1114	CLA	C1C-NC-C4C	2.48	109.06	106.23
17	A	1104	CLA	C2A-C3A-C4A	2.48	106.64	103.78
17	P	5121	CLA	C1C-NC-C4C	2.49	109.07	106.23
17	A	1121	CLA	C1C-NC-C4C	2.49	109.07	106.23
17	P	5104	CLA	C2A-C3A-C4A	2.49	106.65	103.78
17	P	5114	CLA	C1C-NC-C4C	2.49	109.07	106.23
17	Q	5230	CLA	C1C-NC-C4C	2.49	109.07	106.23
17	A	1901	CLA	CHD-C4C-NC	2.49	127.44	124.50
17	Q	5228	CLA	C2A-C1A-CHA	2.49	126.89	122.63
17	A	1140	CLA	C1C-NC-C4C	2.51	109.09	106.23
17	Q	5206	CLA	C2A-C1A-CHA	2.51	126.92	122.63
17	Q	5213	CLA	C2A-C1A-CHA	2.51	126.92	122.63
17	P	5140	CLA	C1C-NC-C4C	2.51	109.10	106.23
17	A	1128	CLA	C3B-C2B-C1B	2.51	108.44	106.29
17	P	5122	CLA	C2A-C1A-CHA	2.52	126.92	122.63
17	P	5127	CLA	C2A-C1A-CHA	2.52	126.92	122.63
17	A	1122	CLA	C2A-C1A-CHA	2.52	126.93	122.63
17	Q	5236	CLA	C1C-NC-C4C	2.52	109.10	106.23
17	B	1206	CLA	C2A-C1A-CHA	2.52	126.93	122.63
17	B	1228	CLA	C2A-C1A-CHA	2.52	126.94	122.63
17	P	5128	CLA	C3B-C2B-C1B	2.53	108.45	106.29
17	B	1236	CLA	C1C-NC-C4C	2.53	109.11	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1127	CLA	C2A-C1A-CHA	2.53	126.95	122.63
17	K	1401	CLA	C2A-C1A-CHA	2.53	126.96	122.63
17	A	1106	CLA	C2A-C1A-CHA	2.53	126.96	122.63
17	5	5401	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	B	1213	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	P	5109	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	B	1211	CLA	C2A-C1A-CHA	2.54	126.96	122.63
17	A	1109	CLA	C2A-C1A-CHA	2.54	126.97	122.63
17	B	1227	CLA	C2A-C1A-CHA	2.55	126.98	122.63
17	P	5106	CLA	C2A-C1A-CHA	2.55	126.98	122.63
17	B	1234	CLA	C2A-C1A-CHA	2.55	126.99	122.63
17	Q	5211	CLA	C2A-C1A-CHA	2.56	127.00	122.63
17	B	1211	CLA	C1C-NC-C4C	2.58	109.17	106.23
17	Q	5234	CLA	C2A-C1A-CHA	2.58	127.03	122.63
17	B	1217	CLA	C1C-NC-C4C	2.58	109.17	106.23
17	A	1138	CLA	C2A-C1A-CHA	2.58	127.04	122.63
17	P	5138	CLA	C2A-C1A-CHA	2.58	127.04	122.63
17	A	1129	CLA	C2A-C1A-CHA	2.59	127.04	122.63
17	P	5110	CLA	C2A-C1A-CHA	2.59	127.05	122.63
17	A	1110	CLA	C2A-C1A-CHA	2.59	127.05	122.63
17	Q	5221	CLA	C1C-NC-C4C	2.59	109.18	106.23
17	Q	5227	CLA	C2A-C1A-CHA	2.59	127.05	122.63
17	B	1221	CLA	C1C-NC-C4C	2.59	109.19	106.23
17	P	5129	CLA	C2A-C1A-CHA	2.59	127.06	122.63
17	A	1102	CLA	C1C-NC-C4C	2.60	109.19	106.23
17	P	5136	CLA	C1C-NC-C4C	2.60	109.20	106.23
17	L	1503	CLA	C1C-NC-C4C	2.60	109.20	106.23
17	P	5102	CLA	C1C-NC-C4C	2.61	109.20	106.23
17	Q	5217	CLA	C1C-NC-C4C	2.61	109.20	106.23
17	V	5233	CLA	C1C-NC-C4C	2.61	109.21	106.23
17	G	1233	CLA	C1C-NC-C4C	2.61	109.21	106.23
17	Q	5208	CLA	C1C-NC-C4C	2.61	109.21	106.23
17	B	1208	CLA	C1C-NC-C4C	2.62	109.21	106.23
17	6	5503	CLA	C1C-NC-C4C	2.62	109.21	106.23
17	A	1136	CLA	C1C-NC-C4C	2.62	109.22	106.23
17	Q	5220	CLA	C2A-C1A-CHA	2.62	127.10	122.63
17	Q	5211	CLA	C1C-NC-C4C	2.63	109.23	106.23
17	Q	5214	CLA	C1C-NC-C4C	2.63	109.23	106.23
17	Q	5223	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	B	1208	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	B	1225	CLA	C2A-C1A-CHA	2.63	127.12	122.63
17	B	1220	CLA	C2A-C1A-CHA	2.63	127.12	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1133	CLA	C1C-NC-C4C	2.63	109.23	106.23
17	B	1214	CLA	C1C-NC-C4C	2.64	109.23	106.23
17	B	1216	CLA	C2A-C1A-CHA	2.64	127.13	122.63
17	Q	5216	CLA	C2A-C1A-CHA	2.64	127.13	122.63
17	Q	5225	CLA	C2A-C1A-CHA	2.64	127.14	122.63
17	Q	5209	CLA	C1C-NC-C4C	2.64	109.24	106.23
17	Q	5208	CLA	C2A-C1A-CHA	2.64	127.14	122.63
17	P	5133	CLA	C1C-NC-C4C	2.65	109.25	106.23
17	Q	5130	CLA	C2A-C1A-CHA	2.65	127.15	122.63
17	B	1223	CLA	C2A-C1A-CHA	2.65	127.15	122.63
17	B	1022	CLA	C2A-C1A-CHA	2.65	127.16	122.63
17	B	1130	CLA	C2A-C1A-CHA	2.65	127.16	122.63
17	B	1209	CLA	C1C-NC-C4C	2.65	109.25	106.23
17	Q	5022	CLA	C2A-C1A-CHA	2.65	127.16	122.63
17	L	1501	CLA	C2A-C1A-CHA	2.66	127.17	122.63
17	B	1201	CLA	C1C-NC-C4C	2.66	109.27	106.23
17	A	1126	CLA	C2A-C1A-CHA	2.66	127.18	122.63
17	P	5126	CLA	C2A-C1A-CHA	2.68	127.20	122.63
17	6	5501	CLA	C2A-C1A-CHA	2.68	127.20	122.63
17	A	1402	CLA	C2A-C1A-CHA	2.68	127.21	122.63
17	A	1121	CLA	C2A-C1A-CHA	2.69	127.22	122.63
17	A	1110	CLA	C1C-NC-C4C	2.69	109.30	106.23
17	P	5402	CLA	C2A-C1A-CHA	2.69	127.22	122.63
17	P	5125	CLA	C2A-C1A-CHA	2.69	127.23	122.63
17	A	1125	CLA	C2A-C1A-CHA	2.69	127.23	122.63
17	P	5121	CLA	C2A-C1A-CHA	2.70	127.23	122.63
17	Q	5201	CLA	C1C-NC-C4C	2.70	109.31	106.23
17	P	5110	CLA	C1C-NC-C4C	2.71	109.33	106.23
17	U	8005	CLA	C2A-C1A-CHA	2.72	127.28	122.63
17	Q	5241	CLA	C2A-C1A-CHA	2.73	127.28	122.63
17	P	5012	CLA	C1C-NC-C4C	2.73	109.34	106.23
17	8	1011	CLA	C2A-C1A-CHA	2.73	127.29	122.63
17	0	1025	CLA	C2A-C1A-CHA	2.73	127.29	122.63
17	Q	5218	CLA	C1C-NC-C4C	2.73	109.34	106.23
17	4	1025	CLA	C2A-C1A-CHA	2.73	127.30	122.63
17	0	1031	CLA	C2A-C1A-CHA	2.73	127.30	122.63
17	4	1031	CLA	C2A-C1A-CHA	2.74	127.30	122.63
17	P	5134	CLA	C1C-NC-C4C	2.74	109.35	106.23
17	Q	5242	CLA	C2A-C1A-CHA	2.74	127.30	122.63
17	F	4005	CLA	C2A-C1A-CHA	2.74	127.30	122.63
17	B	1218	CLA	C1C-NC-C4C	2.74	109.36	106.23
17	8	1021	CLA	C2A-C1A-CHA	2.74	127.31	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1134	CLA	C1C-NC-C4C	2.74	109.36	106.23
17	9	1026	CLA	C2A-C1A-CHA	2.75	127.32	122.63
17	0	1015	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	Q	5240	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	3	1031	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	0	1016	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	2	1011	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	B	1222	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	4	1015	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	B	1241	CLA	C2A-C1A-CHA	2.75	127.33	122.63
17	9	1022	CLA	C2A-C1A-CHA	2.76	127.33	122.63
17	7	1025	CLA	C2A-C1A-CHA	2.76	127.33	122.63
17	B	1242	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	A	1106	CLA	C1C-NC-C4C	2.76	109.37	106.23
17	8	1023	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	G	1701	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	W	5801	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	Q	5222	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	A	1012	CLA	C1C-NC-C4C	2.76	109.38	106.23
17	7	1012	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	1	1021	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	A	1108	CLA	C2A-C1A-CHA	2.76	127.34	122.63
17	2	1033	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	2	1021	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	3	1022	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	J	4008	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	7	1021	CLA	C2A-C1A-CHA	2.76	127.35	122.63
17	A	1122	CLA	C1C-NC-C4C	2.77	109.38	106.23
17	P	5106	CLA	C1C-NC-C4C	2.77	109.38	106.23
17	1	1025	CLA	C2A-C1A-CHA	2.77	127.35	122.63
17	2	1023	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	8	1026	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	Z	8008	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	K	1403	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	7	1014	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	8	1033	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	P	5112	CLA	C1C-NC-C4C	2.77	109.39	106.23
17	B	1240	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	2	1031	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	6	5504	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	2	1026	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	9	1031	CLA	C2A-C1A-CHA	2.77	127.36	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1105	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	8	1012	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	4	1016	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	2	1025	CLA	C2A-C1A-CHA	2.77	127.36	122.63
17	9	1011	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	9	1014	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	3	1011	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	P	5105	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	7	1026	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	Q	8001	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	4	1012	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	3	1026	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	4	1017	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	P	5122	CLA	C1C-NC-C4C	2.78	109.40	106.23
17	1	1014	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	P	5108	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	4	4002	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	2	1017	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	B	4001	CLA	C2A-C1A-CHA	2.78	127.37	122.63
17	F	4004	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	3	1017	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	A	1112	CLA	C1C-NC-C4C	2.78	109.40	106.23
17	P	5114	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	4	1014	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	0	8002	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	8	1013	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	P	8010	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	J	1101	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	8	1017	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	Q	5232	CLA	C1C-NC-C4C	2.78	109.40	106.23
17	2	4007	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	7	1016	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	A	1120	CLA	C1C-NC-C4C	2.78	109.40	106.23
17	1	1012	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	4	1026	CLA	C2A-C1A-CHA	2.78	127.38	122.63
17	3	1021	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	1	1016	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	L	1504	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	8	1015	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	4	1011	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1032	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	9	1017	CLA	C2A-C1A-CHA	2.79	127.39	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	1022	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	1	1017	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	2	1012	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	Q	5214	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	9	1041	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	8	8007	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	2	1013	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	B	1212	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1014	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	H	1801	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	A	4009	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1021	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	V	5701	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	A	4010	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	2	1015	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	7	1031	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	0	1022	CLA	C2A-C1A-CHA	2.79	127.39	122.63
17	5	5403	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	3	1012	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	F	4003	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	4	1021	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	1	1031	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	1	1026	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	A	1138	CLA	C1C-NC-C4C	2.79	109.42	106.23
17	Z	5101	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	K	1404	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	U	8003	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	7	1022	CLA	C2A-C1A-CHA	2.79	127.40	122.63
17	0	1026	CLA	C2A-C1A-CHA	2.80	127.40	122.63
17	A	1116	CLA	C2A-C1A-CHA	2.80	127.40	122.63
17	4	1033	CLA	C2A-C1A-CHA	2.80	127.40	122.63
17	7	1015	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	8	1031	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	2	1022	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	0	1033	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	1	1023	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	8	1025	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	1	1022	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	0	1011	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	7	1023	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	3	1033	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	8	1016	CLA	C2A-C1A-CHA	2.80	127.41	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	8009	CLA	C2A-C1A-CHA	2.80	127.41	122.63
17	U	8006	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	A	1114	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	7	1017	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	F	4006	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	P	5116	CLA	C2A-C1A-CHA	2.80	127.42	122.63
17	4	1032	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	0	1017	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	9	1021	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	3	1041	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	1	1013	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	9	1025	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	B	1214	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	0	1012	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	P	5139	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	2	1016	CLA	C2A-C1A-CHA	2.81	127.42	122.63
17	U	8004	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	4	1023	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	3	1014	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	9	1033	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	3	1016	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	9	1012	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	3	1025	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	1	1015	CLA	C2A-C1A-CHA	2.81	127.43	122.63
17	P	5120	CLA	C1C-NC-C4C	2.81	109.44	106.23
17	4	1013	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	0	1013	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	B	1232	CLA	C1C-NC-C4C	2.82	109.44	106.23
17	B	1237	CLA	C1C-NC-C4C	2.82	109.44	106.23
17	A	1139	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	0	1023	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	Q	5212	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	3	1032	CLA	C2A-C1A-CHA	2.82	127.44	122.63
17	7	1013	CLA	C2A-C1A-CHA	2.82	127.45	122.63
17	9	1016	CLA	C2A-C1A-CHA	2.82	127.45	122.63
17	2	1014	CLA	C2A-C1A-CHA	2.82	127.45	122.63
17	P	5138	CLA	C1C-NC-C4C	2.83	109.45	106.23
17	8	1022	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	8	1014	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	F	1229	CLA	C1C-NC-C4C	2.83	109.45	106.23
17	5	5404	CLA	C2A-C1A-CHA	2.83	127.46	122.63
17	P	5117	CLA	C2A-C1A-CHA	2.83	127.46	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1113	CLA	C2A-C1A-CHA	2.83	127.47	122.63
17	P	5113	CLA	C2A-C1A-CHA	2.83	127.47	122.63
17	1	1011	CLA	C2A-C1A-CHA	2.84	127.47	122.63
17	9	1032	CLA	C2A-C1A-CHA	2.84	127.47	122.63
17	P	5102	CLA	C2A-C1A-CHA	2.84	127.48	122.63
17	A	1102	CLA	C2A-C1A-CHA	2.84	127.48	122.63
17	U	5229	CLA	C1C-NC-C4C	2.84	109.47	106.23
17	7	1011	CLA	C2A-C1A-CHA	2.84	127.48	122.63
17	Q	5237	CLA	C1C-NC-C4C	2.84	109.47	106.23
17	P	5123	CLA	C2A-C1A-CHA	2.85	127.49	122.63
17	3	1015	CLA	C2A-C1A-CHA	2.85	127.49	122.63
17	A	1117	CLA	C2A-C1A-CHA	2.85	127.49	122.63
17	A	1123	CLA	C2A-C1A-CHA	2.85	127.50	122.63
17	9	1015	CLA	C2A-C1A-CHA	2.86	127.52	122.63
17	A	1134	CLA	C2A-C1A-CHA	2.87	127.52	122.63
17	P	5112	CLA	C2A-C1A-CHA	2.87	127.53	122.63
17	Q	5210	CLA	C2A-C1A-CHA	2.88	127.54	122.63
17	A	1120	CLA	C2A-C1A-CHA	2.88	127.54	122.63
17	P	5120	CLA	C2A-C1A-CHA	2.88	127.54	122.63
17	A	1112	CLA	C2A-C1A-CHA	2.88	127.55	122.63
17	B	1210	CLA	C2A-C1A-CHA	2.89	127.56	122.63
17	P	5134	CLA	C2A-C1A-CHA	2.89	127.57	122.63
17	Q	5215	CLA	C1C-NC-C4C	2.90	109.54	106.23
17	B	1215	CLA	C1C-NC-C4C	2.90	109.54	106.23
17	P	5111	CLA	C2A-C1A-CHA	2.90	127.58	122.63
17	A	1111	CLA	C2A-C1A-CHA	2.91	127.60	122.63
17	B	1220	CLA	C1C-NC-C4C	2.93	109.57	106.23
17	L	1502	CLA	C1C-NC-C4C	2.95	109.59	106.23
17	Q	5220	CLA	C1C-NC-C4C	2.96	109.60	106.23
17	A	1119	CLA	C1C-NC-C4C	2.97	109.61	106.23
17	V	5233	CLA	C2A-C1A-CHA	2.97	127.70	122.63
17	A	1129	CLA	C1C-NC-C4C	2.97	109.62	106.23
17	Q	5228	CLA	C1C-NC-C4C	2.97	109.62	106.23
17	G	1233	CLA	C2A-C1A-CHA	2.97	127.70	122.63
17	B	1227	CLA	C1C-NC-C4C	2.97	109.62	106.23
17	A	1135	CLA	C2A-C1A-CHA	2.97	127.71	122.63
17	B	1228	CLA	C1C-NC-C4C	2.98	109.62	106.23
17	Q	5227	CLA	C1C-NC-C4C	2.98	109.62	106.23
17	P	5129	CLA	C1C-NC-C4C	2.98	109.62	106.23
17	P	5135	CLA	C2A-C1A-CHA	2.98	127.72	122.63
17	Q	5231	CLA	C1C-NC-C4C	2.98	109.63	106.23
17	P	5119	CLA	C1C-NC-C4C	2.99	109.64	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	6	5502	CLA	C1C-NC-C4C	2.99	109.64	106.23
17	Q	5235	CLA	C1C-NC-C4C	3.01	109.66	106.23
17	B	1235	CLA	C1C-NC-C4C	3.01	109.66	106.23
17	Q	5232	CLA	C2A-C1A-CHA	3.01	127.77	122.63
17	B	1232	CLA	C2A-C1A-CHA	3.03	127.81	122.63
17	B	1231	CLA	C1C-NC-C4C	3.04	109.70	106.23
17	B	1217	CLA	C2A-C1A-CHA	3.04	127.82	122.63
17	Q	5217	CLA	C2A-C1A-CHA	3.05	127.83	122.63
17	Q	5204	CLA	C1C-NC-C4C	3.05	109.70	106.23
17	B	1204	CLA	C1C-NC-C4C	3.05	109.71	106.23
17	A	1118	CLA	C2A-C1A-CHA	3.06	127.84	122.63
17	B	1218	CLA	C2A-C1A-CHA	3.06	127.84	122.63
17	Q	5218	CLA	C2A-C1A-CHA	3.06	127.85	122.63
17	P	5118	CLA	C2A-C1A-CHA	3.06	127.86	122.63
17	F	1301	CLA	C2A-C1A-CHA	3.09	127.90	122.63
17	J	1302	CLA	C2A-C1A-CHA	3.09	127.91	122.63
17	U	5301	CLA	C2A-C1A-CHA	3.10	127.92	122.63
17	Z	5302	CLA	C2A-C1A-CHA	3.10	127.92	122.63
17	P	5116	CLA	C1C-NC-C4C	3.13	109.80	106.23
17	A	1116	CLA	C1C-NC-C4C	3.14	109.81	106.23
17	P	5901	CLA	C2A-C1A-CHA	3.14	127.99	122.63
17	A	1901	CLA	C2A-C1A-CHA	3.15	128.00	122.63
17	P	5126	CLA	C1C-NC-C4C	3.15	109.82	106.23
17	A	1126	CLA	C1C-NC-C4C	3.15	109.82	106.23
17	B	1221	CLA	C2A-C1A-CHA	3.18	128.06	122.63
17	Q	5221	CLA	C2A-C1A-CHA	3.20	128.09	122.63
17	A	1104	CLA	C2A-C1A-CHA	3.23	128.14	122.63
17	A	1118	CLA	C1C-NC-C4C	3.23	109.91	106.23
17	P	5118	CLA	C1C-NC-C4C	3.24	109.92	106.23
17	P	5104	CLA	C2A-C1A-CHA	3.24	128.17	122.63
17	P	5012	CLA	C2A-C1A-CHA	3.32	128.30	122.63
17	A	1012	CLA	C2A-C1A-CHA	3.32	128.30	122.63
17	B	1023	CLA	C1C-NC-C4C	3.33	110.03	106.23
17	Q	5023	CLA	C1C-NC-C4C	3.39	110.09	106.23
17	P	5107	CLA	C2A-C1A-CHA	3.41	128.44	122.63
17	A	1107	CLA	C2A-C1A-CHA	3.41	128.45	122.63
17	Q	5022	CLA	C1C-NC-C4C	3.42	110.12	106.23
17	B	1022	CLA	C1C-NC-C4C	3.42	110.13	106.23
17	Q	5207	CLA	C2A-C1A-CHA	3.48	128.58	122.63
17	B	1207	CLA	C2A-C1A-CHA	3.49	128.58	122.63
17	B	1225	CLA	C4A-NA-C1A	4.03	110.72	107.17
17	J	1302	CLA	C1C-NC-C4C	4.04	110.83	106.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Z	5302	CLA	C1C-NC-C4C	4.05	110.85	106.23
17	Q	5225	CLA	C4A-NA-C1A	4.06	110.75	107.17
17	B	1219	CLA	C1C-NC-C4C	4.35	111.19	106.23
17	P	5108	CLA	C1C-NC-C4C	4.35	111.19	106.23
17	A	1108	CLA	C1C-NC-C4C	4.36	111.20	106.23
17	Q	5219	CLA	C1C-NC-C4C	4.36	111.20	106.23
17	A	1128	CLA	C4A-NA-C1A	4.39	111.04	107.17
17	B	1226	CLA	C4A-NA-C1A	4.42	111.07	107.17
17	P	5128	CLA	C4A-NA-C1A	4.43	111.08	107.17
17	Q	5226	CLA	C4A-NA-C1A	4.45	111.10	107.17
17	A	1115	CLA	C4A-NA-C1A	4.47	111.11	107.17
17	L	1501	CLA	C4A-NA-C1A	4.48	111.12	107.17
17	P	5115	CLA	C4A-NA-C1A	4.48	111.12	107.17
17	6	5501	CLA	C4A-NA-C1A	4.53	111.16	107.17
17	A	1136	CLA	C4A-NA-C1A	4.57	111.20	107.17
17	P	5136	CLA	C4A-NA-C1A	4.58	111.21	107.17
17	P	5013	CLA	C4A-NA-C1A	4.61	111.23	107.17
17	A	1121	CLA	C4A-NA-C1A	4.62	111.24	107.17
17	A	1113	CLA	C1C-NC-C4C	4.63	111.51	106.23
17	P	5121	CLA	C4A-NA-C1A	4.65	111.27	107.17
17	P	5113	CLA	C1C-NC-C4C	4.65	111.53	106.23
17	A	1013	CLA	C4A-NA-C1A	4.66	111.28	107.17
17	B	1205	CLA	C4A-NA-C1A	4.69	111.30	107.17
17	Q	5205	CLA	C4A-NA-C1A	4.69	111.30	107.17
17	B	1213	CLA	C4A-NA-C1A	4.69	111.31	107.17
17	Q	5213	CLA	C4A-NA-C1A	4.69	111.31	107.17
17	P	5901	CLA	C1C-NC-C4C	4.72	111.60	106.23
17	A	1901	CLA	C1C-NC-C4C	4.76	111.66	106.23
17	P	5112	CLA	C4A-NA-C1A	4.81	111.41	107.17
17	L	1503	CLA	C4A-NA-C1A	4.81	111.41	107.17
17	6	5503	CLA	C4A-NA-C1A	4.81	111.41	107.17
17	B	1238	CLA	C4A-NA-C1A	4.84	111.44	107.17
17	Q	5238	CLA	C4A-NA-C1A	4.84	111.44	107.17
17	A	1112	CLA	C4A-NA-C1A	4.85	111.44	107.17
17	Q	5023	CLA	C4A-NA-C1A	4.86	111.46	107.17
17	B	1023	CLA	C4A-NA-C1A	4.86	111.46	107.17
17	Q	5208	CLA	C4A-NA-C1A	4.87	111.46	107.17
17	A	1126	CLA	C4A-NA-C1A	4.88	111.47	107.17
17	P	5126	CLA	C4A-NA-C1A	4.88	111.47	107.17
17	Q	5022	CLA	C4A-NA-C1A	4.88	111.47	107.17
17	B	1022	CLA	C4A-NA-C1A	4.89	111.48	107.17
17	Q	5232	CLA	C4A-NA-C1A	4.89	111.48	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	1208	CLA	C4A-NA-C1A	4.89	111.48	107.17
17	A	1137	CLA	C1C-NC-C4C	4.90	111.81	106.23
17	B	1232	CLA	C4A-NA-C1A	4.90	111.49	107.17
17	B	1220	CLA	C4A-NA-C1A	4.91	111.50	107.17
17	P	5137	CLA	C1C-NC-C4C	4.92	111.83	106.23
17	P	5119	CLA	C4A-NA-C1A	4.92	111.51	107.17
17	Q	5220	CLA	C4A-NA-C1A	4.94	111.52	107.17
17	B	1216	CLA	C4A-NA-C1A	4.94	111.53	107.17
17	Q	5216	CLA	C4A-NA-C1A	4.95	111.53	107.17
17	A	1119	CLA	C4A-NA-C1A	4.95	111.53	107.17
17	5	5401	CLA	C4A-NA-C1A	4.96	111.54	107.17
17	K	1401	CLA	C4A-NA-C1A	4.97	111.55	107.17
17	L	1502	CLA	C4A-NA-C1A	4.98	111.56	107.17
17	P	5105	CLA	C4A-NA-C1A	4.99	111.57	107.17
17	P	5011	CLA	C4A-NA-C1A	5.00	111.58	107.17
17	A	1132	CLA	C4A-NA-C1A	5.00	111.58	107.17
17	A	1011	CLA	C4A-NA-C1A	5.00	111.58	107.17
17	P	5132	CLA	C4A-NA-C1A	5.00	111.58	107.17
17	P	5117	CLA	C4A-NA-C1A	5.01	111.58	107.17
17	A	1105	CLA	C4A-NA-C1A	5.01	111.58	107.17
17	A	1117	CLA	C4A-NA-C1A	5.01	111.58	107.17
17	A	1139	CLA	C4A-NA-C1A	5.03	111.61	107.17
17	6	5502	CLA	C4A-NA-C1A	5.05	111.62	107.17
17	P	5139	CLA	C4A-NA-C1A	5.05	111.62	107.17
17	B	1236	CLA	C4A-NA-C1A	5.05	111.62	107.17
17	P	5116	CLA	C4A-NA-C1A	5.07	111.64	107.17
17	A	1116	CLA	C4A-NA-C1A	5.08	111.65	107.17
17	Q	5236	CLA	C4A-NA-C1A	5.09	111.66	107.17
17	B	1237	CLA	C4A-NA-C1A	5.11	111.68	107.17
17	B	1227	CLA	C4A-NA-C1A	5.12	111.69	107.17
17	Q	5227	CLA	C4A-NA-C1A	5.13	111.69	107.17
17	P	5120	CLA	C4A-NA-C1A	5.13	111.69	107.17
17	Q	5237	CLA	C4A-NA-C1A	5.13	111.70	107.17
17	B	1215	CLA	C4A-NA-C1A	5.13	111.70	107.17
17	B	1230	CLA	C4A-NA-C1A	5.14	111.70	107.17
17	F	1229	CLA	C4A-NA-C1A	5.15	111.71	107.17
17	A	1109	CLA	C4A-NA-C1A	5.15	111.71	107.17
17	Q	5230	CLA	C4A-NA-C1A	5.15	111.71	107.17
17	A	1120	CLA	C4A-NA-C1A	5.16	111.72	107.17
17	B	1211	CLA	C4A-NA-C1A	5.16	111.72	107.17
17	B	1235	CLA	C4A-NA-C1A	5.17	111.73	107.17
17	Q	5211	CLA	C4A-NA-C1A	5.17	111.73	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	5122	CLA	C4A-NA-C1A	5.18	111.73	107.17
17	A	1138	CLA	C4A-NA-C1A	5.18	111.73	107.17
17	Q	5215	CLA	C4A-NA-C1A	5.18	111.74	107.17
17	A	1122	CLA	C4A-NA-C1A	5.18	111.74	107.17
17	P	5138	CLA	C4A-NA-C1A	5.18	111.74	107.17
17	Q	5235	CLA	C4A-NA-C1A	5.18	111.74	107.17
17	U	5229	CLA	C4A-NA-C1A	5.19	111.74	107.17
17	Q	5222	CLA	C4A-NA-C1A	5.20	111.76	107.17
17	A	1127	CLA	C4A-NA-C1A	5.21	111.76	107.17
17	P	5109	CLA	C4A-NA-C1A	5.21	111.76	107.17
17	P	5102	CLA	C4A-NA-C1A	5.21	111.77	107.17
17	A	1124	CLA	C4A-NA-C1A	5.22	111.77	107.17
17	B	1222	CLA	C4A-NA-C1A	5.22	111.78	107.17
17	A	1102	CLA	C4A-NA-C1A	5.25	111.80	107.17
17	P	5127	CLA	C4A-NA-C1A	5.26	111.80	107.17
17	A	1106	CLA	C4A-NA-C1A	5.27	111.81	107.17
17	P	5124	CLA	C4A-NA-C1A	5.27	111.82	107.17
17	P	5106	CLA	C4A-NA-C1A	5.28	111.82	107.17
17	B	1201	CLA	C4A-NA-C1A	5.28	111.82	107.17
17	Q	5201	CLA	C4A-NA-C1A	5.30	111.84	107.17
17	P	5133	CLA	C4A-NA-C1A	5.30	111.84	107.17
17	B	1228	CLA	C4A-NA-C1A	5.30	111.84	107.17
17	B	1214	CLA	C4A-NA-C1A	5.31	111.85	107.17
17	B	1212	CLA	C4A-NA-C1A	5.32	111.86	107.17
17	A	1133	CLA	C4A-NA-C1A	5.34	111.87	107.17
17	Q	5228	CLA	C4A-NA-C1A	5.34	111.88	107.17
17	Q	5212	CLA	C4A-NA-C1A	5.35	111.88	107.17
17	Q	5214	CLA	C4A-NA-C1A	5.35	111.88	107.17
17	Q	5218	CLA	C4A-NA-C1A	5.35	111.89	107.17
17	P	5107	CLA	C4A-NA-C1A	5.35	111.89	107.17
17	A	1107	CLA	C4A-NA-C1A	5.36	111.90	107.17
17	A	1131	CLA	C4A-NA-C1A	5.37	111.90	107.17
17	P	5131	CLA	C4A-NA-C1A	5.39	111.92	107.17
17	B	1218	CLA	C4A-NA-C1A	5.41	111.94	107.17
17	B	1203	CLA	C4A-NA-C1A	5.41	111.94	107.17
17	P	5129	CLA	C4A-NA-C1A	5.42	111.95	107.17
17	P	5114	CLA	C4A-NA-C1A	5.43	111.95	107.17
17	Q	5203	CLA	C4A-NA-C1A	5.43	111.96	107.17
17	B	1209	CLA	C4A-NA-C1A	5.43	111.96	107.17
17	A	1114	CLA	C4A-NA-C1A	5.43	111.96	107.17
17	F	1301	CLA	C4A-NA-C1A	5.44	111.96	107.17
17	A	1129	CLA	C4A-NA-C1A	5.44	111.96	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	U	5301	CLA	C4A-NA-C1A	5.44	111.96	107.17
17	Q	5209	CLA	C4A-NA-C1A	5.44	111.97	107.17
17	P	5134	CLA	C4A-NA-C1A	5.44	111.97	107.17
17	A	1134	CLA	C4A-NA-C1A	5.45	111.97	107.17
17	2	1021	CLA	C4A-NA-C1A	5.47	111.99	107.17
17	0	1025	CLA	C4A-NA-C1A	5.47	111.99	107.17
17	V	5233	CLA	C4A-NA-C1A	5.47	111.99	107.17
17	Q	5021	CLA	C4A-NA-C1A	5.47	112.00	107.17
17	2	1033	CLA	C4A-NA-C1A	5.48	112.00	107.17
17	A	1012	CLA	C4A-NA-C1A	5.49	112.01	107.17
17	8	1021	CLA	C4A-NA-C1A	5.49	112.01	107.17
17	0	1014	CLA	C4A-NA-C1A	5.49	112.01	107.17
17	8	1033	CLA	C4A-NA-C1A	5.49	112.01	107.17
17	P	5104	CLA	C4A-NA-C1A	5.49	112.01	107.17
17	0	1021	CLA	C4A-NA-C1A	5.50	112.02	107.17
17	9	1016	CLA	C4A-NA-C1A	5.50	112.02	107.17
17	4	1021	CLA	C4A-NA-C1A	5.50	112.02	107.17
17	Q	5224	CLA	C4A-NA-C1A	5.51	112.02	107.17
17	B	1021	CLA	C4A-NA-C1A	5.51	112.02	107.17
17	0	1013	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	0	1012	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	7	1014	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	4	1025	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	Q	5240	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	7	1023	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	P	5012	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	3	1016	CLA	C4A-NA-C1A	5.51	112.03	107.17
17	G	1233	CLA	C4A-NA-C1A	5.52	112.03	107.17
17	A	1104	CLA	C4A-NA-C1A	5.52	112.04	107.17
17	P	5118	CLA	C4A-NA-C1A	5.52	112.04	107.17
17	Q	5234	CLA	C4A-NA-C1A	5.53	112.04	107.17
17	8	1025	CLA	C4A-NA-C1A	5.53	112.04	107.17
17	8	1015	CLA	C4A-NA-C1A	5.53	112.04	107.17
17	1	1023	CLA	C4A-NA-C1A	5.53	112.05	107.17
17	B	1241	CLA	C4A-NA-C1A	5.53	112.05	107.17
17	P	5140	CLA	C4A-NA-C1A	5.53	112.05	107.17
17	0	1023	CLA	C4A-NA-C1A	5.53	112.05	107.17
17	A	1140	CLA	C4A-NA-C1A	5.53	112.05	107.17
17	2	1025	CLA	C4A-NA-C1A	5.53	112.05	107.17
17	4	1012	CLA	C4A-NA-C1A	5.54	112.05	107.17
17	B	1224	CLA	C4A-NA-C1A	5.54	112.05	107.17
17	9	1041	CLA	C4A-NA-C1A	5.54	112.05	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	1118	CLA	C4A-NA-C1A	5.54	112.05	107.17
17	4	1014	CLA	C4A-NA-C1A	5.54	112.05	107.17
17	0	1017	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	0	1026	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	7	1016	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	Q	8001	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	1	1016	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	9	1017	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	B	1234	CLA	C4A-NA-C1A	5.54	112.06	107.17
17	U	8003	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	Q	5242	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	3	1021	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	9	1015	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	Q	5231	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	9	1031	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	4	1023	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	7	1012	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	4	1013	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	2	1012	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	A	4010	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	7	1013	CLA	C4A-NA-C1A	5.55	112.06	107.17
17	7	1021	CLA	C4A-NA-C1A	5.55	112.07	107.17
17	1	1012	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	U	8004	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	2	1017	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	1	1013	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	3	1031	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	0	1016	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	8	1017	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	2	1015	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	B	4001	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	2	1023	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	B	1242	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	L	1504	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	P	8009	CLA	C4A-NA-C1A	5.56	112.07	107.17
17	2	4007	CLA	C4A-NA-C1A	5.56	112.08	107.17
17	6	5504	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	8	1023	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	3	1017	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	7	1031	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	1	1014	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	9	1021	CLA	C4A-NA-C1A	5.57	112.08	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	1240	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	4	1026	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	K	1403	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	V	5701	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	4	1017	CLA	C4A-NA-C1A	5.57	112.08	107.17
17	1	1021	CLA	C4A-NA-C1A	5.58	112.08	107.17
17	8	1011	CLA	C4A-NA-C1A	5.58	112.08	107.17
17	W	5801	CLA	C4A-NA-C1A	5.58	112.08	107.17
17	5	5403	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	0	1033	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	3	1041	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	2	1013	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	P	8010	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	4	1016	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	1	1017	CLA	C4A-NA-C1A	5.58	112.09	107.17
17	3	1011	CLA	C4A-NA-C1A	5.59	112.09	107.17
17	8	1012	CLA	C4A-NA-C1A	5.59	112.09	107.17
17	9	1026	CLA	C4A-NA-C1A	5.59	112.09	107.17
17	4	1033	CLA	C4A-NA-C1A	5.59	112.09	107.17
17	7	1025	CLA	C4A-NA-C1A	5.59	112.09	107.17
17	J	1101	CLA	C4A-NA-C1A	5.59	112.09	107.17
17	1	1026	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	8	8007	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	F	4006	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	3	1015	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	U	8006	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	1	1025	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	A	4009	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	9	1014	CLA	C4A-NA-C1A	5.59	112.10	107.17
17	H	1801	CLA	C4A-NA-C1A	5.60	112.10	107.17
17	3	1014	CLA	C4A-NA-C1A	5.60	112.10	107.17
17	F	4004	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	G	1701	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	Z	8008	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	1	1031	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	0	1031	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	J	4008	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	0	1011	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	4	1011	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	4	1015	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	Q	5241	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	9	1022	CLA	C4A-NA-C1A	5.60	112.11	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	8	1031	CLA	C4A-NA-C1A	5.60	112.11	107.17
17	2	1031	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	F	4003	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	B	1231	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	3	1033	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	3	1026	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	K	1404	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	9	1025	CLA	C4A-NA-C1A	5.61	112.11	107.17
17	2	1022	CLA	C4A-NA-C1A	5.61	112.12	107.17
17	9	1011	CLA	C4A-NA-C1A	5.61	112.12	107.17
17	1	1015	CLA	C4A-NA-C1A	5.61	112.12	107.17
17	2	1011	CLA	C4A-NA-C1A	5.61	112.12	107.17
17	7	1022	CLA	C4A-NA-C1A	5.61	112.12	107.17
17	Z	5101	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	2	1026	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	8	1013	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	F	4005	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	3	1012	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	3	1025	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	7	1026	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	8	1022	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	7	1017	CLA	C4A-NA-C1A	5.62	112.12	107.17
17	0	1015	CLA	C4A-NA-C1A	5.62	112.13	107.17
17	4	1032	CLA	C4A-NA-C1A	5.62	112.13	107.17
17	Q	5217	CLA	C4A-NA-C1A	5.62	112.13	107.17
17	B	1210	CLA	C4A-NA-C1A	5.62	112.13	107.17
17	2	1014	CLA	C4A-NA-C1A	5.62	112.13	107.17
17	Q	5210	CLA	C4A-NA-C1A	5.62	112.13	107.17
17	U	8005	CLA	C4A-NA-C1A	5.63	112.13	107.17
17	7	1015	CLA	C4A-NA-C1A	5.63	112.13	107.17
17	4	1031	CLA	C4A-NA-C1A	5.63	112.13	107.17
17	1	1011	CLA	C4A-NA-C1A	5.63	112.13	107.17
17	9	1032	CLA	C4A-NA-C1A	5.63	112.13	107.17
17	3	1022	CLA	C4A-NA-C1A	5.64	112.14	107.17
17	8	1026	CLA	C4A-NA-C1A	5.64	112.14	107.17
17	7	1011	CLA	C4A-NA-C1A	5.64	112.14	107.17
17	4	1022	CLA	C4A-NA-C1A	5.64	112.14	107.17
17	9	1012	CLA	C4A-NA-C1A	5.64	112.14	107.17
17	0	1022	CLA	C4A-NA-C1A	5.64	112.15	107.17
17	9	1033	CLA	C4A-NA-C1A	5.65	112.15	107.17
17	8	1014	CLA	C4A-NA-C1A	5.65	112.15	107.17
17	8	1016	CLA	C4A-NA-C1A	5.66	112.16	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	1032	CLA	C4A-NA-C1A	5.66	112.16	107.17
17	B	1217	CLA	C4A-NA-C1A	5.66	112.16	107.17
17	1	1022	CLA	C4A-NA-C1A	5.66	112.16	107.17
17	5	5404	CLA	C4A-NA-C1A	5.66	112.16	107.17
17	2	1016	CLA	C4A-NA-C1A	5.66	112.16	107.17
17	0	1032	CLA	C4A-NA-C1A	5.67	112.17	107.17
17	4	4002	CLA	C4A-NA-C1A	5.69	112.19	107.17
17	B	1207	CLA	C4A-NA-C1A	5.70	112.19	107.17
17	Q	5221	CLA	C4A-NA-C1A	5.74	112.23	107.17
17	B	1221	CLA	C4A-NA-C1A	5.74	112.23	107.17
17	0	8002	CLA	C4A-NA-C1A	5.74	112.23	107.17
17	Q	5207	CLA	C4A-NA-C1A	5.75	112.23	107.17
17	A	1110	CLA	C4A-NA-C1A	5.75	112.24	107.17
17	Q	5206	CLA	C4A-NA-C1A	5.76	112.25	107.17
17	B	1206	CLA	C4A-NA-C1A	5.77	112.26	107.17
17	P	5110	CLA	C4A-NA-C1A	5.80	112.28	107.17
17	P	5125	CLA	C4A-NA-C1A	5.80	112.29	107.17
17	A	1125	CLA	C4A-NA-C1A	5.83	112.31	107.17
17	Q	5239	CLA	C4A-NA-C1A	5.84	112.32	107.17
17	B	1239	CLA	C4A-NA-C1A	5.86	112.33	107.17
17	Q	5202	CLA	C4A-NA-C1A	5.91	112.38	107.17
17	B	1202	CLA	C4A-NA-C1A	5.91	112.38	107.17
17	P	5402	CLA	C4A-NA-C1A	5.94	112.41	107.17
17	A	1123	CLA	C4A-NA-C1A	5.94	112.41	107.17
17	P	5123	CLA	C4A-NA-C1A	5.96	112.43	107.17
17	B	1223	CLA	C4A-NA-C1A	5.96	112.43	107.17
17	Q	5223	CLA	C4A-NA-C1A	5.97	112.43	107.17
17	A	1402	CLA	C4A-NA-C1A	6.00	112.46	107.17
17	B	1130	CLA	C4A-NA-C1A	6.04	112.49	107.17
17	B	1204	CLA	C4A-NA-C1A	6.05	112.50	107.17
17	Q	5204	CLA	C4A-NA-C1A	6.05	112.50	107.17
17	Q	5130	CLA	C4A-NA-C1A	6.08	112.53	107.17
17	P	5135	CLA	C4A-NA-C1A	6.09	112.54	107.17
17	A	1111	CLA	C4A-NA-C1A	6.14	112.59	107.17
17	P	5111	CLA	C4A-NA-C1A	6.15	112.59	107.17
17	A	1135	CLA	C4A-NA-C1A	6.15	112.60	107.17
17	A	1137	CLA	C4A-NA-C1A	6.23	112.66	107.17
17	P	5137	CLA	C4A-NA-C1A	6.24	112.67	107.17
17	P	5108	CLA	C4A-NA-C1A	6.44	112.85	107.17
17	A	1103	CLA	C4A-NA-C1A	6.46	112.86	107.17
17	P	5103	CLA	C4A-NA-C1A	6.48	112.88	107.17
17	A	1108	CLA	C4A-NA-C1A	6.49	112.89	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	5219	CLA	C4A-NA-C1A	7.15	113.47	107.17
17	B	1219	CLA	C4A-NA-C1A	7.20	113.52	107.17
17	P	5113	CLA	C4A-NA-C1A	7.33	113.63	107.17
17	A	1113	CLA	C4A-NA-C1A	7.38	113.67	107.17
17	P	5901	CLA	C4A-NA-C1A	7.78	114.03	107.17
17	A	1901	CLA	C4A-NA-C1A	7.81	114.05	107.17
17	J	1302	CLA	C4A-NA-C1A	7.99	114.22	107.17
17	Z	5302	CLA	C4A-NA-C1A	8.02	114.24	107.17

All (924) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	B	1210	CLA	NA
17	B	1210	CLA	NC
17	B	1210	CLA	ND
17	A	1104	CLA	NC
17	A	1104	CLA	ND
17	A	1104	CLA	NA
17	A	1110	CLA	NC
17	A	1110	CLA	ND
17	A	1110	CLA	NA
17	B	1222	CLA	NC
17	B	1222	CLA	ND
17	B	1222	CLA	NA
17	7	1017	CLA	NC
17	7	1017	CLA	ND
17	7	1017	CLA	NA
17	F	4006	CLA	NC
17	F	4006	CLA	ND
17	F	4006	CLA	NA
17	1	1012	CLA	NC
17	1	1012	CLA	ND
17	1	1012	CLA	NA
17	3	1015	CLA	NC
17	3	1015	CLA	ND
17	3	1015	CLA	NA
17	2	1013	CLA	NC
17	2	1013	CLA	ND
17	2	1013	CLA	NA
17	A	1132	CLA	NC
17	A	1132	CLA	ND
17	A	1132	CLA	NA

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Mol	Chain	Res	Type	Atom
17	0	1017	CLA	NC
17	0	1017	CLA	ND
17	0	1017	CLA	NA
17	Z	5101	CLA	NC
17	Z	5101	CLA	ND
17	Z	5101	CLA	NA
17	A	1119	CLA	NC
17	A	1119	CLA	ND
17	A	1119	CLA	NA
17	B	1239	CLA	NC
17	B	1239	CLA	ND
17	A	1103	CLA	NC
17	A	1103	CLA	ND
17	A	1103	CLA	NA
17	1	1021	CLA	NC
17	1	1021	CLA	ND
17	1	1021	CLA	NA
17	Q	5208	CLA	NC
17	Q	5208	CLA	ND
17	Q	5208	CLA	NA
17	Q	5224	CLA	ND
17	B	1238	CLA	NC
17	B	1238	CLA	ND
17	B	1238	CLA	NA
17	2	4007	CLA	NC
17	2	4007	CLA	ND
17	2	4007	CLA	NA
17	2	1033	CLA	NC
17	2	1033	CLA	ND
17	2	1033	CLA	NA
17	Q	5239	CLA	NC
17	Q	5239	CLA	ND
17	0	1022	CLA	NC
17	0	1022	CLA	ND
17	0	1022	CLA	NA
17	P	5134	CLA	NC
17	P	5134	CLA	ND
17	P	5134	CLA	NA
17	P	5102	CLA	NC
17	P	5102	CLA	ND
17	P	5102	CLA	NA
17	0	8002	CLA	NC

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Mol	Chain	Res	Type	Atom
17	0	8002	CLA	ND
17	0	8002	CLA	NA
17	Q	5207	CLA	NC
17	Q	5207	CLA	ND
17	Q	5207	CLA	NA
17	A	1139	CLA	NC
17	A	1139	CLA	ND
17	B	1230	CLA	NC
17	B	1230	CLA	ND
17	B	1230	CLA	NA
17	F	4004	CLA	NC
17	F	4004	CLA	ND
17	F	4004	CLA	NA
17	5	5401	CLA	NC
17	5	5401	CLA	ND
17	5	5401	CLA	NA
17	1	1023	CLA	NC
17	1	1023	CLA	ND
17	1	1023	CLA	NA
17	B	1022	CLA	ND
17	2	1016	CLA	NC
17	2	1016	CLA	ND
17	2	1016	CLA	NA
17	P	5122	CLA	NC
17	P	5122	CLA	ND
17	P	5122	CLA	NA
17	B	1203	CLA	NC
17	B	1203	CLA	ND
17	B	1203	CLA	NA
17	A	1109	CLA	NC
17	A	1109	CLA	ND
17	A	1109	CLA	NA
17	3	1033	CLA	NC
17	3	1033	CLA	ND
17	3	1033	CLA	NA
17	A	1013	CLA	NC
17	A	1013	CLA	ND
17	A	1136	CLA	NC
17	A	1136	CLA	ND
17	A	1136	CLA	NA
17	1	1031	CLA	NC
17	1	1031	CLA	ND

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Mol	Chain	Res	Type	Atom
17	1	1031	CLA	NA
17	B	1232	CLA	NC
17	B	1232	CLA	ND
17	B	1232	CLA	NA
17	7	1011	CLA	NC
17	7	1011	CLA	ND
17	7	1011	CLA	NA
17	8	1025	CLA	NC
17	8	1025	CLA	ND
17	8	1025	CLA	NA
17	Q	5242	CLA	NC
17	Q	5242	CLA	ND
17	Q	5242	CLA	NA
17	Q	8001	CLA	NC
17	Q	8001	CLA	ND
17	Q	8001	CLA	NA
17	4	1014	CLA	NC
17	4	1014	CLA	ND
17	4	1014	CLA	NA
17	4	1026	CLA	NC
17	4	1026	CLA	ND
17	4	1026	CLA	NA
17	Q	5223	CLA	NC
17	Q	5223	CLA	ND
17	Q	5223	CLA	NA
17	P	5109	CLA	NC
17	P	5109	CLA	ND
17	P	5109	CLA	NA
17	9	1041	CLA	NC
17	9	1041	CLA	ND
17	9	1041	CLA	NA
17	A	1012	CLA	ND
17	A	1120	CLA	NC
17	A	1120	CLA	ND
17	A	1120	CLA	NA
17	B	1201	CLA	NC
17	B	1201	CLA	ND
17	B	1201	CLA	NA
17	0	1021	CLA	NC
17	0	1021	CLA	ND
17	0	1021	CLA	NA
17	2	1023	CLA	NC

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Mol	Chain	Res	Type	Atom
17	2	1023	CLA	ND
17	2	1023	CLA	NA
17	3	1021	CLA	NC
17	3	1021	CLA	ND
17	3	1021	CLA	NA
17	9	1033	CLA	NC
17	9	1033	CLA	ND
17	9	1033	CLA	NA
17	K	1401	CLA	NC
17	K	1401	CLA	ND
17	K	1401	CLA	NA
17	8	1021	CLA	NC
17	8	1021	CLA	ND
17	8	1021	CLA	NA
17	A	1134	CLA	NC
17	A	1134	CLA	ND
17	A	1134	CLA	NA
17	Q	5204	CLA	ND
17	Q	5204	CLA	NA
17	4	1012	CLA	NC
17	4	1012	CLA	ND
17	4	1012	CLA	NA
17	3	1012	CLA	NC
17	3	1012	CLA	ND
17	3	1012	CLA	NA
17	U	8006	CLA	NC
17	U	8006	CLA	ND
17	U	8006	CLA	NA
17	9	1026	CLA	NC
17	9	1026	CLA	ND
17	9	1026	CLA	NA
17	Q	5237	CLA	NC
17	Q	5237	CLA	ND
17	A	1129	CLA	NC
17	A	1129	CLA	ND
17	A	1129	CLA	NA
17	Q	5130	CLA	NC
17	Q	5130	CLA	ND
17	Q	5130	CLA	NA
17	B	1202	CLA	NA
17	B	1202	CLA	NC
17	B	1202	CLA	ND

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Mol	Chain	Res	Type	Atom
17	0	1031	CLA	NC
17	0	1031	CLA	ND
17	0	1031	CLA	NA
17	9	1015	CLA	NC
17	9	1015	CLA	ND
17	9	1015	CLA	NA
17	0	1026	CLA	NC
17	0	1026	CLA	ND
17	0	1026	CLA	NA
17	9	1014	CLA	NC
17	9	1014	CLA	ND
17	9	1014	CLA	NA
17	7	1014	CLA	NC
17	7	1014	CLA	ND
17	7	1014	CLA	NA
17	B	1225	CLA	ND
17	2	1021	CLA	NC
17	2	1021	CLA	ND
17	2	1021	CLA	NA
17	A	1131	CLA	ND
17	B	1223	CLA	NC
17	B	1223	CLA	ND
17	B	1223	CLA	NA
17	2	1026	CLA	NC
17	2	1026	CLA	ND
17	2	1026	CLA	NA
17	P	5129	CLA	NC
17	P	5129	CLA	ND
17	P	5129	CLA	NA
17	B	1235	CLA	NC
17	B	1235	CLA	ND
17	B	1235	CLA	NA
17	Q	5218	CLA	NC
17	Q	5218	CLA	ND
17	Q	5218	CLA	NA
17	K	1403	CLA	NC
17	K	1403	CLA	ND
17	K	1403	CLA	NA
17	A	1124	CLA	NC
17	A	1124	CLA	ND
17	A	1124	CLA	NA
17	0	1032	CLA	NC

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Mol	Chain	Res	Type	Atom
17	0	1032	CLA	ND
17	0	1032	CLA	NA
17	A	1116	CLA	NC
17	A	1116	CLA	ND
17	P	5125	CLA	NC
17	P	5125	CLA	ND
17	P	5125	CLA	NA
17	P	5132	CLA	NC
17	P	5132	CLA	ND
17	P	5132	CLA	NA
17	A	1127	CLA	NC
17	A	1127	CLA	ND
17	B	1221	CLA	NC
17	B	1221	CLA	ND
17	B	1221	CLA	NA
17	A	1115	CLA	NC
17	A	1115	CLA	ND
17	A	1115	CLA	NA
17	7	1012	CLA	NC
17	7	1012	CLA	ND
17	7	1012	CLA	NA
17	B	1226	CLA	NC
17	B	1226	CLA	ND
17	B	1226	CLA	NA
17	G	1701	CLA	NC
17	G	1701	CLA	ND
17	G	1701	CLA	NA
17	B	1237	CLA	NC
17	B	1237	CLA	ND
17	P	5111	CLA	NC
17	P	5111	CLA	ND
17	P	5111	CLA	NA
17	P	5107	CLA	NC
17	P	5107	CLA	ND
17	P	5107	CLA	NA
17	U	8005	CLA	NC
17	U	8005	CLA	ND
17	U	8005	CLA	NA
17	Q	5222	CLA	NC
17	Q	5222	CLA	ND
17	Q	5222	CLA	NA
17	A	1113	CLA	NC

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Mol	Chain	Res	Type	Atom
17	A	1113	CLA	ND
17	A	1113	CLA	NA
17	P	5137	CLA	ND
17	3	1011	CLA	NC
17	3	1011	CLA	ND
17	3	1011	CLA	NA
17	1	1011	CLA	NC
17	1	1011	CLA	ND
17	1	1011	CLA	NA
17	P	5105	CLA	NC
17	P	5105	CLA	ND
17	P	5105	CLA	NA
17	B	1213	CLA	NC
17	B	1213	CLA	ND
17	B	1213	CLA	NA
17	4	1032	CLA	NC
17	4	1032	CLA	ND
17	4	1032	CLA	NA
17	4	1015	CLA	NC
17	4	1015	CLA	ND
17	4	1015	CLA	NA
17	B	1204	CLA	ND
17	B	1204	CLA	NA
17	P	5136	CLA	NC
17	P	5136	CLA	ND
17	P	5136	CLA	NA
17	1	1016	CLA	NC
17	1	1016	CLA	ND
17	1	1016	CLA	NA
17	8	1013	CLA	NC
17	8	1013	CLA	ND
17	8	1013	CLA	NA
17	Q	5023	CLA	ND
17	Q	5023	CLA	NA
17	0	1015	CLA	NC
17	0	1015	CLA	ND
17	0	1015	CLA	NA
17	L	1503	CLA	NC
17	L	1503	CLA	ND
17	L	1503	CLA	NA
17	Q	5231	CLA	NC
17	Q	5231	CLA	ND

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Mol	Chain	Res	Type	Atom
17	P	5402	CLA	NC
17	P	5402	CLA	ND
17	P	5402	CLA	NA
17	Q	5210	CLA	NA
17	Q	5210	CLA	NC
17	Q	5210	CLA	ND
17	Q	5228	CLA	NC
17	Q	5228	CLA	ND
17	Q	5228	CLA	NA
17	A	1128	CLA	NC
17	A	1128	CLA	ND
17	A	1128	CLA	NA
17	Q	5225	CLA	ND
17	9	1031	CLA	NC
17	9	1031	CLA	ND
17	9	1031	CLA	NA
17	9	1016	CLA	NC
17	9	1016	CLA	ND
17	9	1016	CLA	NA
17	8	1012	CLA	NC
17	8	1012	CLA	ND
17	8	1012	CLA	NA
17	B	1242	CLA	NC
17	B	1242	CLA	ND
17	B	1242	CLA	NA
17	2	1022	CLA	NC
17	2	1022	CLA	ND
17	2	1022	CLA	NA
17	A	1108	CLA	NC
17	A	1108	CLA	ND
17	P	5108	CLA	NC
17	P	5108	CLA	ND
17	3	1031	CLA	NC
17	3	1031	CLA	ND
17	3	1031	CLA	NA
17	4	1025	CLA	NC
17	4	1025	CLA	ND
17	4	1025	CLA	NA
17	P	5117	CLA	NC
17	P	5117	CLA	ND
17	P	5117	CLA	NA
17	V	5701	CLA	NC

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Mol	Chain	Res	Type	Atom
17	V	5701	CLA	ND
17	V	5701	CLA	NA
17	3	1016	CLA	NC
17	3	1016	CLA	ND
17	3	1016	CLA	NA
17	P	5135	CLA	NC
17	P	5135	CLA	ND
17	P	5135	CLA	NA
17	Q	5238	CLA	NC
17	Q	5238	CLA	ND
17	Q	5238	CLA	NA
17	B	1212	CLA	NC
17	B	1212	CLA	ND
17	Q	5209	CLA	NC
17	Q	5209	CLA	ND
17	Q	5209	CLA	NA
17	F	1301	CLA	NC
17	F	1301	CLA	ND
17	F	1301	CLA	NA
17	Q	5206	CLA	ND
17	8	1015	CLA	NC
17	8	1015	CLA	ND
17	8	1015	CLA	NA
17	B	1216	CLA	NC
17	B	1216	CLA	ND
17	B	1216	CLA	NA
17	L	1501	CLA	ND
17	L	1501	CLA	NA
17	2	1014	CLA	NC
17	2	1014	CLA	ND
17	2	1014	CLA	NA
17	Q	5219	CLA	NC
17	Q	5219	CLA	ND
17	Q	5219	CLA	NA
17	9	1017	CLA	NC
17	9	1017	CLA	ND
17	9	1017	CLA	NA
17	P	5104	CLA	NC
17	P	5104	CLA	ND
17	P	5104	CLA	NA
17	B	1228	CLA	NC
17	B	1228	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	1228	CLA	NA
17	P	5121	CLA	ND
17	B	1214	CLA	NC
17	B	1214	CLA	ND
17	B	1214	CLA	NA
17	7	1021	CLA	NC
17	7	1021	CLA	ND
17	7	1021	CLA	NA
17	1	1025	CLA	NC
17	1	1025	CLA	ND
17	1	1025	CLA	NA
17	4	1013	CLA	NC
17	4	1013	CLA	ND
17	4	1013	CLA	NA
17	A	1133	CLA	NC
17	A	1133	CLA	ND
17	A	1133	CLA	NA
17	P	5131	CLA	ND
17	4	1031	CLA	NC
17	4	1031	CLA	ND
17	4	1031	CLA	NA
17	7	1023	CLA	NC
17	7	1023	CLA	ND
17	7	1023	CLA	NA
17	Q	5213	CLA	NC
17	Q	5213	CLA	ND
17	Q	5213	CLA	NA
17	8	1033	CLA	NC
17	8	1033	CLA	ND
17	8	1033	CLA	NA
17	3	1025	CLA	NC
17	3	1025	CLA	ND
17	3	1025	CLA	NA
17	P	8010	CLA	NC
17	P	8010	CLA	ND
17	P	8010	CLA	NA
17	4	4002	CLA	NC
17	4	4002	CLA	ND
17	4	4002	CLA	NA
17	U	5301	CLA	NC
17	U	5301	CLA	ND
17	U	5301	CLA	NA

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Mol	Chain	Res	Type	Atom
17	L	1504	CLA	NC
17	L	1504	CLA	ND
17	L	1504	CLA	NA
17	2	1031	CLA	NC
17	2	1031	CLA	ND
17	2	1031	CLA	NA
17	F	4003	CLA	NC
17	F	4003	CLA	ND
17	F	4003	CLA	NA
17	U	8004	CLA	NC
17	U	8004	CLA	ND
17	U	8004	CLA	NA
17	P	5112	CLA	NC
17	P	5112	CLA	ND
17	P	5112	CLA	NA
17	0	1011	CLA	NC
17	0	1011	CLA	ND
17	0	1011	CLA	NA
17	Q	5021	CLA	ND
17	A	1138	CLA	NC
17	A	1138	CLA	ND
17	A	1138	CLA	NA
17	A	1107	CLA	NC
17	A	1107	CLA	ND
17	A	1107	CLA	NA
17	1	1015	CLA	NC
17	1	1015	CLA	ND
17	1	1015	CLA	NA
17	6	5502	CLA	NC
17	6	5502	CLA	NA
17	3	1026	CLA	NC
17	3	1026	CLA	ND
17	3	1026	CLA	NA
17	4	1022	CLA	NC
17	4	1022	CLA	ND
17	4	1022	CLA	NA
17	4	1033	CLA	NC
17	4	1033	CLA	ND
17	4	1033	CLA	NA
17	0	1016	CLA	NC
17	0	1016	CLA	ND
17	0	1016	CLA	NA

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Mol	Chain	Res	Type	Atom
17	9	1021	CLA	NC
17	9	1021	CLA	ND
17	9	1021	CLA	NA
17	6	5501	CLA	ND
17	6	5501	CLA	NA
17	6	5504	CLA	NC
17	6	5504	CLA	ND
17	6	5504	CLA	NA
17	4	1017	CLA	NC
17	4	1017	CLA	ND
17	4	1017	CLA	NA
17	P	5140	CLA	NC
17	P	5140	CLA	ND
17	P	5140	CLA	NA
17	L	1502	CLA	NC
17	L	1502	CLA	NA
17	A	4010	CLA	NC
17	A	4010	CLA	ND
17	A	4010	CLA	NA
17	7	1025	CLA	NC
17	7	1025	CLA	ND
17	7	1025	CLA	NA
17	Q	5241	CLA	NC
17	Q	5241	CLA	ND
17	Q	5241	CLA	NA
17	A	1135	CLA	NC
17	A	1135	CLA	ND
17	A	1135	CLA	NA
17	3	1022	CLA	NC
17	3	1022	CLA	ND
17	3	1022	CLA	NA
17	U	8003	CLA	NC
17	U	8003	CLA	ND
17	U	8003	CLA	NA
17	J	4008	CLA	NC
17	J	4008	CLA	ND
17	J	4008	CLA	NA
17	8	1023	CLA	NC
17	8	1023	CLA	ND
17	8	1023	CLA	NA
17	2	1017	CLA	NC
17	2	1017	CLA	ND

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Mol	Chain	Res	Type	Atom
17	2	1017	CLA	NA
17	Q	5203	CLA	NC
17	Q	5203	CLA	ND
17	Q	5203	CLA	NA
17	9	1022	CLA	NC
17	9	1022	CLA	ND
17	9	1022	CLA	NA
17	P	5106	CLA	NC
17	P	5106	CLA	ND
17	P	5106	CLA	NA
17	1	1017	CLA	NC
17	1	1017	CLA	ND
17	1	1017	CLA	NA
17	3	1017	CLA	NC
17	3	1017	CLA	ND
17	3	1017	CLA	NA
17	B	1215	CLA	ND
17	B	1215	CLA	NA
17	B	1209	CLA	NC
17	B	1209	CLA	ND
17	B	1209	CLA	NA
17	P	5128	CLA	NC
17	P	5128	CLA	ND
17	P	5128	CLA	NA
17	8	1014	CLA	NC
17	8	1014	CLA	ND
17	8	1014	CLA	NA
17	F	4005	CLA	NC
17	F	4005	CLA	ND
17	F	4005	CLA	NA
17	A	1117	CLA	NC
17	A	1117	CLA	ND
17	A	1117	CLA	NA
17	B	1219	CLA	NC
17	B	1219	CLA	ND
17	B	1219	CLA	NA
17	B	1234	CLA	NC
17	B	1234	CLA	ND
17	B	1234	CLA	NA
17	Q	5214	CLA	NC
17	Q	5214	CLA	ND
17	Q	5214	CLA	NA

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Mol	Chain	Res	Type	Atom
17	7	1015	CLA	NC
17	7	1015	CLA	ND
17	7	1015	CLA	NA
17	0	1014	CLA	NC
17	0	1014	CLA	ND
17	0	1014	CLA	NA
17	B	1241	CLA	NC
17	B	1241	CLA	ND
17	B	1241	CLA	NA
17	Q	5226	CLA	NC
17	Q	5226	CLA	ND
17	Q	5226	CLA	NA
17	J	1101	CLA	NC
17	J	1101	CLA	ND
17	J	1101	CLA	NA
17	Q	5221	CLA	NC
17	Q	5221	CLA	ND
17	Q	5221	CLA	NA
17	B	1211	CLA	NC
17	B	1211	CLA	ND
17	B	1211	CLA	NA
17	8	1017	CLA	NC
17	8	1017	CLA	ND
17	8	1017	CLA	NA
17	P	5901	CLA	NC
17	P	5901	CLA	ND
17	P	5901	CLA	NA
17	A	1126	CLA	ND
17	P	5118	CLA	NC
17	P	5118	CLA	ND
17	P	5118	CLA	NA
17	8	1016	CLA	NC
17	8	1016	CLA	ND
17	8	1016	CLA	NA
17	H	1801	CLA	NC
17	H	1801	CLA	ND
17	H	1801	CLA	NA
17	2	1015	CLA	NC
17	2	1015	CLA	ND
17	2	1015	CLA	NA
17	P	5133	CLA	NC
17	P	5133	CLA	ND

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Mol	Chain	Res	Type	Atom
17	P	5133	CLA	NA
17	K	1404	CLA	NC
17	K	1404	CLA	ND
17	K	1404	CLA	NA
17	P	5114	CLA	NC
17	P	5114	CLA	ND
17	P	5114	CLA	NA
17	Q	5240	CLA	NC
17	Q	5240	CLA	ND
17	Q	5240	CLA	NA
17	B	1220	CLA	NC
17	B	1220	CLA	ND
17	B	1220	CLA	NA
17	7	1016	CLA	NC
17	7	1016	CLA	ND
17	7	1016	CLA	NA
17	Q	5227	CLA	NC
17	Q	5227	CLA	ND
17	Q	5227	CLA	NA
17	8	1026	CLA	NC
17	8	1026	CLA	ND
17	8	1026	CLA	NA
17	8	1031	CLA	NC
17	8	1031	CLA	ND
17	8	1031	CLA	NA
17	G	1233	CLA	NC
17	G	1233	CLA	ND
17	G	1233	CLA	NA
17	4	1016	CLA	NC
17	4	1016	CLA	ND
17	4	1016	CLA	NA
17	P	5119	CLA	NC
17	P	5119	CLA	ND
17	P	5119	CLA	NA
17	A	1901	CLA	NC
17	A	1901	CLA	ND
17	A	1901	CLA	NA
17	3	1041	CLA	NC
17	3	1041	CLA	ND
17	3	1041	CLA	NA
17	B	1217	CLA	NC
17	B	1217	CLA	ND

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Mol	Chain	Res	Type	Atom
17	B	1217	CLA	NA
17	0	1025	CLA	NC
17	0	1025	CLA	ND
17	0	1025	CLA	NA
17	A	1011	CLA	NC
17	A	1011	CLA	ND
17	P	5126	CLA	ND
17	7	1013	CLA	NC
17	7	1013	CLA	ND
17	7	1013	CLA	NA
17	0	1023	CLA	NC
17	0	1023	CLA	ND
17	0	1023	CLA	NA
17	A	1112	CLA	NC
17	A	1112	CLA	ND
17	A	1112	CLA	NA
17	7	1022	CLA	NC
17	7	1022	CLA	ND
17	7	1022	CLA	NA
17	B	1236	CLA	ND
17	8	8007	CLA	NC
17	8	8007	CLA	ND
17	8	8007	CLA	NA
17	A	1402	CLA	NC
17	A	1402	CLA	ND
17	A	1402	CLA	NA
17	B	1206	CLA	ND
17	P	5127	CLA	NC
17	P	5127	CLA	ND
17	Q	5217	CLA	NC
17	Q	5217	CLA	ND
17	Q	5217	CLA	NA
17	Q	5216	CLA	NC
17	Q	5216	CLA	ND
17	Q	5216	CLA	NA
17	P	5120	CLA	NC
17	P	5120	CLA	ND
17	P	5120	CLA	NA
17	Q	5235	CLA	NC
17	Q	5235	CLA	ND
17	Q	5235	CLA	NA
17	Z	5302	CLA	NC

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Mol	Chain	Res	Type	Atom
17	Z	5302	CLA	ND
17	Z	5302	CLA	NA
17	A	1140	CLA	NC
17	A	1140	CLA	ND
17	A	1140	CLA	NA
17	5	5403	CLA	NC
17	5	5403	CLA	ND
17	5	5403	CLA	NA
17	P	5138	CLA	NC
17	P	5138	CLA	ND
17	P	5138	CLA	NA
17	B	1021	CLA	ND
17	P	5124	CLA	NC
17	P	5124	CLA	ND
17	P	5124	CLA	NA
17	0	1033	CLA	NC
17	0	1033	CLA	ND
17	0	1033	CLA	NA
17	Q	5212	CLA	NC
17	Q	5212	CLA	ND
17	P	5011	CLA	NC
17	P	5011	CLA	ND
17	B	1207	CLA	NC
17	B	1207	CLA	ND
17	B	1207	CLA	NA
17	Q	5220	CLA	NC
17	Q	5220	CLA	ND
17	Q	5220	CLA	NA
17	A	1137	CLA	ND
17	0	1013	CLA	NC
17	0	1013	CLA	ND
17	0	1013	CLA	NA
17	A	1123	CLA	NC
17	A	1123	CLA	ND
17	A	1123	CLA	NA
17	P	5115	CLA	NC
17	P	5115	CLA	ND
17	P	5115	CLA	NA
17	1	1013	CLA	NC
17	1	1013	CLA	ND
17	1	1013	CLA	NA
17	B	1224	CLA	ND

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Mol	Chain	Res	Type	Atom
17	4	1023	CLA	NC
17	4	1023	CLA	ND
17	4	1023	CLA	NA
17	P	5113	CLA	NC
17	P	5113	CLA	ND
17	P	5113	CLA	NA
17	1	1014	CLA	NC
17	1	1014	CLA	ND
17	1	1014	CLA	NA
17	P	5103	CLA	NC
17	P	5103	CLA	ND
17	P	5103	CLA	NA
17	Q	5022	CLA	ND
17	9	1012	CLA	NC
17	9	1012	CLA	ND
17	9	1012	CLA	NA
17	B	1205	CLA	ND
17	3	1014	CLA	NC
17	3	1014	CLA	ND
17	3	1014	CLA	NA
17	4	1011	CLA	NC
17	4	1011	CLA	ND
17	4	1011	CLA	NA
17	B	1208	CLA	NC
17	B	1208	CLA	ND
17	B	1208	CLA	NA
17	A	1118	CLA	NC
17	A	1118	CLA	ND
17	A	1118	CLA	NA
17	6	5503	CLA	NC
17	6	5503	CLA	ND
17	6	5503	CLA	NA
17	7	1031	CLA	NC
17	7	1031	CLA	ND
17	7	1031	CLA	NA
17	P	5116	CLA	NC
17	P	5116	CLA	ND
17	9	1025	CLA	NC
17	9	1025	CLA	ND
17	9	1025	CLA	NA
17	Q	5234	CLA	NC
17	Q	5234	CLA	ND

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Mol	Chain	Res	Type	Atom
17	Q	5234	CLA	NA
17	A	1106	CLA	NC
17	A	1106	CLA	ND
17	A	1106	CLA	NA
17	P	8009	CLA	NC
17	P	8009	CLA	ND
17	P	8009	CLA	NA
17	Q	5232	CLA	NC
17	Q	5232	CLA	ND
17	Q	5232	CLA	NA
17	B	1231	CLA	NC
17	B	1231	CLA	ND
17	Q	5201	CLA	NC
17	Q	5201	CLA	ND
17	Q	5201	CLA	NA
17	Z	8008	CLA	NC
17	Z	8008	CLA	ND
17	Z	8008	CLA	NA
17	8	1011	CLA	NC
17	8	1011	CLA	ND
17	8	1011	CLA	NA
17	F	1229	CLA	NC
17	F	1229	CLA	ND
17	F	1229	CLA	NA
17	A	1111	CLA	NC
17	A	1111	CLA	ND
17	A	1111	CLA	NA
17	3	1032	CLA	NC
17	3	1032	CLA	ND
17	3	1032	CLA	NA
17	2	1025	CLA	NC
17	2	1025	CLA	ND
17	2	1025	CLA	NA
17	P	5139	CLA	NC
17	P	5139	CLA	ND
17	Q	5230	CLA	NC
17	Q	5230	CLA	ND
17	Q	5230	CLA	NA
17	Q	5215	CLA	ND
17	Q	5215	CLA	NA
17	P	5110	CLA	NC
17	P	5110	CLA	ND

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Mol	Chain	Res	Type	Atom
17	P	5110	CLA	NA
17	0	1012	CLA	NC
17	0	1012	CLA	ND
17	0	1012	CLA	NA
17	2	1012	CLA	NC
17	2	1012	CLA	ND
17	2	1012	CLA	NA
17	A	1105	CLA	NC
17	A	1105	CLA	ND
17	A	1105	CLA	NA
17	1	1022	CLA	NC
17	1	1022	CLA	ND
17	1	1022	CLA	NA
17	9	1032	CLA	NC
17	9	1032	CLA	ND
17	9	1032	CLA	NA
17	8	1022	CLA	NC
17	8	1022	CLA	ND
17	8	1022	CLA	NA
17	7	1026	CLA	NC
17	7	1026	CLA	ND
17	7	1026	CLA	NA
17	Q	5211	CLA	NC
17	Q	5211	CLA	ND
17	Q	5211	CLA	NA
17	A	1125	CLA	NC
17	A	1125	CLA	ND
17	A	1125	CLA	NA
17	A	4009	CLA	NC
17	A	4009	CLA	ND
17	A	4009	CLA	NA
17	9	1011	CLA	NC
17	9	1011	CLA	ND
17	9	1011	CLA	NA
17	4	1021	CLA	NC
17	4	1021	CLA	ND
17	4	1021	CLA	NA
17	2	1011	CLA	NC
17	2	1011	CLA	ND
17	2	1011	CLA	NA
17	W	5801	CLA	NC
17	W	5801	CLA	ND

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Mol	Chain	Res	Type	Atom
17	W	5801	CLA	NA
17	A	1122	CLA	NC
17	A	1122	CLA	ND
17	A	1122	CLA	NA
17	A	1114	CLA	NC
17	A	1114	CLA	ND
17	A	1114	CLA	NA
17	5	5404	CLA	NC
17	5	5404	CLA	ND
17	5	5404	CLA	NA
17	J	1302	CLA	NC
17	J	1302	CLA	ND
17	J	1302	CLA	NA
17	B	1023	CLA	ND
17	B	1023	CLA	NA
17	U	5229	CLA	NC
17	U	5229	CLA	ND
17	U	5229	CLA	NA
17	B	1240	CLA	NC
17	B	1240	CLA	ND
17	B	1240	CLA	NA
17	B	1227	CLA	NC
17	B	1227	CLA	ND
17	B	1227	CLA	NA
17	1	1026	CLA	NC
17	1	1026	CLA	ND
17	1	1026	CLA	NA
17	P	5013	CLA	NC
17	P	5013	CLA	ND
17	Q	5205	CLA	ND
17	B	4001	CLA	NC
17	B	4001	CLA	ND
17	B	4001	CLA	NA
17	P	5012	CLA	ND
17	A	1102	CLA	NC
17	A	1102	CLA	ND
17	A	1102	CLA	NA
17	P	5123	CLA	NC
17	P	5123	CLA	ND
17	P	5123	CLA	NA
17	Q	5236	CLA	ND
17	V	5233	CLA	NC

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Mol	Chain	Res	Type	Atom
17	V	5233	CLA	ND
17	V	5233	CLA	NA
17	Q	5202	CLA	NA
17	Q	5202	CLA	NC
17	Q	5202	CLA	ND
17	B	1218	CLA	NC
17	B	1218	CLA	ND
17	B	1218	CLA	NA
17	B	1130	CLA	NC
17	B	1130	CLA	ND
17	B	1130	CLA	NA
17	A	1121	CLA	ND

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.