



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 20, 2017 – 02:15 AM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

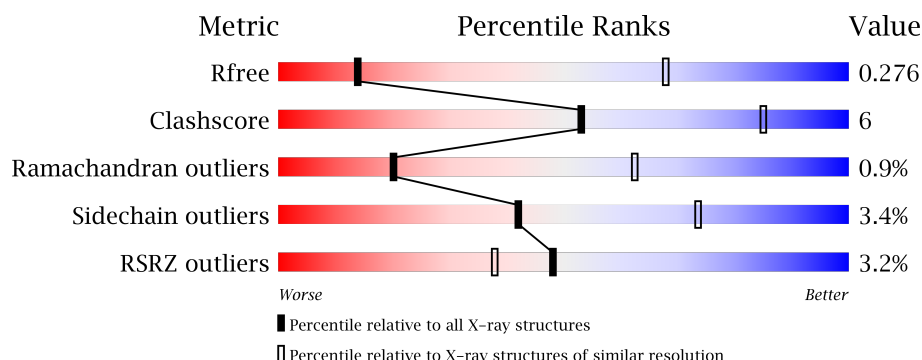
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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

Mol	Chain	Length	Quality of chain
1	1	751	
1	A	751	
1	a	751	
2	2	731	
2	B	731	

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

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

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

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

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

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

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

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

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

2 Entry composition [i](#)

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	a	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			
1	1	739	Total	C	N	O	S	0	0	0
			5772	3783	982	980	27			

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

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

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

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

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

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

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

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

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

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

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

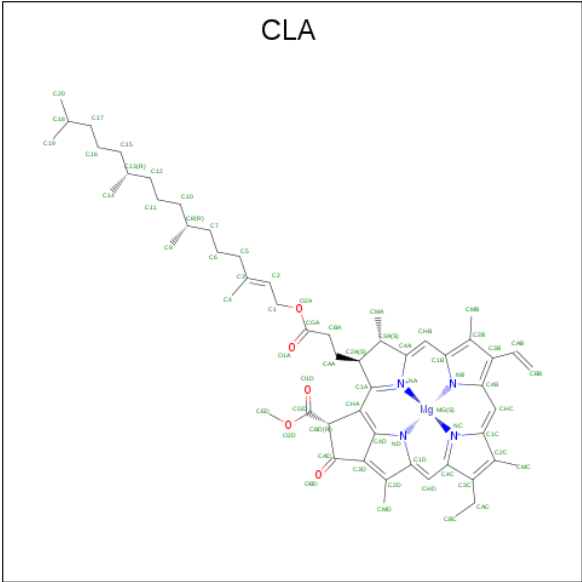
- Molecule 9 is a protein called Photosystem I subunit III.

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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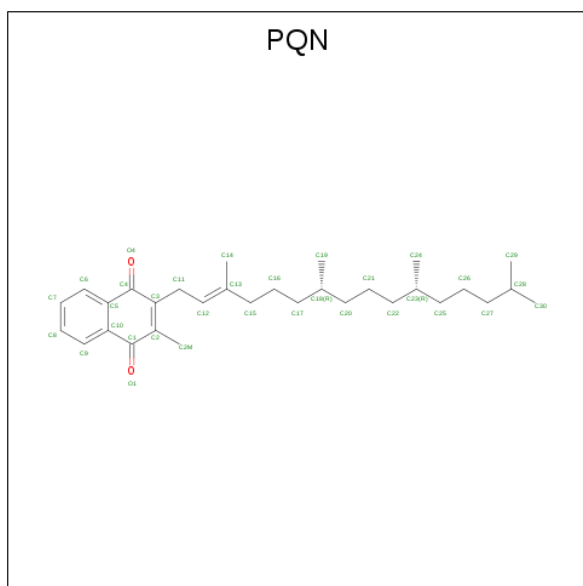
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	2	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
11	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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

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



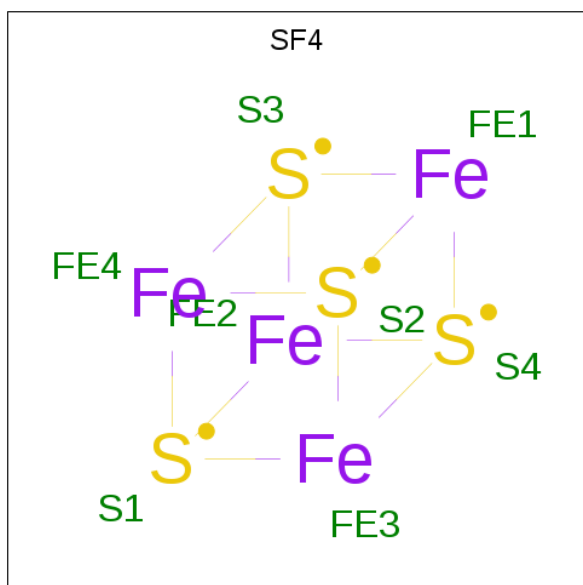
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			33	31	2		
12	B	1	Total	C	O	0	0
			33	31	2		
12	a	1	Total	C	O	0	0
			33	31	2		
12	b	1	Total	C	O	0	0
			33	31	2		

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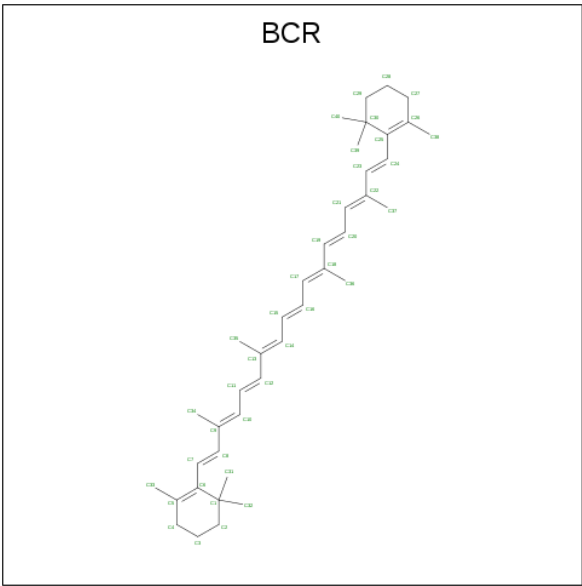
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	1	1	Total	C	O	0	0
			33	31	2		
12	2	1	Total	C	O	0	0
			33	31	2		

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



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

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



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

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

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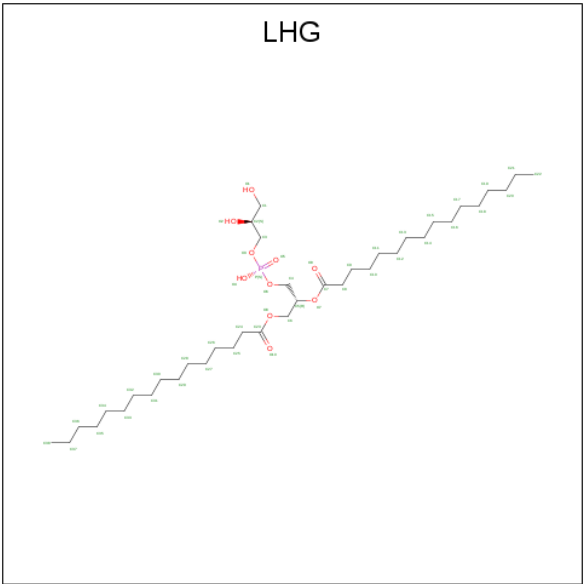
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	f	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	l	1	Total C 40 40	0	0
14	m	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	1	1	Total C 40 40	0	0
14	2	1	Total C 40 40	0	0
14	2	1	Total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

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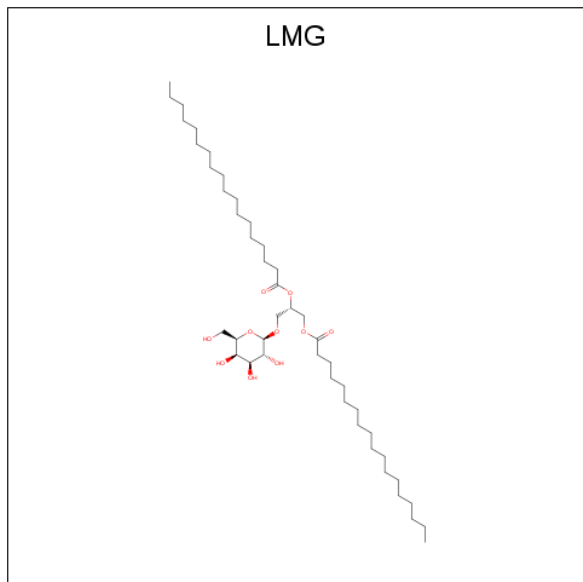
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	8	1	Total C 40 40	0	0
14	7	1	Total C 40 40	0	0

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



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

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).

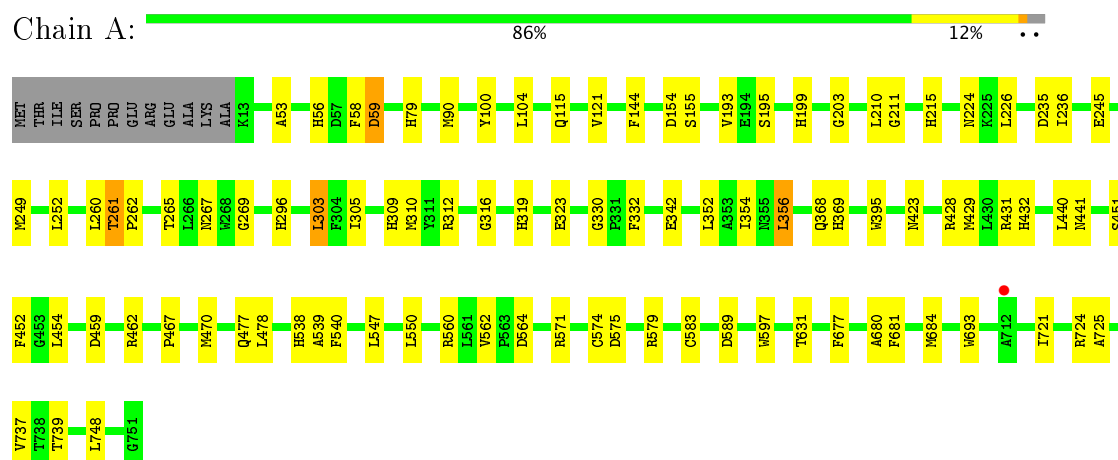


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	B	1	Total	C	O	0	0
			55	45	10		
16	b	1	Total	C	O	0	0
			55	45	10		
16	2	1	Total	C	O	0	0
			55	45	10		

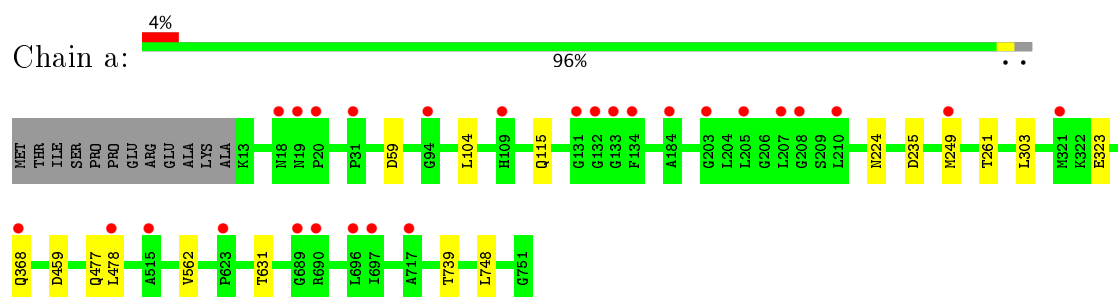
3 Residue-property plots [i](#)

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

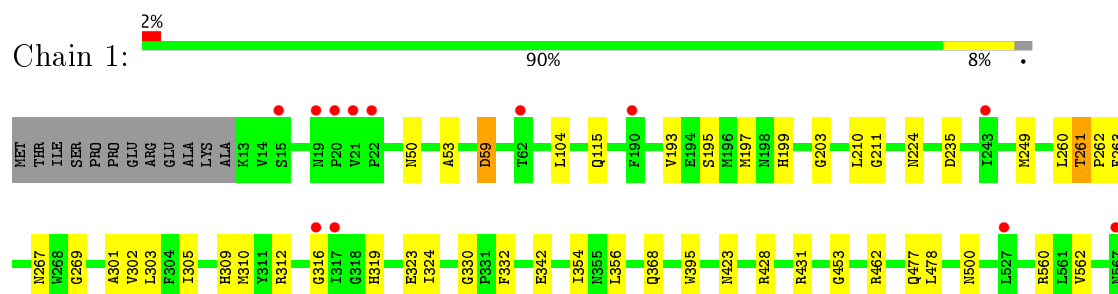
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

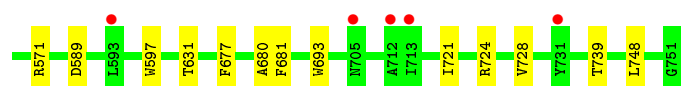


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



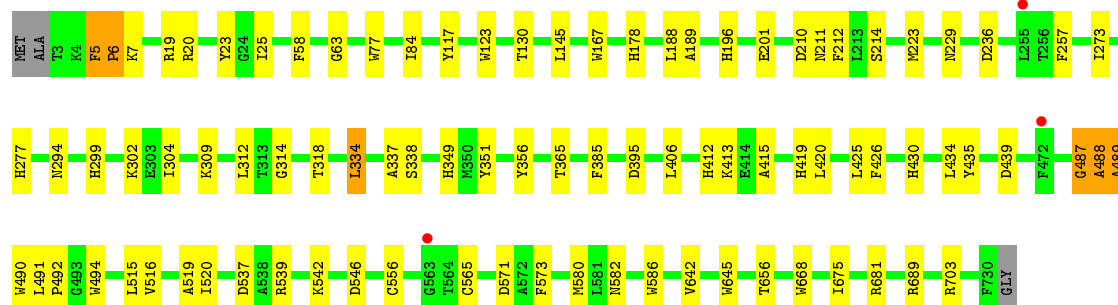
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





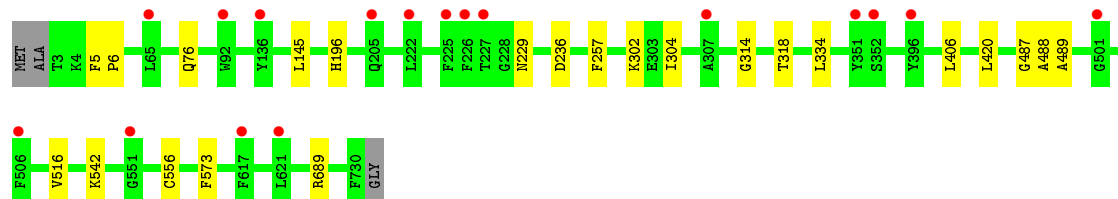
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 87% 11% .



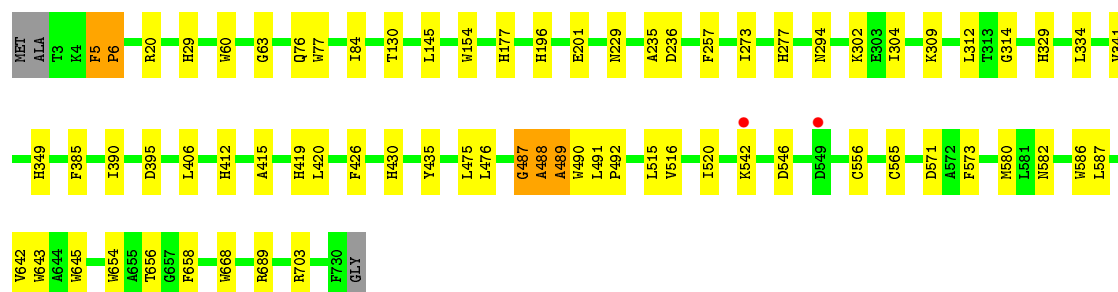
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 2% 96% .



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2: 90% 9% .



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 84% 10% 5% .




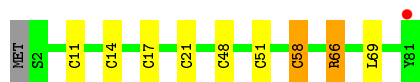
- Molecule 3: Photosystem I iron-sulfur center

Chain c:  94% 5%




- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  88% 9%



- Molecule 4: Photosystem I subunit II

Chain D:  88% 8%



- Molecule 4: Photosystem I subunit II

Chain d:  94%




- Molecule 4: Photosystem I subunit II

Chain 4:  91%




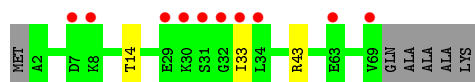
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  84% 7% 8%

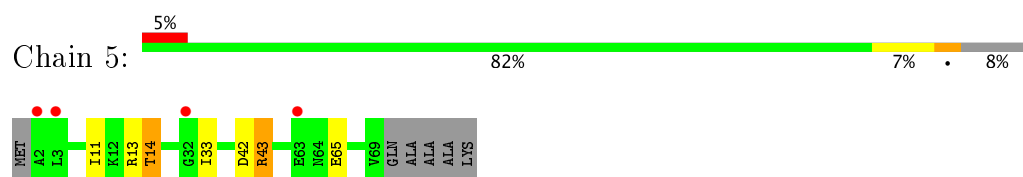


- Molecule 5: Photosystem I reaction center subunit IV

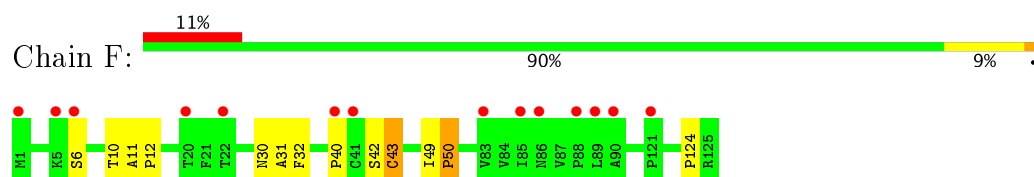
Chain e:  88% 8%



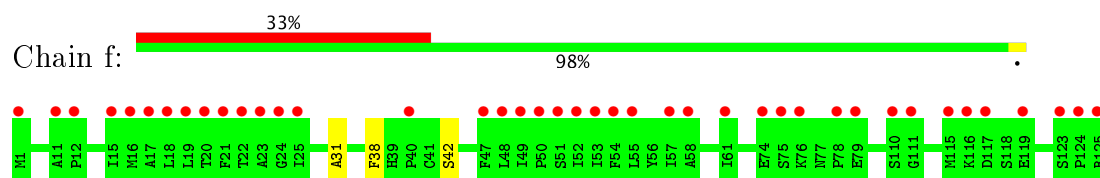
- Molecule 5: Photosystem I reaction center subunit IV



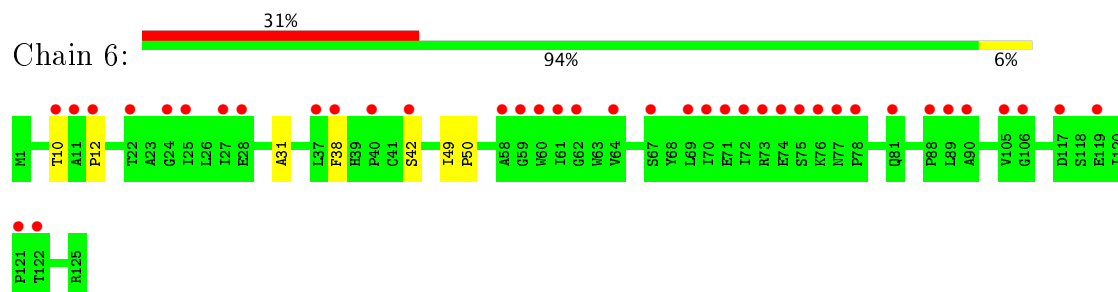
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



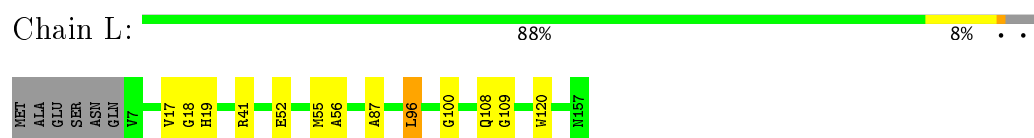
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



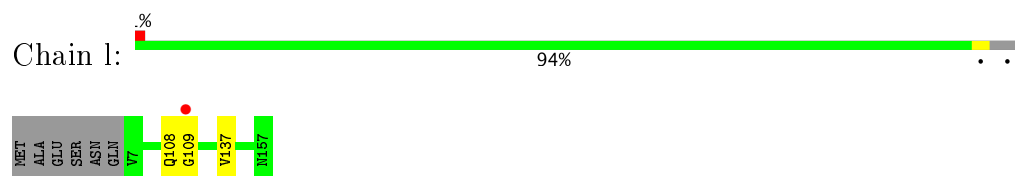
- Molecule 6: Fusion protein of Photosystem I subunit III and subunit IX



- Molecule 7: Photosystem I reaction center subunit XI



- Molecule 7: Photosystem I reaction center subunit XI

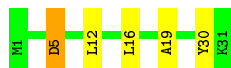
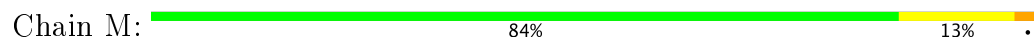


- Molecule 7: Photosystem I reaction center subunit XI





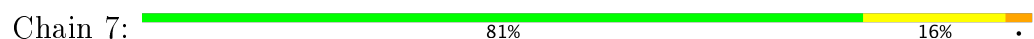
- Molecule 8: Photosystem I reaction center subunit XII



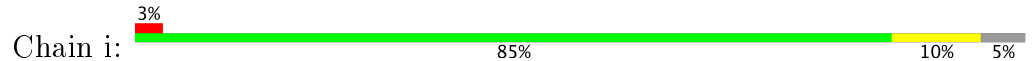
- Molecule 8: Photosystem I reaction center subunit XII



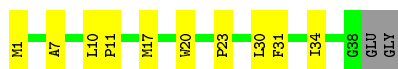
- Molecule 8: Photosystem I reaction center subunit XII



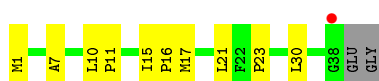
- Molecule 9: Photosystem I subunit III



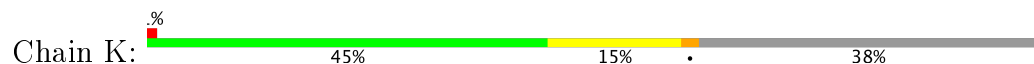
- Molecule 9: Photosystem I subunit III

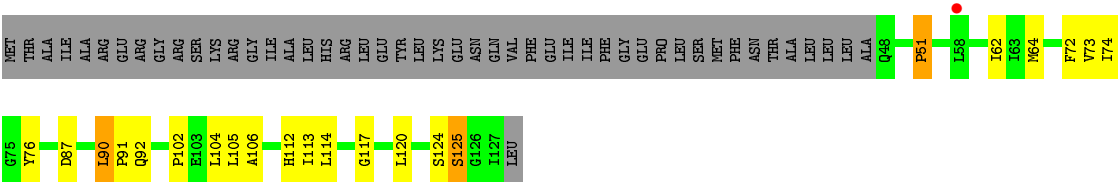


- Molecule 9: Photosystem I subunit III

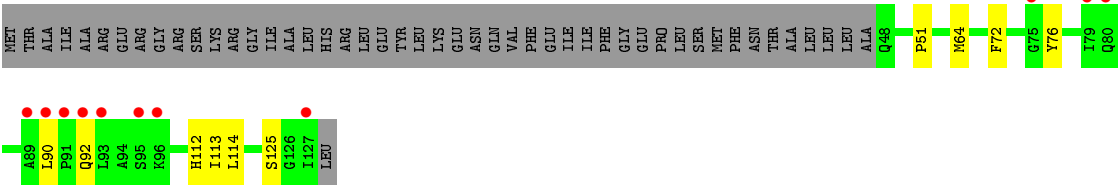


- Molecule 10: Photosystem I reaction center subunit VIII

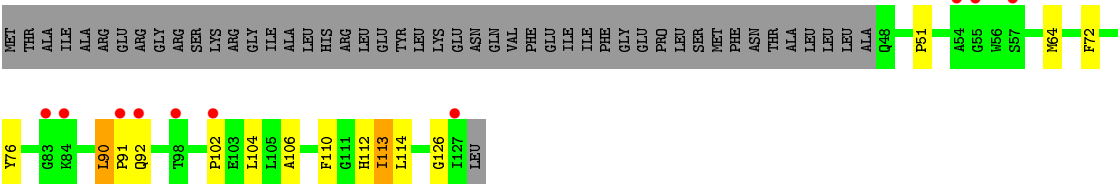




● Molecule 10: Photosystem I reaction center subunit VIII



● Molecule 10: Photosystem I reaction center subunit VIII



4 Data and refinement statistics

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

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
4	4	0	1
4	D	0	1
4	d	0	1
6	F	0	1
10	k	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

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

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	1	5772	0	5621	48	0
1	A	5772	0	5621	94	0
1	a	5772	0	5621	0	0
2	2	5765	0	5546	48	0
2	B	5765	0	5546	64	0
2	b	5765	0	5545	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	3	600	0	588	22	0
3	C	600	0	586	25	0
3	c	600	0	587	0	0
4	4	1079	0	1073	5	0
4	D	1079	0	1073	9	0
4	d	1079	0	1073	0	0
5	5	529	0	506	4	0
5	E	529	0	506	2	0
5	e	529	0	506	0	0
6	6	685	0	411	3	0
6	F	676	0	395	11	0
6	f	685	0	411	0	0
7	8	1133	0	1108	5	0
7	L	1133	0	1108	9	0
7	l	1133	0	1108	0	0
8	7	235	0	253	7	0
8	M	235	0	253	7	0
8	m	235	0	253	0	0
9	9	297	0	295	10	0
9	I	297	0	295	7	0
9	i	297	0	295	0	0
10	0	496	0	439	4	0
10	K	496	0	439	12	0
10	k	496	0	439	0	0
11	0	115	0	111	4	0
11	1	2546	0	2430	89	0
11	2	2313	0	2213	84	0
11	8	176	0	177	8	0
11	A	2546	0	2435	159	0
11	B	2313	0	2213	127	0
11	K	115	0	111	8	0
11	L	176	0	177	8	0
11	a	2546	0	2434	0	0
11	b	2313	0	2213	0	0
11	k	115	0	111	0	0
11	l	176	0	177	0	0
12	1	33	0	45	1	0
12	2	33	0	45	3	0
12	A	33	0	45	5	0
12	B	33	0	45	4	0
12	a	33	0	46	0	0
12	b	33	0	45	0	0

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

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

The worst 5 of 831 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:CYS:SG	13:C:3002:SF4:FE4	0.75	1.74
3:3:48:CYS:SG	13:3:3002:SF4:FE4	0.87	1.64
1:A:56:HIS:CG	11:A:1103:CLA:HBB2	3.55	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:11:CYS:SG	13:3:3003:SF4:FE3	0.88	1.61
3:C:58:CYS:SG	13:C:3003:SF4:FE1	1.08	1.57

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	737/751 (98%)	697 (95%)	38 (5%)	2 (0%)	44	81
1	A	737/751 (98%)	693 (94%)	42 (6%)	2 (0%)	44	81
1	a	737/751 (98%)	698 (95%)	37 (5%)	2 (0%)	44	81
2	2	726/731 (99%)	691 (95%)	28 (4%)	7 (1%)	18	61
2	B	726/731 (99%)	690 (95%)	30 (4%)	6 (1%)	22	65
2	b	726/731 (99%)	692 (95%)	28 (4%)	6 (1%)	22	65
3	3	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	121 (89%)	14 (10%)	1 (1%)	25	68
4	D	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	25	68
4	d	136/141 (96%)	122 (90%)	13 (10%)	1 (1%)	25	68
5	5	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	12	53
5	E	66/74 (89%)	57 (86%)	8 (12%)	1 (2%)	12	53
5	e	66/74 (89%)	58 (88%)	7 (11%)	1 (2%)	12	53
6	6	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	11	52
6	F	123/125 (98%)	114 (93%)	6 (5%)	3 (2%)	7	45
6	f	123/125 (98%)	115 (94%)	6 (5%)	2 (2%)	11	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	8	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	14	56
7	L	149/157 (95%)	135 (91%)	11 (7%)	3 (2%)	9	49
7	l	149/157 (95%)	135 (91%)	12 (8%)	2 (1%)	14	56
8	7	29/31 (94%)	29 (100%)	0	0	100	100
8	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
8	m	29/31 (94%)	29 (100%)	0	0	100	100
9	9	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	I	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
9	i	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
10	0	78/128 (61%)	65 (83%)	9 (12%)	4 (5%)	2	29
10	K	78/128 (61%)	66 (85%)	7 (9%)	5 (6%)	1	25
10	k	78/128 (61%)	66 (85%)	9 (12%)	3 (4%)	4	36
All	All	6474/6777 (96%)	6056 (94%)	361 (6%)	57 (1%)	20	62

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	THR
2	B	6	PRO
4	D	99	PRO
6	F	43	CYS
1	a	261	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	588/603 (98%)	573 (97%)	15 (3%)	51	78
1	A	588/603 (98%)	570 (97%)	18 (3%)	45	75
1	a	588/603 (98%)	573 (97%)	15 (3%)	51	78
2	2	582/583 (100%)	565 (97%)	17 (3%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	582/583 (100%)	562 (97%)	20 (3%)	42	73
2	b	582/583 (100%)	566 (97%)	16 (3%)	50	77
3	3	68/69 (99%)	65 (96%)	3 (4%)	33	68
3	C	68/69 (99%)	61 (90%)	7 (10%)	8	38
3	c	68/69 (99%)	64 (94%)	4 (6%)	23	60
4	4	113/116 (97%)	109 (96%)	4 (4%)	41	73
4	D	113/116 (97%)	111 (98%)	2 (2%)	64	85
4	d	113/116 (97%)	110 (97%)	3 (3%)	50	77
5	5	56/60 (93%)	54 (96%)	2 (4%)	40	72
5	E	56/60 (93%)	54 (96%)	2 (4%)	40	72
5	e	56/60 (93%)	54 (96%)	2 (4%)	40	72
6	6	21/106 (20%)	20 (95%)	1 (5%)	30	66
6	F	19/106 (18%)	19 (100%)	0	100	100
6	f	21/106 (20%)	20 (95%)	1 (5%)	30	66
7	8	113/118 (96%)	113 (100%)	0	100	100
7	L	113/118 (96%)	112 (99%)	1 (1%)	82	92
7	l	113/118 (96%)	112 (99%)	1 (1%)	82	92
8	7	24/25 (96%)	23 (96%)	1 (4%)	34	68
8	M	24/25 (96%)	23 (96%)	1 (4%)	34	68
8	m	24/25 (96%)	23 (96%)	1 (4%)	34	68
9	9	31/32 (97%)	28 (90%)	3 (10%)	9	40
9	I	31/32 (97%)	27 (87%)	4 (13%)	5	29
9	i	31/32 (97%)	27 (87%)	4 (13%)	5	29
10	0	37/100 (37%)	30 (81%)	7 (19%)	2	13
10	K	37/100 (37%)	30 (81%)	7 (19%)	2	13
10	k	37/100 (37%)	31 (84%)	6 (16%)	3	20
All	All	4897/5436 (90%)	4729 (97%)	168 (3%)	42	73

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	334	LEU
9	i	21	LEU

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Mol	Chain	Res	Type
10	k	64	MET
2	b	516	VAL
3	c	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	34	HIS
1	1	76	HIS
2	2	437	HIS
2	b	437	HIS
2	b	582	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

357 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	CLA	0	1401	-	56,73,73	1.85	12 (21%)	65,113,113	2.18	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	0	1402	-	41,58,73	2.24	13 (31%)	47,95,113	2.28	11 (23%)
11	CLA	1	1011	-	56,73,73	1.82	13 (23%)	65,113,113	2.53	18 (27%)
11	CLA	1	1012	-	56,73,73	1.88	12 (21%)	65,113,113	2.37	19 (29%)
11	CLA	1	1022	-	56,73,73	1.86	13 (23%)	65,113,113	2.14	14 (21%)
11	CLA	1	1101	-	56,73,73	1.84	12 (21%)	65,113,113	2.13	17 (26%)
11	CLA	1	1102	-	56,73,73	1.88	12 (21%)	65,113,113	1.99	11 (16%)
11	CLA	1	1103	-	56,73,73	1.85	12 (21%)	65,113,113	2.11	18 (27%)
11	CLA	1	1104	-	56,73,73	1.86	12 (21%)	65,113,113	2.12	16 (24%)
11	CLA	1	1105	-	39,56,73	2.23	12 (30%)	45,92,113	2.40	13 (28%)
11	CLA	1	1106	1	56,73,73	1.89	12 (21%)	65,113,113	2.04	15 (23%)
11	CLA	1	1107	-	56,73,73	1.89	12 (21%)	65,113,113	2.14	15 (23%)
11	CLA	1	1108	-	33,53,73	2.29	12 (36%)	37,89,113	2.33	9 (24%)
11	CLA	1	1109	-	56,73,73	1.88	12 (21%)	65,113,113	2.12	14 (21%)
11	CLA	1	1110	-	45,62,73	2.06	12 (26%)	51,99,113	2.48	15 (29%)
11	CLA	1	1111	-	51,68,73	1.93	11 (21%)	59,107,113	2.14	17 (28%)
11	CLA	1	1112	-	33,53,73	2.27	11 (33%)	37,89,113	2.35	11 (29%)
11	CLA	1	1113	-	33,53,73	2.27	12 (36%)	37,89,113	2.32	9 (24%)
11	CLA	1	1114	-	37,54,73	2.39	13 (35%)	43,90,113	2.33	13 (30%)
11	CLA	1	1115	-	37,54,73	2.36	13 (35%)	43,90,113	2.45	13 (30%)
11	CLA	1	1116	-	45,62,73	2.09	12 (26%)	51,99,113	2.31	16 (31%)
11	CLA	1	1117	-	56,73,73	1.87	12 (21%)	65,113,113	2.07	17 (26%)
11	CLA	1	1118	-	52,69,73	1.93	12 (23%)	60,108,113	2.12	17 (28%)
11	CLA	1	1119	-	56,73,73	1.87	12 (21%)	65,113,113	2.11	16 (24%)
11	CLA	1	1120	-	37,54,73	2.39	13 (35%)	43,90,113	2.39	13 (30%)
11	CLA	1	1121	-	37,54,73	2.37	12 (32%)	43,90,113	2.35	12 (27%)
11	CLA	1	1122	-	50,67,73	2.00	13 (26%)	57,105,113	2.25	15 (26%)
11	CLA	1	1123	-	56,73,73	1.85	13 (23%)	65,113,113	2.15	14 (21%)
11	CLA	1	1124	-	46,63,73	2.05	13 (28%)	53,101,113	2.25	14 (26%)
11	CLA	1	1125	-	43,60,73	2.10	13 (30%)	49,97,113	2.38	16 (32%)
11	CLA	1	1126	-	56,73,73	1.87	13 (23%)	65,113,113	2.12	17 (26%)
11	CLA	1	1127	-	56,73,73	1.89	12 (21%)	65,113,113	1.98	14 (21%)
11	CLA	1	1128	-	56,73,73	1.86	12 (21%)	65,113,113	2.05	15 (23%)
11	CLA	1	1129	-	37,54,73	2.39	13 (35%)	43,90,113	2.38	12 (27%)
11	CLA	1	1130	-	37,54,73	2.40	13 (35%)	43,90,113	2.27	11 (25%)
11	CLA	1	1131	-	56,73,73	1.86	13 (23%)	65,113,113	2.10	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	1	1132	-	56,73,73	1.85	12 (21%)	65,113,113	2.00	13 (20%)
11	CLA	1	1133	-	37,54,73	2.39	12 (32%)	43,90,113	2.41	14 (32%)
11	CLA	1	1134	-	37,54,73	2.39	12 (32%)	43,90,113	2.37	13 (30%)
11	CLA	1	1135	-	42,59,73	2.16	13 (30%)	48,96,113	2.48	15 (31%)
11	CLA	1	1136	-	37,54,73	2.39	12 (32%)	43,90,113	2.25	12 (27%)
11	CLA	1	1137	-	56,73,73	1.89	13 (23%)	65,113,113	2.29	18 (27%)
11	CLA	1	1138	-	37,54,73	2.38	12 (32%)	43,90,113	2.20	13 (30%)
11	CLA	1	1139	-	41,58,73	2.18	13 (31%)	47,95,113	2.40	16 (34%)
11	CLA	1	1140	-	56,73,73	1.88	13 (23%)	65,113,113	2.17	17 (26%)
11	CLA	1	1237	-	46,63,73	2.02	12 (26%)	53,101,113	2.26	17 (32%)
11	CLA	1	1801	15	43,60,73	2.16	13 (30%)	49,97,113	2.47	16 (32%)
12	PQN	1	2001	-	34,34,34	1.45	2 (5%)	43,45,45	1.05	2 (4%)
13	SF4	1	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	1	4001	-	41,41,41	2.74	6 (14%)	56,56,56	6.51	27 (48%)
14	BCR	1	4002	-	41,41,41	2.73	6 (14%)	56,56,56	6.91	23 (41%)
14	BCR	1	4003	-	41,41,41	2.80	6 (14%)	56,56,56	6.35	28 (50%)
14	BCR	1	4007	-	41,41,41	2.73	6 (14%)	56,56,56	6.63	26 (46%)
14	BCR	1	4008	-	41,41,41	2.73	6 (14%)	56,56,56	6.76	28 (50%)
15	LHG	1	5001	-	48,48,48	0.93	2 (4%)	49,54,54	1.13	3 (6%)
15	LHG	1	5003	11	48,48,48	0.94	2 (4%)	49,54,54	1.08	3 (6%)
11	CLA	2	1013	-	56,73,73	1.87	12 (21%)	65,113,113	2.09	17 (26%)
11	CLA	2	1021	-	56,73,73	1.85	12 (21%)	65,113,113	2.29	19 (29%)
11	CLA	2	1023	-	56,73,73	1.85	12 (21%)	65,113,113	2.23	17 (26%)
11	CLA	2	1201	-	45,62,73	2.11	12 (26%)	51,99,113	2.24	14 (27%)
11	CLA	2	1202	-	56,73,73	1.88	12 (21%)	65,113,113	2.06	17 (26%)
11	CLA	2	1203	-	56,73,73	1.84	12 (21%)	65,113,113	2.07	16 (24%)
11	CLA	2	1204	-	56,73,73	1.87	12 (21%)	65,113,113	2.03	14 (21%)
11	CLA	2	1205	-	46,63,73	2.04	13 (28%)	53,101,113	2.38	13 (24%)
11	CLA	2	1206	2	56,73,73	1.83	12 (21%)	65,113,113	2.13	13 (20%)
11	CLA	2	1207	-	56,73,73	1.86	12 (21%)	65,113,113	2.17	16 (24%)
11	CLA	2	1208	-	33,53,73	2.29	11 (33%)	37,89,113	2.28	9 (24%)
11	CLA	2	1209	-	33,53,73	2.26	11 (33%)	37,89,113	2.40	12 (32%)
11	CLA	2	1210	-	56,73,73	1.84	12 (21%)	65,113,113	2.11	19 (29%)
11	CLA	2	1211	-	37,54,73	2.40	11 (29%)	43,90,113	2.35	13 (30%)
11	CLA	2	1212	-	33,53,73	2.28	12 (36%)	37,89,113	2.42	12 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	2	1213	-	56,73,73	1.94	13 (23%)	65,113,113	2.27	15 (23%)
11	CLA	2	1214	-	50,67,73	1.96	12 (24%)	57,105,113	2.16	16 (28%)
11	CLA	2	1215	-	56,73,73	1.88	12 (21%)	65,113,113	2.28	18 (27%)
11	CLA	2	1216	-	56,73,73	1.86	12 (21%)	65,113,113	2.19	15 (23%)
11	CLA	2	1217	-	38,55,73	2.22	12 (31%)	44,91,113	2.53	16 (36%)
11	CLA	2	1218	-	33,53,73	2.25	11 (33%)	37,89,113	2.24	11 (29%)
11	CLA	2	1219	-	46,63,73	2.11	13 (28%)	53,101,113	2.29	15 (28%)
11	CLA	2	1220	-	37,54,73	2.37	12 (32%)	43,90,113	2.33	12 (27%)
11	CLA	2	1221	-	45,62,73	2.07	13 (28%)	51,99,113	2.35	15 (29%)
11	CLA	2	1222	-	47,64,73	2.04	13 (27%)	54,102,113	2.33	16 (29%)
11	CLA	2	1223	-	56,73,73	1.87	12 (21%)	65,113,113	2.06	17 (26%)
11	CLA	2	1224	-	46,63,73	2.04	13 (28%)	53,101,113	2.40	16 (30%)
11	CLA	2	1225	-	56,73,73	1.85	11 (19%)	65,113,113	2.05	15 (23%)
11	CLA	2	1226	-	56,73,73	1.88	11 (19%)	65,113,113	2.16	15 (23%)
11	CLA	2	1227	-	33,53,73	2.25	11 (33%)	37,89,113	2.42	10 (27%)
11	CLA	2	1228	-	41,58,73	2.19	13 (31%)	47,95,113	2.39	14 (29%)
11	CLA	2	1229	-	56,73,73	1.85	13 (23%)	65,113,113	2.05	14 (21%)
11	CLA	2	1230	-	49,66,73	2.03	12 (24%)	56,104,113	2.29	18 (32%)
11	CLA	2	1231	-	33,53,73	2.26	12 (36%)	37,89,113	2.43	14 (37%)
11	CLA	2	1232	-	33,53,73	2.25	12 (36%)	37,89,113	2.27	9 (24%)
11	CLA	2	1234	-	51,68,73	1.92	12 (23%)	59,107,113	2.21	14 (23%)
11	CLA	2	1235	-	51,68,73	1.96	13 (25%)	59,107,113	2.16	19 (32%)
11	CLA	2	1236	-	38,55,73	2.24	12 (31%)	44,91,113	2.52	14 (31%)
11	CLA	2	1238	-	56,73,73	1.88	13 (23%)	65,113,113	2.01	12 (18%)
11	CLA	2	1239	-	37,54,73	2.41	13 (35%)	43,90,113	2.41	13 (30%)
11	CLA	2	1240	15	33,53,73	2.28	11 (33%)	37,89,113	2.32	10 (27%)
12	PQN	2	2002	-	34,34,34	1.43	2 (5%)	43,45,45	1.04	5 (11%)
14	BCR	2	4004	-	41,41,41	2.73	6 (14%)	56,56,56	6.43	29 (51%)
14	BCR	2	4005	-	41,41,41	2.75	6 (14%)	56,56,56	6.34	21 (37%)
14	BCR	2	4006	-	41,41,41	2.74	6 (14%)	56,56,56	6.79	28 (50%)
14	BCR	2	4009	-	41,41,41	2.73	6 (14%)	56,56,56	6.72	24 (42%)
14	BCR	2	4010	-	41,41,41	2.86	6 (14%)	56,56,56	6.36	27 (48%)
14	BCR	2	4011	-	41,41,41	2.81	6 (14%)	56,56,56	6.74	26 (46%)
14	BCR	2	4014	-	41,41,41	2.82	6 (14%)	56,56,56	6.40	24 (42%)
14	BCR	2	4017	-	41,41,41	2.80	7 (17%)	56,56,56	6.50	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LMG	2	5002	-	55,55,55	0.89	2 (3%)	63,63,63	1.09	4 (6%)
15	LHG	2	5004	11	48,48,48	0.94	2 (4%)	49,54,54	1.10	3 (6%)
13	SF4	3	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
13	SF4	3	3003	-	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	6	4013	-	41,41,41	2.71	6 (14%)	56,56,56	6.59	24 (42%)
14	BCR	6	4018	-	41,41,41	2.89	7 (17%)	56,56,56	6.26	26 (46%)
14	BCR	6	4020	-	41,41,41	2.87	7 (17%)	56,56,56	6.50	23 (41%)
14	BCR	7	4021	-	41,41,41	2.79	6 (14%)	56,56,56	6.57	21 (37%)
11	CLA	8	1501	-	56,73,73	1.84	12 (21%)	65,113,113	2.19	16 (24%)
11	CLA	8	1502	-	37,54,73	2.37	12 (32%)	43,90,113	2.43	14 (32%)
11	CLA	8	1503	-	56,73,73	1.90	13 (23%)	65,113,113	2.06	14 (21%)
14	BCR	8	4019	-	41,41,41	2.77	6 (14%)	56,56,56	6.61	24 (42%)
14	BCR	8	4022	-	41,41,41	2.80	6 (14%)	56,56,56	6.46	31 (55%)
11	CLA	A	1011	-	56,73,73	1.83	12 (21%)	65,113,113	2.14	16 (24%)
11	CLA	A	1012	-	56,73,73	1.87	13 (23%)	65,113,113	2.44	19 (29%)
11	CLA	A	1022	-	56,73,73	1.85	12 (21%)	65,113,113	2.10	16 (24%)
11	CLA	A	1101	-	56,73,73	1.85	12 (21%)	65,113,113	2.01	15 (23%)
11	CLA	A	1102	11	56,73,73	1.88	13 (23%)	65,113,113	2.14	17 (26%)
11	CLA	A	1103	-	56,73,73	1.87	11 (19%)	65,113,113	1.96	17 (26%)
11	CLA	A	1104	-	56,73,73	1.85	12 (21%)	65,113,113	2.18	18 (27%)
11	CLA	A	1105	-	39,56,73	2.22	13 (33%)	45,92,113	2.38	14 (31%)
11	CLA	A	1106	1	56,73,73	1.86	12 (21%)	65,113,113	2.08	13 (20%)
11	CLA	A	1107	1	56,73,73	1.86	11 (19%)	65,113,113	2.13	16 (24%)
11	CLA	A	1108	-	33,53,73	2.27	11 (33%)	37,89,113	2.30	11 (29%)
11	CLA	A	1109	11	56,73,73	1.90	12 (21%)	65,113,113	2.06	15 (23%)
11	CLA	A	1110	-	45,62,73	2.10	12 (26%)	51,99,113	2.46	15 (29%)
11	CLA	A	1111	-	51,68,73	1.92	12 (23%)	59,107,113	2.11	16 (27%)
11	CLA	A	1112	-	33,53,73	2.25	11 (33%)	37,89,113	2.31	11 (29%)
11	CLA	A	1113	-	33,53,73	2.27	12 (36%)	37,89,113	2.35	13 (35%)
11	CLA	A	1114	-	37,54,73	2.38	12 (32%)	43,90,113	2.30	12 (27%)
11	CLA	A	1115	-	37,54,73	2.41	13 (35%)	43,90,113	2.26	13 (30%)
11	CLA	A	1116	-	45,62,73	2.09	12 (26%)	51,99,113	2.29	16 (31%)
11	CLA	A	1117	-	56,73,73	1.94	12 (21%)	65,113,113	2.05	14 (21%)
11	CLA	A	1118	-	52,69,73	1.92	12 (23%)	60,108,113	2.16	17 (28%)
11	CLA	A	1119	-	56,73,73	1.84	12 (21%)	65,113,113	2.02	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	1120	-	37,54,73	2.38	13 (35%)	43,90,113	2.30	14 (32%)
11	CLA	A	1121	-	37,54,73	2.38	13 (35%)	43,90,113	2.28	12 (27%)
11	CLA	A	1122	-	50,67,73	1.98	11 (22%)	57,105,113	2.31	17 (29%)
11	CLA	A	1123	-	56,73,73	1.80	12 (21%)	65,113,113	2.18	18 (27%)
11	CLA	A	1124	-	46,63,73	2.04	12 (26%)	53,101,113	2.28	16 (30%)
11	CLA	A	1125	-	43,60,73	2.11	12 (27%)	49,97,113	2.65	16 (32%)
11	CLA	A	1126	-	56,73,73	1.88	11 (19%)	65,113,113	2.09	16 (24%)
11	CLA	A	1127	-	56,73,73	1.85	13 (23%)	65,113,113	2.15	16 (24%)
11	CLA	A	1128	-	56,73,73	1.86	11 (19%)	65,113,113	2.04	15 (23%)
11	CLA	A	1129	-	37,54,73	2.37	12 (32%)	43,90,113	2.29	12 (27%)
11	CLA	A	1130	-	37,54,73	2.38	13 (35%)	43,90,113	2.29	12 (27%)
11	CLA	A	1131	-	56,73,73	1.88	12 (21%)	65,113,113	2.10	17 (26%)
11	CLA	A	1132	-	56,73,73	1.88	12 (21%)	65,113,113	2.14	13 (20%)
11	CLA	A	1133	-	37,54,73	2.37	12 (32%)	43,90,113	2.50	15 (34%)
11	CLA	A	1134	1	37,54,73	2.36	12 (32%)	43,90,113	2.40	14 (32%)
11	CLA	A	1135	-	42,59,73	2.14	12 (28%)	48,96,113	2.40	15 (31%)
11	CLA	A	1136	-	37,54,73	2.38	12 (32%)	43,90,113	2.35	12 (27%)
11	CLA	A	1137	-	56,73,73	1.91	12 (21%)	65,113,113	2.28	18 (27%)
11	CLA	A	1138	-	37,54,73	2.35	12 (32%)	43,90,113	2.33	16 (37%)
11	CLA	A	1139	-	41,58,73	2.19	12 (29%)	47,95,113	2.32	14 (29%)
11	CLA	A	1140	-	56,73,73	1.87	12 (21%)	65,113,113	2.15	16 (24%)
11	CLA	A	1237	-	46,63,73	2.06	11 (23%)	53,101,113	2.29	14 (26%)
11	CLA	A	1801	15	43,60,73	2.17	12 (27%)	49,97,113	2.51	15 (30%)
12	PQN	A	2001	-	34,34,34	1.44	2 (5%)	43,45,45	1.08	5 (11%)
13	SF4	A	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	A	4001	-	41,41,41	2.79	6 (14%)	56,56,56	6.35	27 (48%)
14	BCR	A	4002	-	41,41,41	2.76	6 (14%)	56,56,56	6.28	24 (42%)
14	BCR	A	4003	-	41,41,41	2.86	6 (14%)	56,56,56	6.25	24 (42%)
14	BCR	A	4007	-	41,41,41	2.78	6 (14%)	56,56,56	6.77	23 (41%)
14	BCR	A	4008	-	41,41,41	2.73	7 (17%)	56,56,56	6.65	30 (53%)
15	LHG	A	5001	-	48,48,48	0.91	2 (4%)	49,54,54	1.18	4 (8%)
15	LHG	A	5003	11	48,48,48	0.94	2 (4%)	49,54,54	1.18	4 (8%)
11	CLA	B	1013	-	56,73,73	1.88	12 (21%)	65,113,113	2.10	16 (24%)
11	CLA	B	1021	-	56,73,73	1.83	13 (23%)	65,113,113	2.33	18 (27%)
11	CLA	B	1023	-	56,73,73	1.83	11 (19%)	65,113,113	2.10	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1201	-	45,62,73	2.08	12 (26%)	51,99,113	2.35	16 (31%)
11	CLA	B	1202	-	56,73,73	1.92	13 (23%)	65,113,113	2.08	14 (21%)
11	CLA	B	1203	-	56,73,73	1.85	12 (21%)	65,113,113	2.02	13 (20%)
11	CLA	B	1204	-	56,73,73	1.83	11 (19%)	65,113,113	2.06	15 (23%)
11	CLA	B	1205	-	46,63,73	2.02	11 (23%)	53,101,113	2.44	14 (26%)
11	CLA	B	1206	2	56,73,73	1.83	12 (21%)	65,113,113	2.11	16 (24%)
11	CLA	B	1207	-	56,73,73	1.84	11 (19%)	65,113,113	2.15	14 (21%)
11	CLA	B	1208	-	33,53,73	2.29	11 (33%)	37,89,113	2.28	10 (27%)
11	CLA	B	1209	-	33,53,73	2.26	11 (33%)	37,89,113	2.44	13 (35%)
11	CLA	B	1210	-	56,73,73	1.88	12 (21%)	65,113,113	2.08	17 (26%)
11	CLA	B	1211	-	37,54,73	2.37	11 (29%)	43,90,113	2.31	13 (30%)
11	CLA	B	1212	-	33,53,73	2.28	12 (36%)	37,89,113	2.30	10 (27%)
11	CLA	B	1213	-	56,73,73	1.89	12 (21%)	65,113,113	2.09	15 (23%)
11	CLA	B	1214	-	50,67,73	1.97	13 (26%)	57,105,113	2.34	19 (33%)
11	CLA	B	1215	-	56,73,73	1.85	12 (21%)	65,113,113	2.27	18 (27%)
11	CLA	B	1216	-	56,73,73	1.87	12 (21%)	65,113,113	2.05	15 (23%)
11	CLA	B	1217	-	38,55,73	2.22	12 (31%)	44,91,113	2.45	13 (29%)
11	CLA	B	1218	-	33,53,73	2.27	11 (33%)	37,89,113	2.29	10 (27%)
11	CLA	B	1219	-	46,63,73	2.06	13 (28%)	53,101,113	2.23	16 (30%)
11	CLA	B	1220	-	37,54,73	2.34	12 (32%)	43,90,113	2.26	11 (25%)
11	CLA	B	1221	-	45,62,73	2.07	12 (26%)	51,99,113	2.41	15 (29%)
11	CLA	B	1222	-	47,64,73	2.10	12 (25%)	54,102,113	2.54	19 (35%)
11	CLA	B	1223	-	56,73,73	1.86	13 (23%)	65,113,113	2.16	18 (27%)
11	CLA	B	1224	-	46,63,73	2.07	12 (26%)	53,101,113	2.35	15 (28%)
11	CLA	B	1225	-	56,73,73	1.85	12 (21%)	65,113,113	2.06	15 (23%)
11	CLA	B	1226	-	56,73,73	1.84	11 (19%)	65,113,113	2.20	17 (26%)
11	CLA	B	1227	-	33,53,73	2.25	11 (33%)	37,89,113	2.53	12 (32%)
11	CLA	B	1228	-	41,58,73	2.20	12 (29%)	47,95,113	2.34	14 (29%)
11	CLA	B	1229	-	56,73,73	1.85	12 (21%)	65,113,113	2.10	17 (26%)
11	CLA	B	1230	-	49,66,73	2.02	12 (24%)	56,104,113	2.33	17 (30%)
11	CLA	B	1231	-	33,53,73	2.24	11 (33%)	37,89,113	2.55	14 (37%)
11	CLA	B	1232	-	33,53,73	2.24	11 (33%)	37,89,113	2.43	11 (29%)
11	CLA	B	1234	-	51,68,73	1.93	12 (23%)	59,107,113	2.29	16 (27%)
11	CLA	B	1235	-	51,68,73	1.99	13 (25%)	59,107,113	2.13	13 (22%)
11	CLA	B	1236	-	38,55,73	2.20	12 (31%)	44,91,113	2.47	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	1238	-	56,73,73	1.86	11 (19%)	65,113,113	1.98	14 (21%)
11	CLA	B	1239	-	37,54,73	2.38	12 (32%)	43,90,113	2.32	12 (27%)
11	CLA	B	1240	15	33,53,73	2.31	11 (33%)	37,89,113	2.32	9 (24%)
12	PQN	B	2002	-	34,34,34	1.44	2 (5%)	43,45,45	1.09	3 (6%)
14	BCR	B	4004	-	41,41,41	2.81	6 (14%)	56,56,56	6.52	27 (48%)
14	BCR	B	4005	-	41,41,41	2.81	7 (17%)	56,56,56	6.50	25 (44%)
14	BCR	B	4006	-	41,41,41	2.76	6 (14%)	56,56,56	6.78	26 (46%)
14	BCR	B	4009	-	41,41,41	2.76	6 (14%)	56,56,56	6.67	22 (39%)
14	BCR	B	4010	-	41,41,41	2.73	6 (14%)	56,56,56	6.37	26 (46%)
14	BCR	B	4011	-	41,41,41	2.83	7 (17%)	56,56,56	6.67	27 (48%)
14	BCR	B	4014	-	41,41,41	2.79	7 (17%)	56,56,56	6.25	25 (44%)
14	BCR	B	4017	-	41,41,41	2.78	6 (14%)	56,56,56	6.56	31 (55%)
16	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	1.10	4 (6%)
15	LHG	B	5004	11	48,48,48	0.94	2 (4%)	49,54,54	1.18	4 (8%)
13	SF4	C	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
13	SF4	C	3003	3	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	F	4013	-	41,41,41	2.79	6 (14%)	56,56,56	6.75	21 (37%)
14	BCR	F	4018	-	41,41,41	2.92	7 (17%)	56,56,56	6.53	24 (42%)
14	BCR	F	4020	-	41,41,41	2.80	6 (14%)	56,56,56	6.37	23 (41%)
11	CLA	K	1401	-	56,73,73	1.85	12 (21%)	65,113,113	2.18	16 (24%)
11	CLA	K	1402	-	41,58,73	2.21	12 (29%)	47,95,113	2.28	12 (25%)
11	CLA	L	1501	7	56,73,73	1.86	12 (21%)	65,113,113	2.06	15 (23%)
11	CLA	L	1502	-	37,54,73	2.38	11 (29%)	43,90,113	2.39	12 (27%)
11	CLA	L	1503	-	56,73,73	1.84	11 (19%)	65,113,113	2.14	13 (20%)
14	BCR	L	4019	-	41,41,41	2.71	6 (14%)	56,56,56	6.55	24 (42%)
14	BCR	L	4022	-	41,41,41	2.71	6 (14%)	56,56,56	6.07	25 (44%)
14	BCR	M	4021	-	41,41,41	2.81	6 (14%)	56,56,56	6.54	21 (37%)
11	CLA	a	1011	-	56,73,73	1.88	13 (23%)	65,113,113	2.22	16 (24%)
11	CLA	a	1012	-	56,73,73	1.88	13 (23%)	65,113,113	2.26	16 (24%)
11	CLA	a	1022	-	56,73,73	1.86	13 (23%)	65,113,113	2.17	14 (21%)
11	CLA	a	1101	-	56,73,73	1.88	12 (21%)	65,113,113	2.13	17 (26%)
11	CLA	a	1102	11	56,73,73	1.87	13 (23%)	65,113,113	2.07	13 (20%)
11	CLA	a	1103	-	56,73,73	1.87	13 (23%)	65,113,113	2.11	14 (21%)
11	CLA	a	1104	-	56,73,73	1.84	12 (21%)	65,113,113	2.06	17 (26%)
11	CLA	a	1105	-	39,56,73	2.26	12 (30%)	45,92,113	2.52	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	a	1106	1	56,73,73	1.88	13 (23%)	65,113,113	2.13	16 (24%)
11	CLA	a	1107	1	56,73,73	1.84	12 (21%)	65,113,113	2.26	18 (27%)
11	CLA	a	1108	-	33,53,73	2.28	11 (33%)	37,89,113	2.37	11 (29%)
11	CLA	a	1109	11	56,73,73	1.89	13 (23%)	65,113,113	2.10	15 (23%)
11	CLA	a	1110	-	45,62,73	2.10	13 (28%)	51,99,113	2.34	14 (27%)
11	CLA	a	1111	-	51,68,73	1.92	13 (25%)	59,107,113	2.17	17 (28%)
11	CLA	a	1112	-	33,53,73	2.26	11 (33%)	37,89,113	2.24	12 (32%)
11	CLA	a	1113	-	33,53,73	2.28	11 (33%)	37,89,113	2.33	11 (29%)
11	CLA	a	1114	-	37,54,73	2.38	13 (35%)	43,90,113	2.35	12 (27%)
11	CLA	a	1115	-	37,54,73	2.41	12 (32%)	43,90,113	2.20	11 (25%)
11	CLA	a	1116	-	45,62,73	2.11	12 (26%)	51,99,113	2.28	14 (27%)
11	CLA	a	1117	-	56,73,73	1.89	12 (21%)	65,113,113	2.04	16 (24%)
11	CLA	a	1118	-	52,69,73	1.94	11 (21%)	60,108,113	2.12	15 (25%)
11	CLA	a	1119	-	56,73,73	1.86	12 (21%)	65,113,113	2.13	18 (27%)
11	CLA	a	1120	-	37,54,73	2.39	13 (35%)	43,90,113	2.41	13 (30%)
11	CLA	a	1121	-	37,54,73	2.37	13 (35%)	43,90,113	2.37	13 (30%)
11	CLA	a	1122	-	50,67,73	2.01	12 (24%)	57,105,113	2.27	16 (28%)
11	CLA	a	1123	-	56,73,73	1.86	12 (21%)	65,113,113	2.11	16 (24%)
11	CLA	a	1124	-	46,63,73	2.05	13 (28%)	53,101,113	2.36	15 (28%)
11	CLA	a	1125	-	43,60,73	2.09	13 (30%)	49,97,113	2.34	14 (28%)
11	CLA	a	1126	-	56,73,73	1.89	11 (19%)	65,113,113	2.10	15 (23%)
11	CLA	a	1127	-	56,73,73	1.86	12 (21%)	65,113,113	2.23	20 (30%)
11	CLA	a	1128	-	56,73,73	1.88	12 (21%)	65,113,113	2.09	16 (24%)
11	CLA	a	1129	-	37,54,73	2.39	11 (29%)	43,90,113	2.39	13 (30%)
11	CLA	a	1130	-	37,54,73	2.41	12 (32%)	43,90,113	2.31	12 (27%)
11	CLA	a	1131	-	56,73,73	1.88	12 (21%)	65,113,113	2.09	19 (29%)
11	CLA	a	1132	-	56,73,73	1.88	13 (23%)	65,113,113	2.03	14 (21%)
11	CLA	a	1133	-	37,54,73	2.38	12 (32%)	43,90,113	2.44	12 (27%)
11	CLA	a	1134	-	37,54,73	2.38	12 (32%)	43,90,113	2.33	15 (34%)
11	CLA	a	1135	-	42,59,73	2.15	12 (28%)	48,96,113	2.46	15 (31%)
11	CLA	a	1136	-	37,54,73	2.38	12 (32%)	43,90,113	2.36	11 (25%)
11	CLA	a	1137	-	56,73,73	1.89	13 (23%)	65,113,113	2.21	17 (26%)
11	CLA	a	1138	-	37,54,73	2.36	12 (32%)	43,90,113	2.35	16 (37%)
11	CLA	a	1139	-	41,58,73	2.17	13 (31%)	47,95,113	2.46	13 (27%)
11	CLA	a	1140	-	56,73,73	1.87	12 (21%)	65,113,113	2.09	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	a	1237	-	46,63,73	2.08	11 (23%)	53,101,113	2.23	13 (24%)
11	CLA	a	1801	15	43,60,73	2.15	13 (30%)	49,97,113	2.43	13 (26%)
12	PQN	a	2001	-	34,34,34	1.43	2 (5%)	43,45,45	0.99	4 (9%)
13	SF4	a	3001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	a	4001	-	41,41,41	2.75	6 (14%)	56,56,56	6.48	27 (48%)
14	BCR	a	4002	-	41,41,41	2.78	6 (14%)	56,56,56	6.56	25 (44%)
14	BCR	a	4003	-	41,41,41	2.76	6 (14%)	56,56,56	6.16	26 (46%)
14	BCR	a	4007	-	41,41,41	2.74	6 (14%)	56,56,56	6.70	25 (44%)
14	BCR	a	4008	-	41,41,41	2.75	7 (17%)	56,56,56	6.53	29 (51%)
15	LHG	a	5001	-	48,48,48	0.94	2 (4%)	49,54,54	1.11	3 (6%)
15	LHG	a	5003	11	48,48,48	0.92	2 (4%)	49,54,54	1.08	3 (6%)
11	CLA	b	1013	-	56,73,73	1.88	12 (21%)	65,113,113	2.04	15 (23%)
11	CLA	b	1021	-	56,73,73	1.88	12 (21%)	65,113,113	2.33	22 (33%)
11	CLA	b	1023	-	56,73,73	1.85	12 (21%)	65,113,113	2.10	17 (26%)
11	CLA	b	1201	-	45,62,73	2.13	11 (24%)	51,99,113	2.33	16 (31%)
11	CLA	b	1202	-	56,73,73	1.88	12 (21%)	65,113,113	2.01	14 (21%)
11	CLA	b	1203	-	56,73,73	1.85	13 (23%)	65,113,113	2.10	15 (23%)
11	CLA	b	1204	-	56,73,73	1.85	12 (21%)	65,113,113	2.02	13 (20%)
11	CLA	b	1205	-	46,63,73	2.05	11 (23%)	53,101,113	2.32	14 (26%)
11	CLA	b	1206	2	56,73,73	1.85	12 (21%)	65,113,113	2.09	17 (26%)
11	CLA	b	1207	-	56,73,73	1.86	12 (21%)	65,113,113	2.22	13 (20%)
11	CLA	b	1208	-	33,53,73	2.28	11 (33%)	37,89,113	2.44	10 (27%)
11	CLA	b	1209	-	33,53,73	2.30	11 (33%)	37,89,113	2.37	12 (32%)
11	CLA	b	1210	-	56,73,73	1.88	13 (23%)	65,113,113	2.05	19 (29%)
11	CLA	b	1211	-	37,54,73	2.39	13 (35%)	43,90,113	2.38	13 (30%)
11	CLA	b	1212	-	33,53,73	2.27	12 (36%)	37,89,113	2.39	9 (24%)
11	CLA	b	1213	-	56,73,73	1.90	12 (21%)	65,113,113	2.09	14 (21%)
11	CLA	b	1214	-	50,67,73	1.97	13 (26%)	57,105,113	2.17	17 (29%)
11	CLA	b	1215	-	56,73,73	1.87	12 (21%)	65,113,113	2.23	18 (27%)
11	CLA	b	1216	-	56,73,73	1.88	12 (21%)	65,113,113	2.14	19 (29%)
11	CLA	b	1217	-	38,55,73	2.24	13 (34%)	44,91,113	2.47	13 (29%)
11	CLA	b	1218	-	33,53,73	2.28	12 (36%)	37,89,113	2.31	10 (27%)
11	CLA	b	1219	-	46,63,73	2.10	12 (26%)	53,101,113	2.37	15 (28%)
11	CLA	b	1220	-	37,54,73	2.41	13 (35%)	43,90,113	2.37	13 (30%)
11	CLA	b	1221	-	45,62,73	2.09	12 (26%)	51,99,113	2.45	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	b	1222	-	47,64,73	2.04	13 (27%)	54,102,113	2.45	16 (29%)
11	CLA	b	1223	-	56,73,73	1.89	12 (21%)	65,113,113	2.08	16 (24%)
11	CLA	b	1224	-	46,63,73	2.08	13 (28%)	53,101,113	2.35	16 (30%)
11	CLA	b	1225	-	56,73,73	1.87	13 (23%)	65,113,113	2.08	15 (23%)
11	CLA	b	1226	-	56,73,73	1.85	13 (23%)	65,113,113	2.14	16 (24%)
11	CLA	b	1227	-	33,53,73	2.27	12 (36%)	37,89,113	2.47	11 (29%)
11	CLA	b	1228	-	41,58,73	2.19	12 (29%)	47,95,113	2.37	14 (29%)
11	CLA	b	1229	-	56,73,73	1.87	13 (23%)	65,113,113	2.03	15 (23%)
11	CLA	b	1230	-	49,66,73	2.04	13 (26%)	56,104,113	2.41	16 (28%)
11	CLA	b	1231	-	33,53,73	2.25	12 (36%)	37,89,113	2.26	12 (32%)
11	CLA	b	1232	-	33,53,73	2.28	12 (36%)	37,89,113	2.35	10 (27%)
11	CLA	b	1234	-	51,68,73	1.95	12 (23%)	59,107,113	2.24	15 (25%)
11	CLA	b	1235	-	51,68,73	1.99	13 (25%)	59,107,113	2.23	18 (30%)
11	CLA	b	1236	-	38,55,73	2.23	11 (28%)	44,91,113	2.42	13 (29%)
11	CLA	b	1238	-	56,73,73	1.87	12 (21%)	65,113,113	2.01	13 (20%)
11	CLA	b	1239	-	37,54,73	2.38	12 (32%)	43,90,113	2.42	14 (32%)
11	CLA	b	1240	-	33,53,73	2.30	12 (36%)	37,89,113	2.30	10 (27%)
12	PQN	b	2002	-	34,34,34	1.43	2 (5%)	43,45,45	1.06	4 (9%)
14	BCR	b	4004	-	41,41,41	2.75	6 (14%)	56,56,56	6.53	26 (46%)
14	BCR	b	4005	-	41,41,41	2.77	6 (14%)	56,56,56	6.54	25 (44%)
14	BCR	b	4006	-	41,41,41	2.78	6 (14%)	56,56,56	6.90	27 (48%)
14	BCR	b	4009	-	41,41,41	2.66	6 (14%)	56,56,56	6.89	26 (46%)
14	BCR	b	4010	-	41,41,41	2.80	6 (14%)	56,56,56	6.67	24 (42%)
14	BCR	b	4011	-	41,41,41	2.77	6 (14%)	56,56,56	6.76	25 (44%)
14	BCR	b	4014	-	41,41,41	2.75	7 (17%)	56,56,56	6.45	24 (42%)
14	BCR	b	4017	-	41,41,41	2.83	7 (17%)	56,56,56	6.62	27 (48%)
16	LMG	b	5002	-	55,55,55	0.87	2 (3%)	63,63,63	1.07	5 (7%)
15	LHG	b	5004	-	48,48,48	0.92	2 (4%)	49,54,54	1.09	3 (6%)
13	SF4	c	3002	3	0,12,12	0.00	-	0,24,24	0.00	-
13	SF4	c	3003	3	0,12,12	0.00	-	0,24,24	0.00	-
14	BCR	f	4013	-	41,41,41	2.77	6 (14%)	56,56,56	6.58	24 (42%)
14	BCR	f	4018	-	41,41,41	2.87	7 (17%)	56,56,56	6.32	24 (42%)
14	BCR	f	4020	-	41,41,41	2.81	6 (14%)	56,56,56	6.54	22 (39%)
11	CLA	k	1401	-	56,73,73	1.86	12 (21%)	65,113,113	2.19	16 (24%)
11	CLA	k	1402	-	41,58,73	2.23	12 (29%)	47,95,113	2.33	14 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	l	1501	7	56,73,73	1.88	13 (23%)	65,113,113	2.15	16 (24%)
11	CLA	l	1502	-	37,54,73	2.39	12 (32%)	43,90,113	2.43	12 (27%)
11	CLA	l	1503	-	56,73,73	1.86	12 (21%)	65,113,113	2.08	13 (20%)
14	BCR	l	4019	-	41,41,41	2.77	6 (14%)	56,56,56	6.67	23 (41%)
14	BCR	l	4022	-	41,41,41	2.75	6 (14%)	56,56,56	6.38	26 (46%)
14	BCR	m	4021	-	41,41,41	2.86	6 (14%)	56,56,56	6.47	24 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	0	1401	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	0	1402	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	1	1011	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1012	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1022	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1102	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1104	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1105	-	3/3/16/25	0/17/115/135	0/0/9/9
11	CLA	1	1106	1	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1107	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	1	1109	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1110	-	2/2/17/25	0/24/122/135	0/0/9/9
11	CLA	1	1111	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	1	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	1	1113	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	1	1114	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1115	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1116	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	1	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1118	-	3/3/19/25	0/33/131/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	1	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1121	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1122	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	1	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	1	1125	-	2/2/17/25	0/22/120/135	0/0/9/9
11	CLA	1	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1129	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1130	-	1/1/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1131	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1134	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1135	-	2/2/17/25	0/21/119/135	0/0/9/9
11	CLA	1	1136	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1137	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1138	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	1	1139	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	1	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	1	1237	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	1	1801	15	3/3/17/25	0/22/120/135	0/0/9/9
12	PQN	1	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	1	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	1	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	1	4008	-	-	1/29/63/63	0/2/2/2
15	LHG	1	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	1	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	2	1013	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1023	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1201	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	2	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1203	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1204	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1205	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	2	1206	2	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1207	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1208	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1209	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	2	1212	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1213	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1214	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	2	1215	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1217	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	2	1218	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1219	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	2	1220	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	2	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	2	1222	-	3/3/18/25	0/27/125/135	0/0/9/9
11	CLA	2	1223	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1224	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	2	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1227	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	2	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1230	-	2/2/18/25	0/29/127/135	0/0/9/9
11	CLA	2	1231	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1232	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	2	1234	-	2/2/19/25	0/31/129/135	0/0/9/9
11	CLA	2	1235	-	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	2	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	2	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	2	1239	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	2	1240	15	3/3/16/25	0/11/111/135	0/0/9/9
12	PQN	2	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	2	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4006	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4014	-	-	0/29/63/63	0/2/2/2
14	BCR	2	4017	-	-	2/29/63/63	0/2/2/2
16	LMG	2	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	2	5004	11	-	0/53/53/53	0/0/0/0
13	SF4	3	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	3	3003	-	-	0/0/48/48	0/6/5/5
14	BCR	6	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	6	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	6	4020	-	-	1/29/63/63	0/2/2/2
14	BCR	7	4021	-	-	0/29/63/63	0/2/2/2
11	CLA	8	1501	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	8	1502	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	8	1503	-	3/3/20/25	0/37/135/135	0/0/9/9
14	BCR	8	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	8	4022	-	-	0/29/63/63	0/2/2/2
11	CLA	A	1011	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1012	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1022	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1102	11	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1105	-	3/3/16/25	0/17/115/135	0/0/9/9
11	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	A	1109	11	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	1110	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	A	1111	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	A	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	A	1113	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	A	1114	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1115	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1116	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	A	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1118	-	3/3/19/25	0/33/131/135	0/0/9/9
11	CLA	A	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1121	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1122	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	A	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	A	1125	-	2/2/17/25	0/22/120/135	0/0/9/9
11	CLA	A	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1129	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1130	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1131	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1134	1	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1135	-	3/3/17/25	0/21/119/135	0/0/9/9
11	CLA	A	1136	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1137	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1138	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	A	1139	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	A	1140	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	A	1237	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	A	1801	15	3/3/17/25	0/22/120/135	0/0/9/9
12	PQN	A	2001	-	-	0/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	A	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	A	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	3/29/63/63	0/2/2/2
15	LHG	A	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	A	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	B	1013	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1201	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	B	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1203	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1204	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1205	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	B	1206	2	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1207	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1208	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1209	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	B	1212	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1213	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1214	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	B	1215	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1217	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	B	1218	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1219	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	B	1220	-	1/1/16/25	0/15/113/135	0/0/9/9
11	CLA	B	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	B	1222	-	3/3/18/25	0/27/125/135	0/0/9/9
11	CLA	B	1223	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1224	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	B	1225	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1227	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	B	1229	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1230	-	2/2/18/25	0/29/127/135	0/0/9/9
11	CLA	B	1231	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1232	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	B	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	B	1235	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	B	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	B	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	B	1239	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	B	1240	15	3/3/16/25	0/11/111/135	0/0/9/9
12	PQN	B	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	B	4004	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	2/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4014	-	-	0/29/63/63	0/2/2/2
14	BCR	B	4017	-	-	1/29/63/63	0/2/2/2
16	LMG	B	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	B	5004	11	-	0/53/53/53	0/0/0/0
13	SF4	C	3002	3	-	0/0/48/48	0/6/5/5
13	SF4	C	3003	3	-	0/0/48/48	0/6/5/5
14	BCR	F	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	F	4020	-	-	0/29/63/63	0/2/2/2
11	CLA	K	1401	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	K	1402	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	L	1501	7	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	L	1502	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	L	1503	-	2/2/20/25	0/37/135/135	0/0/9/9
14	BCR	L	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	L	4022	-	-	0/29/63/63	0/2/2/2
14	BCR	M	4021	-	-	0/29/63/63	0/2/2/2
11	CLA	a	1011	-	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1012	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1022	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1102	11	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1103	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1104	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1105	-	3/3/16/25	0/17/115/135	0/0/9/9
11	CLA	a	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1107	1	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	a	1109	11	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1110	-	2/2/17/25	0/24/122/135	0/0/9/9
11	CLA	a	1111	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	a	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	a	1113	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	a	1114	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1115	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1116	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	a	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1118	-	3/3/19/25	0/33/131/135	0/0/9/9
11	CLA	a	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1121	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1122	-	3/3/18/25	0/30/128/135	0/0/9/9
11	CLA	a	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	a	1125	-	2/2/17/25	0/22/120/135	0/0/9/9
11	CLA	a	1126	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1129	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1130	-	2/2/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1131	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1132	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	a	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1134	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1135	-	2/2/17/25	0/21/119/135	0/0/9/9
11	CLA	a	1136	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1137	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1138	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	a	1139	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	a	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	a	1237	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	a	1801	15	3/3/17/25	0/22/120/135	0/0/9/9
12	PQN	a	2001	-	-	0/23/43/43	0/2/2/2
13	SF4	a	3001	1,2	-	0/0/48/48	0/6/5/5
14	BCR	a	4001	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4002	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4003	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4007	-	-	0/29/63/63	0/2/2/2
14	BCR	a	4008	-	-	1/29/63/63	0/2/2/2
15	LHG	a	5001	-	-	0/53/53/53	0/0/0/0
15	LHG	a	5003	11	-	0/53/53/53	0/0/0/0
11	CLA	b	1013	-	1/1/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1021	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1023	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1201	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	b	1202	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1203	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1204	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1205	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	b	1206	2	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1207	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1208	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1209	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1211	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	b	1212	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1213	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1214	-	3/3/18/25	0/30/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	b	1215	-	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1217	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	b	1218	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1219	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	b	1220	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	b	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
11	CLA	b	1222	-	3/3/18/25	0/27/125/135	0/0/9/9
11	CLA	b	1223	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1224	-	3/3/18/25	0/25/123/135	0/0/9/9
11	CLA	b	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1227	-	2/2/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	b	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1230	-	3/3/18/25	0/29/127/135	0/0/9/9
11	CLA	b	1231	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1232	-	3/3/16/25	0/11/111/135	0/0/9/9
11	CLA	b	1234	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	b	1235	-	3/3/19/25	0/31/129/135	0/0/9/9
11	CLA	b	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
11	CLA	b	1238	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	b	1239	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	b	1240	-	3/3/16/25	0/11/111/135	0/0/9/9
12	PQN	b	2002	-	-	0/23/43/43	0/2/2/2
14	BCR	b	4004	-	-	1/29/63/63	0/2/2/2
14	BCR	b	4005	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4006	-	-	2/29/63/63	0/2/2/2
14	BCR	b	4009	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4010	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4011	-	-	0/29/63/63	0/2/2/2
14	BCR	b	4014	-	-	2/29/63/63	0/2/2/2
14	BCR	b	4017	-	-	1/29/63/63	0/2/2/2
16	LMG	b	5002	-	-	0/50/70/70	0/1/1/1
15	LHG	b	5004	-	-	0/53/53/53	0/0/0/0
13	SF4	c	3002	3	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	c	3003	3	-	0/0/48/48	0/6/5/5
14	BCR	f	4013	-	-	0/29/63/63	0/2/2/2
14	BCR	f	4018	-	-	0/29/63/63	0/2/2/2
14	BCR	f	4020	-	-	0/29/63/63	0/2/2/2
11	CLA	k	1401	-	3/3/20/25	0/37/135/135	0/0/9/9
11	CLA	k	1402	-	3/3/17/25	0/19/117/135	0/0/9/9
11	CLA	l	1501	7	2/2/20/25	0/37/135/135	0/0/9/9
11	CLA	l	1502	-	3/3/16/25	0/15/113/135	0/0/9/9
11	CLA	l	1503	-	2/2/20/25	0/37/135/135	0/0/9/9
14	BCR	l	4019	-	-	0/29/63/63	0/2/2/2
14	BCR	l	4022	-	-	0/29/63/63	0/2/2/2
14	BCR	m	4021	-	-	0/29/63/63	0/2/2/2

The worst 5 of 3697 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	4003	BCR	C11-C10	-8.40	1.17	1.43
14	F	4018	BCR	C11-C10	-8.36	1.18	1.43
14	2	4010	BCR	C11-C10	-8.32	1.18	1.43
14	m	4021	BCR	C8-C9	-8.32	1.27	1.45
14	m	4021	BCR	C11-C10	-8.30	1.18	1.43

The worst 5 of 5490 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	4003	BCR	C24-C23-C22	-7.24	115.34	126.21
14	6	4018	BCR	C24-C23-C22	-7.00	115.70	126.21
14	L	4019	BCR	C24-C23-C22	-6.91	115.83	126.21
14	f	4018	BCR	C24-C23-C22	-6.62	116.26	126.21
14	b	4017	BCR	C34-C9-C10	-6.48	113.84	122.92

5 of 748 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	2	1218	CLA	NC
11	2	1218	CLA	ND
11	2	1218	CLA	NA
11	a	1122	CLA	NC
11	a	1122	CLA	ND

5 of 17 torsion outliers are listed below:

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

There are no ring outliers.

208 monomers are involved in 696 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	0	1401	CLA	3	0
11	0	1402	CLA	1	0
11	1	1011	CLA	1	0
11	1	1012	CLA	5	0
11	1	1022	CLA	5	0
11	1	1101	CLA	3	0
11	1	1102	CLA	1	0
11	1	1103	CLA	2	0
11	1	1104	CLA	1	0
11	1	1105	CLA	1	0
11	1	1106	CLA	8	0
11	1	1107	CLA	3	0
11	1	1109	CLA	2	0
11	1	1110	CLA	2	0
11	1	1111	CLA	1	0
11	1	1112	CLA	3	0
11	1	1113	CLA	3	0
11	1	1115	CLA	4	0
11	1	1117	CLA	2	0
11	1	1118	CLA	2	0
11	1	1119	CLA	4	0
11	1	1121	CLA	1	0
11	1	1122	CLA	1	0
11	1	1123	CLA	5	0
11	1	1124	CLA	2	0
11	1	1125	CLA	2	0
11	1	1126	CLA	4	0
11	1	1127	CLA	4	0
11	1	1128	CLA	9	0
11	1	1129	CLA	2	0
11	1	1130	CLA	2	0
11	1	1131	CLA	2	0
11	1	1132	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1	1133	CLA	2	0
11	1	1134	CLA	3	0
11	1	1137	CLA	4	0
11	1	1140	CLA	2	0
11	1	1237	CLA	3	0
11	1	1801	CLA	5	0
12	1	2001	PQN	1	0
13	1	3001	SF4	1	0
14	1	4001	BCR	8	0
14	1	4002	BCR	5	0
14	1	4003	BCR	2	0
14	1	4007	BCR	7	0
14	1	4008	BCR	4	0
15	1	5001	LHG	10	0
15	1	5003	LHG	6	0
11	2	1013	CLA	5	0
11	2	1021	CLA	6	0
11	2	1023	CLA	3	0
11	2	1201	CLA	2	0
11	2	1202	CLA	3	0
11	2	1203	CLA	1	0
11	2	1204	CLA	3	0
11	2	1205	CLA	4	0
11	2	1206	CLA	6	0
11	2	1207	CLA	4	0
11	2	1208	CLA	1	0
11	2	1209	CLA	1	0
11	2	1210	CLA	2	0
11	2	1211	CLA	2	0
11	2	1212	CLA	4	0
11	2	1214	CLA	2	0
11	2	1220	CLA	1	0
11	2	1222	CLA	3	0
11	2	1223	CLA	2	0
11	2	1225	CLA	1	0
11	2	1227	CLA	3	0
11	2	1229	CLA	5	0
11	2	1230	CLA	3	0
11	2	1231	CLA	8	0
11	2	1232	CLA	3	0
11	2	1234	CLA	4	0
11	2	1235	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	2	1238	CLA	5	0
11	2	1239	CLA	4	0
11	2	1240	CLA	2	0
12	2	2002	PQN	3	0
14	2	4004	BCR	2	0
14	2	4005	BCR	3	0
14	2	4006	BCR	1	0
14	2	4009	BCR	5	0
14	2	4010	BCR	6	0
14	2	4011	BCR	7	0
14	2	4014	BCR	7	0
14	2	4017	BCR	9	0
16	2	5002	LMG	1	0
15	2	5004	LHG	7	0
13	3	3002	SF4	9	0
13	3	3003	SF4	12	0
14	6	4013	BCR	7	0
14	6	4018	BCR	9	0
14	6	4020	BCR	4	0
14	7	4021	BCR	6	0
11	8	1501	CLA	6	0
11	8	1503	CLA	3	0
14	8	4019	BCR	7	0
14	8	4022	BCR	8	0
11	A	1011	CLA	3	0
11	A	1012	CLA	5	0
11	A	1022	CLA	6	0
11	A	1101	CLA	4	0
11	A	1102	CLA	4	0
11	A	1103	CLA	20	0
11	A	1104	CLA	8	0
11	A	1105	CLA	1	0
11	A	1106	CLA	6	0
11	A	1107	CLA	5	0
11	A	1108	CLA	2	0
11	A	1109	CLA	1	0
11	A	1110	CLA	2	0
11	A	1111	CLA	4	0
11	A	1112	CLA	7	0
11	A	1113	CLA	2	0
11	A	1114	CLA	2	0
11	A	1115	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1116	CLA	2	0
11	A	1117	CLA	2	0
11	A	1118	CLA	5	0
11	A	1119	CLA	11	0
11	A	1121	CLA	4	0
11	A	1122	CLA	2	0
11	A	1123	CLA	6	0
11	A	1124	CLA	3	0
11	A	1125	CLA	7	0
11	A	1126	CLA	9	0
11	A	1127	CLA	3	0
11	A	1128	CLA	6	0
11	A	1129	CLA	4	0
11	A	1131	CLA	4	0
11	A	1132	CLA	4	0
11	A	1133	CLA	4	0
11	A	1134	CLA	1	0
11	A	1135	CLA	1	0
11	A	1136	CLA	4	0
11	A	1137	CLA	5	0
11	A	1138	CLA	6	0
11	A	1140	CLA	1	0
11	A	1237	CLA	4	0
11	A	1801	CLA	8	0
12	A	2001	PQN	5	0
13	A	3001	SF4	4	0
14	A	4001	BCR	6	0
14	A	4002	BCR	9	0
14	A	4003	BCR	9	0
14	A	4007	BCR	9	0
14	A	4008	BCR	5	0
15	A	5001	LHG	5	0
15	A	5003	LHG	10	0
11	B	1013	CLA	9	0
11	B	1021	CLA	7	0
11	B	1023	CLA	8	0
11	B	1201	CLA	4	0
11	B	1202	CLA	1	0
11	B	1203	CLA	2	0
11	B	1204	CLA	3	0
11	B	1205	CLA	5	0
11	B	1206	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	1207	CLA	3	0
11	B	1208	CLA	3	0
11	B	1209	CLA	6	0
11	B	1210	CLA	3	0
11	B	1211	CLA	5	0
11	B	1212	CLA	5	0
11	B	1214	CLA	2	0
11	B	1215	CLA	1	0
11	B	1217	CLA	2	0
11	B	1219	CLA	2	0
11	B	1220	CLA	3	0
11	B	1221	CLA	4	0
11	B	1222	CLA	7	0
11	B	1223	CLA	20	0
11	B	1224	CLA	1	0
11	B	1225	CLA	3	0
11	B	1226	CLA	1	0
11	B	1227	CLA	4	0
11	B	1228	CLA	2	0
11	B	1229	CLA	6	0
11	B	1230	CLA	5	0
11	B	1231	CLA	3	0
11	B	1234	CLA	2	0
11	B	1235	CLA	3	0
11	B	1238	CLA	7	0
11	B	1240	CLA	1	0
12	B	2002	PQN	4	0
14	B	4004	BCR	4	0
14	B	4005	BCR	7	0
14	B	4006	BCR	3	0
14	B	4009	BCR	7	0
14	B	4010	BCR	15	0
14	B	4011	BCR	10	0
14	B	4014	BCR	6	0
14	B	4017	BCR	10	0
16	B	5002	LMG	1	0
15	B	5004	LHG	8	0
13	C	3002	SF4	11	0
13	C	3003	SF4	11	0
14	F	4013	BCR	6	0
14	F	4018	BCR	11	0
14	F	4020	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1401	CLA	4	0
11	K	1402	CLA	4	0
11	L	1501	CLA	8	0
11	L	1503	CLA	3	0
14	L	4019	BCR	13	0
14	L	4022	BCR	9	0
14	M	4021	BCR	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	132	GLY	12.4
6	f	50	PRO	11.5
10	k	92	GLN	10.6
6	f	125	ARG	10.4
6	f	51	SER	9.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	BCR	1	4003	40/40	0.62	1.31	15.39	193,227,269,270	0
14	BCR	2	4014	40/40	0.55	1.01	15.04	184,206,223,228	0
14	BCR	f	4018	40/40	0.90	0.73	14.02	132,138,152,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	BCR	b	4010	40/40	0.82	1.16	12.05	230,257,283,284	0
14	BCR	2	4011	40/40	0.68	1.23	10.17	187,207,215,220	0
15	LHG	2	5004	49/49	0.93	0.62	9.82	183,200,224,236	0
14	BCR	1	4002	40/40	0.53	1.04	8.67	220,241,266,270	0
14	BCR	F	4018	40/40	0.91	0.41	8.54	94,101,113,114	0
14	BCR	l	4019	40/40	0.85	0.97	8.40	122,133,149,151	0
16	LMG	B	5002	55/55	0.88	0.71	7.85	110,116,120,125	0
14	BCR	B	4014	40/40	0.81	0.91	7.63	138,157,191,200	0
14	BCR	B	4005	40/40	0.81	0.85	7.55	118,135,161,162	0
14	BCR	8	4019	40/40	0.89	0.85	7.35	125,129,144,154	0
14	BCR	b	4005	40/40	0.62	1.20	7.26	193,207,227,230	0
15	LHG	1	5003	49/49	0.91	0.49	6.86	154,173,196,198	0
14	BCR	6	4018	40/40	0.94	0.51	6.48	93,97,107,113	0
14	BCR	b	4011	40/40	0.67	0.96	6.46	204,219,248,251	0
15	LHG	a	5003	49/49	0.94	0.35	6.36	144,147,154,158	0
14	BCR	2	4010	40/40	0.88	0.69	5.82	132,140,147,150	0
14	BCR	1	4007	40/40	0.82	0.75	5.80	202,218,231,231	0
14	BCR	a	4007	40/40	0.82	0.61	5.58	144,153,167,170	0
11	CLA	2	1223	65/65	0.93	0.44	5.49	131,134,148,153	0
14	BCR	m	4021	40/40	0.74	0.76	5.48	175,183,191,194	0
12	PQN	2	2002	33/33	0.94	0.48	5.41	106,118,130,131	0
14	BCR	L	4019	40/40	0.92	0.79	5.31	87,90,93,93	0
14	BCR	A	4008	40/40	0.92	0.49	5.21	82,86,94,95	0
11	CLA	2	1234	60/65	0.92	0.51	5.16	151,164,196,206	0
11	CLA	1	1104	65/65	0.94	0.44	5.13	205,230,242,264	0
14	BCR	2	4017	40/40	0.90	0.59	5.08	96,102,117,117	0
11	CLA	2	1227	45/65	0.77	0.50	5.01	197,210,223,231	0
14	BCR	7	4021	40/40	0.86	0.47	5.01	106,110,121,131	0
14	BCR	M	4021	40/40	0.81	0.36	4.98	103,111,125,126	0
14	BCR	b	4017	40/40	0.87	0.62	4.97	143,150,160,162	0
14	BCR	B	4011	40/40	0.91	0.59	4.90	108,121,138,141	0
14	BCR	A	4003	40/40	0.87	0.54	4.73	100,112,129,132	0
14	BCR	f	4020	40/40	0.89	0.67	4.53	113,119,125,126	0
14	BCR	8	4022	40/40	0.85	0.54	4.46	123,131,145,146	0
11	CLA	a	1137	65/65	0.91	0.58	4.40	153,164,174,179	0
12	PQN	b	2002	33/33	0.91	0.57	4.22	140,146,156,158	0
12	PQN	B	2002	33/33	0.93	0.41	4.20	86,88,98,133	0
14	BCR	2	4005	40/40	0.81	0.66	4.16	102,108,118,120	0
14	BCR	l	4022	40/40	0.79	0.65	4.14	121,122,124,124	0
14	BCR	1	4008	40/40	0.89	0.57	4.04	169,180,189,192	0
14	BCR	B	4017	40/40	0.90	0.42	3.92	80,85,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	BCR	2	4004	40/40	0.78	0.65	3.84	123,137,161,163	0
14	BCR	a	4001	40/40	0.83	0.82	3.83	173,199,227,229	0
11	CLA	1	1127	65/65	0.95	0.57	3.81	214,223,233,237	0
11	CLA	b	1221	54/65	0.87	0.52	3.80	241,253,261,266	0
11	CLA	1	1102	65/65	0.88	0.53	3.79	199,219,239,246	0
14	BCR	B	4010	40/40	0.88	0.52	3.60	128,141,167,171	0
16	LMG	b	5002	55/55	0.89	0.56	3.60	149,160,167,167	0
12	PQN	A	2001	33/33	0.90	0.44	3.53	104,115,128,137	0
12	PQN	a	2001	33/33	0.71	1.19	3.47	181,201,225,229	0
11	CLA	B	1225	65/65	0.95	0.47	3.47	110,123,143,148	0
14	BCR	2	4006	40/40	0.88	0.37	3.47	98,105,120,122	0
11	CLA	b	1202	65/65	0.90	0.60	3.37	169,187,198,202	0
14	BCR	b	4006	40/40	0.54	0.75	3.36	193,210,237,241	0
16	LMG	2	5002	55/55	0.84	0.42	3.36	122,136,148,155	0
15	LHG	1	5001	49/49	0.89	0.41	3.33	182,196,208,213	0
11	CLA	B	1203	65/65	0.95	0.37	3.32	104,109,117,121	0
11	CLA	B	1240	45/65	0.83	0.53	3.30	211,230,239,242	0
11	CLA	A	1012	65/65	0.94	0.44	3.26	105,116,126,129	0
14	BCR	f	4013	40/40	0.71	1.73	3.23	275,292,321,326	0
11	CLA	A	1140	65/65	0.94	0.51	3.18	124,136,172,178	0
11	CLA	1	1107	65/65	0.90	0.44	3.18	207,232,269,282	0
11	CLA	b	1206	65/65	0.94	0.64	3.16	135,142,149,151	0
15	LHG	B	5004	49/49	0.90	0.47	3.13	158,169,178,183	0
11	CLA	a	1128	65/65	0.94	0.45	3.08	185,196,213,224	0
14	BCR	1	4001	40/40	0.84	0.80	3.04	241,254,269,271	0
11	CLA	B	1209	45/65	0.90	0.36	3.02	149,160,170,173	0
11	CLA	B	1219	55/65	0.94	0.31	3.01	158,173,186,192	0
11	CLA	B	1239	46/65	0.95	0.34	3.01	87,91,94,95	0
11	CLA	B	1226	65/65	0.94	0.43	2.97	104,114,121,124	0
11	CLA	A	1111	60/65	0.94	0.31	2.97	106,111,121,124	0
11	CLA	1	1106	65/65	0.94	0.41	2.95	187,201,212,222	0
11	CLA	b	1210	65/65	0.83	0.64	2.91	207,221,229,232	0
11	CLA	A	1127	65/65	0.96	0.46	2.89	94,101,108,110	0
11	CLA	A	1117	65/65	0.96	0.46	2.83	92,103,111,114	0
14	BCR	b	4014	40/40	0.42	2.06	2.83	230,259,294,299	0
11	CLA	1	1137	65/65	0.92	0.40	2.82	155,167,185,189	0
14	BCR	L	4022	40/40	0.78	0.59	2.76	110,121,132,133	0
11	CLA	A	1118	61/65	0.90	0.35	2.74	130,138,152,163	0
11	CLA	b	1225	65/65	0.92	0.50	2.73	183,198,210,214	0
11	CLA	1	1131	65/65	0.93	0.34	2.61	108,119,126,130	0
11	CLA	A	1125	52/65	0.94	0.38	2.61	95,99,105,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	1	1117	65/65	0.93	0.47	2.56	185,202,216,219	0
11	CLA	2	1235	60/65	0.91	0.34	2.55	154,169,185,191	0
14	BCR	A	4001	40/40	0.85	0.41	2.54	110,115,129,130	0
11	CLA	a	1131	65/65	0.95	0.36	2.54	121,124,131,134	0
11	CLA	a	1134	46/65	0.89	0.22	2.52	160,175,184,187	0
11	CLA	A	1124	55/65	0.96	0.34	2.52	85,89,93,93	0
11	CLA	A	1103	65/65	0.93	0.38	2.52	93,100,116,120	0
11	CLA	1	1128	65/65	0.95	0.39	2.52	197,213,223,224	0
11	CLA	1	1012	65/65	0.93	0.62	2.51	147,161,195,201	0
11	CLA	a	1126	65/65	0.89	0.42	2.50	210,232,258,266	0
11	CLA	b	1214	59/65	0.92	0.41	2.49	229,247,262,266	0
11	CLA	a	1132	65/65	0.94	0.37	2.49	113,128,133,136	0
11	CLA	B	1228	50/65	0.89	0.33	2.48	181,188,206,208	0
11	CLA	2	1222	56/65	0.92	0.42	2.46	141,153,179,185	0
14	BCR	a	4002	40/40	0.75	1.15	2.46	214,227,233,235	0
11	CLA	B	1227	45/65	0.87	0.28	2.44	168,175,199,212	0
11	CLA	b	1216	65/65	0.91	0.42	2.42	221,239,260,264	0
11	CLA	2	1225	65/65	0.95	0.34	2.39	100,105,110,112	0
11	CLA	b	1208	45/65	0.74	0.57	2.38	227,240,247,250	0
11	CLA	2	1013	65/65	0.94	0.54	2.37	153,169,194,196	0
15	LHG	a	5001	49/49	0.90	0.49	2.35	181,190,210,212	0
15	LHG	A	5001	49/49	0.93	0.37	2.33	94,99,108,110	0
14	BCR	6	4020	40/40	0.88	0.37	2.30	93,104,116,117	0
11	CLA	B	1206	65/65	0.94	0.41	2.30	94,99,104,106	0
11	CLA	b	1222	56/65	0.93	0.35	2.29	230,254,284,293	0
11	CLA	l	1501	65/65	0.88	0.47	2.27	137,139,157,168	0
11	CLA	2	1207	65/65	0.93	0.36	2.26	99,103,107,121	0
11	CLA	a	1117	65/65	0.89	0.67	2.23	167,191,206,211	0
11	CLA	B	1207	65/65	0.94	0.38	2.22	99,106,116,180	0
11	CLA	B	1223	65/65	0.92	0.41	2.22	154,166,176,183	0
15	LHG	b	5004	49/49	0.89	0.37	2.20	270,283,301,308	0
11	CLA	B	1222	56/65	0.91	0.37	2.19	121,136,161,169	0
11	CLA	1	1125	52/65	0.88	0.37	2.12	168,181,193,200	0
11	CLA	2	1211	46/65	0.94	0.34	2.10	98,104,109,112	0
14	BCR	a	4003	40/40	0.78	1.13	2.10	192,210,235,238	0
11	CLA	2	1204	65/65	0.94	0.34	2.10	88,90,94,99	0
11	CLA	B	1210	65/65	0.92	0.51	2.08	126,135,144,149	0
11	CLA	A	1126	65/65	0.92	0.41	2.05	95,105,125,130	0
14	BCR	A	4007	40/40	0.88	0.36	2.00	91,93,99,109	0
11	CLA	0	1401	65/65	0.80	0.43	1.99	251,268,277,306	0
11	CLA	b	1203	65/65	0.92	0.54	1.97	169,178,189,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	BCR	B	4004	40/40	0.77	0.54	1.97	168,175,187,190	0
11	CLA	b	1240	45/65	0.84	0.59	1.96	286,304,319,324	0
11	CLA	B	1235	60/65	0.95	0.37	1.91	141,154,163,166	0
11	CLA	B	1229	65/65	0.87	0.47	1.91	151,164,176,181	0
11	CLA	A	1133	46/65	0.94	0.35	1.89	89,96,101,103	0
11	CLA	B	1238	65/65	0.93	0.40	1.87	82,86,90,93	0
11	CLA	1	1103	65/65	0.95	0.42	1.87	218,234,261,272	0
11	CLA	1	1124	55/65	0.94	0.34	1.87	176,181,188,196	0
11	CLA	0	1402	50/65	0.86	0.52	1.86	282,304,319,325	0
11	CLA	A	1106	65/65	0.93	0.45	1.86	123,134,140,152	0
11	CLA	1	1129	46/65	0.93	0.41	1.86	166,179,190,191	0
11	CLA	A	1130	46/65	0.93	0.35	1.84	88,90,93,107	0
11	CLA	2	1206	65/65	0.95	0.34	1.84	91,95,98,100	0
14	BCR	A	4002	40/40	0.92	0.39	1.83	118,122,130,131	0
11	CLA	A	1129	46/65	0.94	0.34	1.82	82,85,88,89	0
11	CLA	2	1215	65/65	0.94	0.39	1.82	107,116,134,140	0
11	CLA	b	1219	55/65	0.91	0.53	1.81	267,284,296,299	0
11	CLA	B	1204	65/65	0.94	0.28	1.81	100,109,115,117	0
11	CLA	A	1134	46/65	0.93	0.28	1.77	98,106,111,113	0
11	CLA	A	1110	54/65	0.95	0.23	1.74	113,119,131,135	0
11	CLA	B	1224	55/65	0.95	0.35	1.74	116,122,128,136	0
11	CLA	L	1503	65/65	0.94	0.36	1.72	106,116,134,148	0
11	CLA	b	1205	55/65	0.96	0.30	1.72	146,156,165,167	0
11	CLA	2	1021	65/65	0.95	0.49	1.72	122,129,148,156	0
11	CLA	2	1238	65/65	0.94	0.38	1.71	93,106,113,116	0
11	CLA	B	1021	65/65	0.95	0.33	1.69	110,119,135,150	0
11	CLA	a	1130	46/65	0.95	0.27	1.68	117,123,125,128	0
11	CLA	b	1013	65/65	0.85	0.61	1.67	201,226,239,244	0
11	CLA	2	1213	65/65	0.88	0.46	1.66	142,149,160,181	0
11	CLA	1	1133	46/65	0.93	0.33	1.63	179,192,203,206	0
11	CLA	A	1011	65/65	0.95	0.37	1.62	85,97,106,141	0
11	CLA	8	1501	65/65	0.94	0.33	1.60	131,138,145,158	0
11	CLA	B	1221	54/65	0.94	0.43	1.60	126,134,140,146	0
11	CLA	B	1202	65/65	0.96	0.42	1.60	107,117,127,130	0
11	CLA	l	1503	65/65	0.92	0.32	1.59	125,130,137,187	0
11	CLA	b	1239	46/65	0.97	0.29	1.59	155,159,164,171	0
11	CLA	1	1126	65/65	0.93	0.44	1.58	179,200,211,215	0
11	CLA	a	1104	65/65	0.94	0.40	1.58	189,200,213,217	0
11	CLA	a	1113	45/65	0.81	0.47	1.56	233,253,273,278	0
11	CLA	2	1228	50/65	0.91	0.31	1.54	191,205,224,232	0
11	CLA	K	1401	65/65	0.85	0.36	1.54	141,148,155,157	0
11	CLA	b	1238	65/65	0.94	0.32	1.53	121,126,133,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	B	1216	65/65	0.88	0.38	1.52	151,164,179,185	0
11	CLA	a	1129	46/65	0.94	0.31	1.52	141,147,154,156	0
11	CLA	A	1135	51/65	0.95	0.31	1.50	90,94,97,99	0
11	CLA	1	1116	54/65	0.93	0.38	1.50	201,212,225,236	0
11	CLA	B	1234	60/65	0.88	0.32	1.50	124,143,166,172	0
11	CLA	b	1220	46/65	0.93	0.32	1.50	254,281,294,297	0
11	CLA	A	1102	65/65	0.96	0.27	1.49	123,130,142,144	0
11	CLA	a	1237	55/65	0.95	0.30	1.48	116,121,126,128	0
11	CLA	A	1128	65/65	0.95	0.34	1.46	102,108,118,128	0
11	CLA	2	1210	65/65	0.90	0.47	1.46	104,112,120,123	0
11	CLA	A	1116	54/65	0.94	0.34	1.46	96,102,108,123	0
11	CLA	2	1221	54/65	0.90	0.38	1.44	120,128,140,143	0
11	CLA	1	1132	65/65	0.95	0.34	1.44	99,105,118,123	0
11	CLA	2	1224	55/65	0.93	0.41	1.42	103,107,124,141	0
11	CLA	a	1123	65/65	0.92	0.53	1.42	159,181,191,193	0
11	CLA	1	1109	65/65	0.87	0.57	1.41	239,261,278,283	0
11	CLA	b	1217	47/65	0.89	0.28	1.41	240,259,267,270	0
11	CLA	2	1216	65/65	0.93	0.34	1.41	141,156,169,176	0
14	BCR	F	4020	40/40	0.93	0.28	1.40	84,87,94,94	0
11	CLA	B	1023	65/65	0.96	0.31	1.39	80,82,87,88	0
11	CLA	B	1205	55/65	0.95	0.34	1.38	97,104,114,127	0
11	CLA	b	1226	65/65	0.95	0.39	1.38	165,186,192,194	0
11	CLA	A	1237	55/65	0.95	0.30	1.31	80,83,86,87	0
11	CLA	b	1218	45/65	0.85	0.23	1.31	273,286,303,305	0
11	CLA	2	1214	59/65	0.95	0.31	1.30	120,130,139,145	0
11	CLA	L	1501	65/65	0.92	0.39	1.29	116,126,140,160	0
11	CLA	A	1120	46/65	0.94	0.27	1.28	99,107,111,112	0
11	CLA	a	1106	65/65	0.94	0.37	1.28	212,222,232,234	0
11	CLA	a	1102	65/65	0.90	0.34	1.28	213,223,246,250	0
15	LHG	A	5003	49/49	0.92	0.32	1.27	92,97,104,115	0
11	CLA	2	1218	45/65	0.89	0.24	1.25	164,178,189,194	0
11	CLA	b	1023	65/65	0.93	0.34	1.25	135,142,156,159	0
11	CLA	B	1201	54/65	0.93	0.32	1.24	99,107,110,111	0
11	CLA	A	1137	65/65	0.94	0.30	1.24	81,83,91,110	0
14	BCR	a	4008	40/40	0.78	0.42	1.24	150,152,155,155	0
11	CLA	a	1109	65/65	0.84	0.41	1.22	224,238,254,259	0
11	CLA	1	1112	45/65	0.88	0.48	1.20	263,286,301,303	0
11	CLA	A	1123	65/65	0.94	0.31	1.19	89,95,99,100	0
11	CLA	a	1124	55/65	0.94	0.43	1.19	156,166,174,176	0
11	CLA	a	1127	65/65	0.94	0.48	1.19	186,200,211,220	0
11	CLA	1	1113	45/65	0.87	0.51	1.18	235,255,277,284	0
11	CLA	2	1202	65/65	0.95	0.47	1.18	114,123,128,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	8	1503	65/65	0.93	0.42	1.17	137,142,156,177	0
11	CLA	2	1239	46/65	0.97	0.28	1.16	103,112,115,119	0
11	CLA	B	1236	47/65	0.96	0.33	1.15	136,145,152,153	0
11	CLA	B	1215	65/65	0.94	0.39	1.14	135,141,147,154	0
14	BCR	B	4006	40/40	0.80	0.39	1.14	128,148,172,176	0
11	CLA	1	1118	61/65	0.88	0.52	1.13	279,308,317,321	0
11	CLA	b	1207	65/65	0.93	0.40	1.13	120,127,132,133	0
11	CLA	A	1119	65/65	0.94	0.35	1.13	82,95,99,109	0
11	CLA	b	1209	45/65	0.78	0.32	1.13	226,238,250,254	0
11	CLA	2	1231	45/65	0.93	0.24	1.11	139,147,159,168	0
11	CLA	1	1123	65/65	0.94	0.44	1.11	208,227,237,242	0
11	CLA	k	1402	50/65	0.88	0.37	1.10	225,232,238,242	0
11	CLA	1	1119	65/65	0.92	0.39	1.10	197,237,248,254	0
11	CLA	a	1801	52/65	0.92	0.27	1.09	156,164,182,184	0
11	CLA	A	1801	52/65	0.92	0.25	1.07	89,95,98,103	0
11	CLA	A	1132	65/65	0.94	0.30	1.06	90,92,97,100	0
11	CLA	A	1121	46/65	0.93	0.29	1.06	97,103,120,155	0
14	BCR	6	4013	40/40	0.47	1.32	1.06	254,275,285,291	0
11	CLA	a	1118	61/65	0.93	0.58	1.06	202,218,238,243	0
11	CLA	B	1213	65/65	0.70	0.43	1.06	190,205,222,228	0
11	CLA	A	1104	65/65	0.95	0.33	1.04	93,99,105,107	0
11	CLA	A	1131	65/65	0.94	0.33	1.03	81,84,88,109	0
11	CLA	A	1122	59/65	0.95	0.34	0.99	83,88,92,94	0
11	CLA	A	1109	65/65	0.94	0.26	0.99	111,119,129,132	0
11	CLA	l	1502	46/65	0.95	0.40	0.99	111,114,119,120	0
11	CLA	b	1213	65/65	0.78	0.40	0.98	261,273,288,291	0
12	PQN	1	2001	33/33	0.91	0.60	0.97	184,204,226,230	0
11	CLA	B	1217	47/65	0.90	0.30	0.96	159,172,182,186	0
11	CLA	1	1105	48/65	0.90	0.30	0.96	208,225,238,242	0
11	CLA	a	1103	65/65	0.94	0.34	0.95	199,214,239,246	0
11	CLA	1	1237	55/65	0.93	0.29	0.94	113,120,130,133	0
11	CLA	b	1204	65/65	0.94	0.39	0.94	163,169,175,177	0
11	CLA	B	1220	46/65	0.94	0.25	0.93	133,148,155,158	0
11	CLA	2	1023	65/65	0.94	0.37	0.91	117,135,145,149	0
11	CLA	a	1107	65/65	0.91	0.34	0.91	235,255,266,271	0
11	CLA	1	1122	59/65	0.94	0.34	0.91	168,189,205,209	0
11	CLA	1	1111	60/65	0.91	0.40	0.90	229,246,266,273	0
11	CLA	b	1227	45/65	0.85	0.19	0.89	277,302,310,314	0
11	CLA	B	1013	65/65	0.96	0.28	0.89	99,112,120,139	0
11	CLA	a	1022	65/65	0.92	0.35	0.88	142,156,166,168	0
11	CLA	2	1201	54/65	0.92	0.31	0.87	91,100,104,107	0
11	CLA	1	1135	51/65	0.94	0.40	0.87	174,178,184,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	a	1121	46/65	0.87	0.29	0.87	162,173,180,183	0
11	CLA	2	1236	47/65	0.91	0.35	0.84	149,159,173,177	0
11	CLA	A	1139	50/65	0.93	0.42	0.83	112,126,138,142	0
11	CLA	a	1111	60/65	0.95	0.36	0.83	198,205,225,229	0
11	CLA	A	1022	65/65	0.95	0.33	0.82	82,88,92,93	0
11	CLA	a	1138	46/65	0.91	0.28	0.81	226,242,255,260	0
11	CLA	a	1105	48/65	0.91	0.41	0.81	249,270,280,285	0
11	CLA	2	1226	65/65	0.94	0.31	0.81	99,113,120,122	0
11	CLA	2	1220	46/65	0.95	0.31	0.80	145,153,163,167	0
11	CLA	k	1401	65/65	0.87	0.32	0.79	196,201,206,207	0
11	CLA	b	1234	60/65	0.84	0.46	0.79	220,242,268,270	0
13	SF4	A	3001	8/8	0.97	0.24	0.76	50,62,210,290	0
11	CLA	L	1502	46/65	0.94	0.33	0.76	86,91,96,114	0
11	CLA	A	1138	46/65	0.94	0.28	0.76	121,131,139,143	0
11	CLA	b	1235	60/65	0.93	0.24	0.73	235,252,263,268	0
11	CLA	a	1136	46/65	0.95	0.30	0.71	140,148,157,173	0
11	CLA	a	1135	51/65	0.93	0.39	0.71	140,155,162,167	0
11	CLA	a	1116	54/65	0.95	0.30	0.70	170,177,186,189	0
11	CLA	1	1011	65/65	0.95	0.36	0.69	124,133,140,142	0
11	CLA	A	1101	65/65	0.94	0.39	0.68	143,151,160,175	0
11	CLA	A	1107	65/65	0.92	0.38	0.67	122,130,137,141	0
14	BCR	b	4004	40/40	0.77	0.56	0.66	242,256,279,281	0
11	CLA	K	1402	50/65	0.90	0.34	0.66	169,178,200,223	0
11	CLA	a	1140	65/65	0.93	0.53	0.64	203,218,260,267	0
11	CLA	b	1201	54/65	0.90	0.27	0.64	150,157,164,166	0
11	CLA	b	1215	65/65	0.95	0.30	0.63	226,238,256,265	0
11	CLA	a	1011	65/65	0.92	0.41	0.63	161,188,194,198	0
11	CLA	a	1122	59/65	0.94	0.29	0.63	134,144,153,156	0
11	CLA	1	1130	46/65	0.91	0.29	0.60	131,140,148,150	0
11	CLA	A	1113	45/65	0.92	0.27	0.56	121,133,146,148	0
11	CLA	1	1022	65/65	0.94	0.39	0.53	101,124,132,137	0
11	CLA	b	1228	50/65	0.90	0.22	0.53	262,267,290,297	0
11	CLA	a	1012	65/65	0.93	0.41	0.52	185,204,226,230	0
11	CLA	A	1136	46/65	0.95	0.25	0.52	82,86,88,89	0
11	CLA	b	1224	55/65	0.93	0.28	0.52	163,171,178,179	0
11	CLA	8	1502	46/65	0.95	0.27	0.51	153,164,178,197	0
11	CLA	a	1110	54/65	0.83	0.27	0.51	211,224,241,244	0
11	CLA	A	1115	46/65	0.95	0.26	0.48	111,121,126,126	0
11	CLA	2	1205	55/65	0.96	0.28	0.43	92,96,98,99	0
11	CLA	1	1140	65/65	0.94	0.48	0.43	180,188,218,225	0
11	CLA	b	1236	47/65	0.93	0.20	0.43	239,254,268,270	0
11	CLA	b	1021	65/65	0.94	0.37	0.41	185,193,223,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	a	1119	65/65	0.92	0.42	0.40	143,162,172,177	0
11	CLA	a	1133	46/65	0.93	0.26	0.38	158,171,178,183	0
11	CLA	1	1121	46/65	0.87	0.23	0.38	195,211,221,226	0
11	CLA	a	1112	45/65	0.85	0.29	0.36	233,251,261,266	0
11	CLA	b	1231	45/65	0.91	0.37	0.36	275,294,305,311	0
11	CLA	b	1223	65/65	0.94	0.47	0.35	218,233,240,242	0
11	CLA	B	1230	58/65	0.85	0.34	0.34	159,178,203,214	0
13	SF4	1	3001	8/8	0.98	0.19	0.34	50,62,210,290	0
11	CLA	a	1101	65/65	0.93	0.39	0.33	236,245,257,265	0
13	SF4	C	3003	8/8	0.98	0.21	0.29	60,67,100,115	0
11	CLA	2	1209	45/65	0.91	0.21	0.27	124,135,140,143	0
11	CLA	2	1230	58/65	0.88	0.37	0.27	222,240,273,278	0
11	CLA	2	1203	65/65	0.94	0.24	0.26	97,104,108,110	0
11	CLA	1	1134	46/65	0.90	0.21	0.26	212,228,242,244	0
11	CLA	B	1211	46/65	0.95	0.26	0.19	137,146,156,161	0
11	CLA	A	1112	45/65	0.97	0.21	0.17	132,143,149,153	0
11	CLA	1	1101	65/65	0.93	0.47	0.17	214,232,245,253	0
11	CLA	b	1230	58/65	0.84	0.38	0.16	250,275,310,317	0
11	CLA	B	1212	45/65	0.92	0.27	0.15	160,174,184,187	0
11	CLA	1	1136	46/65	0.95	0.27	0.14	154,164,170,176	0
11	CLA	B	1218	45/65	0.94	0.23	0.14	168,176,189,196	0
11	CLA	2	1217	47/65	0.94	0.20	0.14	127,139,146,149	0
11	CLA	B	1232	45/65	0.91	0.23	0.11	168,184,196,202	0
11	CLA	2	1229	65/65	0.87	0.33	0.11	177,187,202,209	0
11	CLA	a	1125	52/65	0.92	0.34	0.11	157,167,173,177	0
11	CLA	A	1114	46/65	0.93	0.26	0.10	150,165,173,175	0
11	CLA	B	1214	59/65	0.92	0.24	0.08	143,159,171,177	0
11	CLA	B	1231	45/65	0.92	0.24	0.07	154,169,180,185	0
11	CLA	a	1114	46/65	0.85	0.25	0.06	248,267,279,284	0
11	CLA	b	1211	46/65	0.87	0.25	0.06	210,224,234,240	0
11	CLA	B	1208	45/65	0.94	0.27	0.05	128,136,143,147	0
11	CLA	1	1115	46/65	0.90	0.24	0.04	236,256,261,267	0
11	CLA	A	1105	48/65	0.92	0.28	0.04	118,132,139,142	0
11	CLA	A	1108	45/65	0.93	0.23	0.01	111,120,127,130	0
11	CLA	1	1801	52/65	0.91	0.24	-0.01	199,212,225,231	0
13	SF4	C	3002	8/8	0.95	0.24	-0.11	60,88,151,152	0
11	CLA	1	1138	46/65	0.92	0.29	-0.13	175,188,205,208	0
11	CLA	a	1120	46/65	0.93	0.28	-0.16	190,204,214,230	0
11	CLA	1	1120	46/65	0.90	0.32	-0.16	227,248,258,262	0
11	CLA	1	1114	46/65	0.80	0.40	-0.20	262,279,288,293	0
11	CLA	1	1139	50/65	0.93	0.27	-0.20	181,204,222,225	0
11	CLA	a	1139	50/65	0.83	0.23	-0.23	210,233,255,263	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	CLA	2	1212	45/65	0.94	0.25	-0.28	114,120,125,126	0
11	CLA	a	1115	46/65	0.92	0.19	-0.30	188,200,211,232	0
11	CLA	b	1229	65/65	0.88	0.50	-0.32	249,269,282,289	0
11	CLA	1	1108	45/65	0.83	0.19	-0.41	247,270,284,289	0
11	CLA	a	1108	45/65	0.87	0.21	-0.47	215,233,245,250	0
11	CLA	b	1212	45/65	0.88	0.22	-0.50	248,260,269,270	0
13	SF4	3	3002	8/8	0.97	0.19	-0.54	60,88,151,152	0
11	CLA	1	1110	54/65	0.89	0.27	-0.56	258,268,295,299	0
11	CLA	2	1208	45/65	0.93	0.28	-0.73	102,111,118,120	0
13	SF4	c	3002	8/8	0.97	0.16	-0.83	60,88,151,152	0
13	SF4	a	3001	8/8	0.98	0.16	-1.19	50,62,210,290	0
13	SF4	3	3003	8/8	0.97	0.10	-1.38	60,67,100,115	0
13	SF4	c	3003	8/8	0.97	0.11	-1.47	60,67,100,115	0
14	BCR	F	4013	40/40	0.65	1.11	-	163,191,214,225	0
14	BCR	B	4009	40/40	0.75	1.11	-	169,203,225,226	0
11	CLA	2	1232	45/65	0.94	0.23	-	148,157,170,176	0
14	BCR	b	4009	40/40	0.82	1.31	-	254,280,313,316	0
14	BCR	2	4009	40/40	0.60	1.70	-	189,224,256,263	0
11	CLA	2	1219	55/65	0.91	0.30	-	177,196,211,233	0
11	CLA	b	1232	45/65	0.90	0.28	-	249,265,277,284	0
11	CLA	2	1240	45/65	0.85	0.34	-	224,246,269,289	0

6.5 Other polymers [i](#)

There are no such residues in this entry.