



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3LW5
Title : Improved model of plant photosystem I
Authors : Nelson, N.; Toporik, H.
Deposited on : 2010-02-23
Resolution : 3.30 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

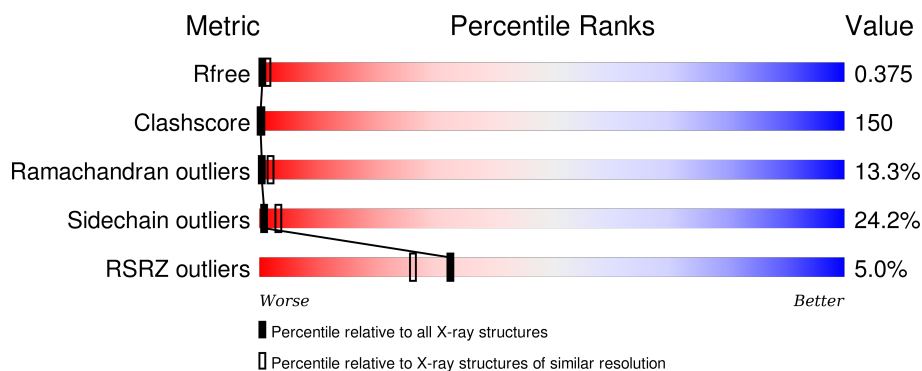
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	A	738	
2	B	733	
3	C	81	
4	D	138	
5	E	64	

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Mol	Chain	Length	Quality of chain
6	F	154	
7	G	95	
8	H	69	
9	I	30	
10	J	42	
11	K	84	
12	L	161	
13	N	85	
14	R	53	
15	1	170	
16	2	176	
17	3	172	
18	4	166	

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
19	CLA	1	1001	X	-	-	-
19	CLA	1	1002	X	-	-	-
19	CLA	1	1003	X	-	-	-
19	CLA	1	1005	X	-	-	-
19	CLA	1	1006	X	-	-	X
19	CLA	1	1007	X	-	-	-
19	CLA	1	1008	X	-	-	-
19	CLA	1	1010	X	-	-	-
19	CLA	1	1011	X	-	-	-
19	CLA	1	1012	X	-	-	-
19	CLA	1	1013	X	-	-	-
19	CLA	1	1014	X	-	-	-
19	CLA	1	1015	X	-	-	-
19	CLA	1	1303	X	-	-	-
19	CLA	1	1310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	1307	X	-	-	-
19	CLA	2	2001	X	-	-	-
19	CLA	2	2002	X	-	-	-
19	CLA	2	2003	X	-	-	-
19	CLA	2	2004	X	-	-	-
19	CLA	2	2005	X	-	-	-
19	CLA	2	2006	X	-	-	-
19	CLA	2	2007	X	-	-	-
19	CLA	2	2008	X	-	-	-
19	CLA	2	2010	X	-	-	-
19	CLA	2	2011	X	-	-	-
19	CLA	2	2012	X	-	-	-
19	CLA	2	2013	X	-	-	-
19	CLA	2	2014	X	-	X	-
19	CLA	2	4009	X	-	-	-
19	CLA	3	1118	X	-	-	-
19	CLA	3	1147	X	-	-	-
19	CLA	3	2009	X	-	X	-
19	CLA	3	3001	X	-	-	-
19	CLA	3	3002	X	-	-	-
19	CLA	3	3003	X	-	-	-
19	CLA	3	3004	X	-	-	-
19	CLA	3	3005	X	-	-	-
19	CLA	3	3006	X	-	-	-
19	CLA	3	3007	X	-	-	-
19	CLA	3	3008	X	-	-	-
19	CLA	3	3010	X	-	-	-
19	CLA	3	3011	X	-	-	-
19	CLA	3	3012	X	-	-	-
19	CLA	3	3013	X	-	-	-
19	CLA	3	3014	X	-	-	-
19	CLA	3	3015	X	-	-	-
19	CLA	3	3016	X	-	-	-
19	CLA	3	3017	X	-	-	-
19	CLA	4	1004	X	-	X	-
19	CLA	4	1009	X	-	-	-
19	CLA	4	1304	X	-	X	-
19	CLA	4	1306	X	-	-	-
19	CLA	4	4001	X	-	-	X
19	CLA	4	4002	X	-	X	-
19	CLA	4	4003	X	-	-	-
19	CLA	4	4004	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	4	4005	X	-	-	-
19	CLA	4	4006	X	-	-	-
19	CLA	4	4007	X	-	-	-
19	CLA	4	4010	X	-	-	-
19	CLA	4	4011	X	-	-	-
19	CLA	4	4012	X	-	-	-
19	CLA	4	4013	X	-	-	-
19	CLA	4	4014	X	-	-	-
19	CLA	4	4015	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	X	-
19	CLA	A	1106	X	-	X	-
19	CLA	A	1107	X	-	X	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	X	-
19	CLA	A	1112	X	-	X	X
19	CLA	A	1113	X	-	-	-
19	CLA	A	1115	X	-	X	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	X	-
19	CLA	A	1119	X	-	X	X
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	X	-
19	CLA	A	1123	X	-	X	-
19	CLA	A	1124	X	-	X	-
19	CLA	A	1125	X	-	X	-
19	CLA	A	1126	X	-	X	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	X	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1131	X	-	X	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	X	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	X	-
19	CLA	A	1136	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	X	-
19	CLA	A	1139	X	-	X	-
19	CLA	A	1140	X	-	X	-
19	CLA	A	1141	X	-	X	-
19	CLA	A	1149	X	-	-	-
19	CLA	A	1151	X	-	-	-
19	CLA	A	1237	X	-	X	-
19	CLA	A	1309	X	-	-	-
19	CLA	A	9011	X	-	-	-
19	CLA	A	9012	X	-	X	-
19	CLA	A	9013	X	-	X	-
19	CLA	A	9022	X	-	X	-
19	CLA	A	9023	X	-	X	-
19	CLA	B	1201	X	-	-	X
19	CLA	B	1202	X	-	X	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1205	X	-	X	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	X	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	X
19	CLA	B	1214	X	-	X	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	X	-
19	CLA	B	1221	X	-	X	-
19	CLA	B	1222	X	-	X	-
19	CLA	B	1223	X	-	X	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	X	-
19	CLA	B	1226	X	-	X	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	X
19	CLA	B	1233	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	X	-
19	CLA	B	1236	X	-	X	-
19	CLA	B	1238	X	-	X	-
19	CLA	B	1239	X	-	X	-
19	CLA	B	1301	X	-	-	-
19	CLA	B	9010	X	-	-	-
19	CLA	F	1240	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	F	1305	X	-	-	-
19	CLA	G	1242	X	-	-	-
19	CLA	H	1145	X	-	X	-
19	CLA	H	1207	X	-	X	-
19	CLA	H	1241	X	-	-	-
19	CLA	H	1505	X	-	-	-
19	CLA	I	1204	X	-	-	-
19	CLA	J	1308	X	-	X	-
19	CLA	J	1311	X	-	-	-
19	CLA	K	1142	X	-	-	-
19	CLA	K	1143	X	-	X	-
19	CLA	K	1146	X	-	-	-
19	CLA	K	3009	X	-	-	-
19	CLA	L	1130	X	-	X	-
19	CLA	L	1148	X	-	X	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	X	-
19	CLA	L	1503	X	-	-	-
19	CLA	L	1504	X	-	X	X
19	CLA	R	1144	X	-	-	-
19	CLA	R	1150	X	-	-	-
20	PQN	A	5001	X	-	-	-
20	PQN	B	5002	X	-	X	-
21	BCR	A	6002	-	-	X	X
21	BCR	A	6007	-	-	X	X
21	BCR	A	6008	-	-	X	X
21	BCR	A	6011	-	-	X	-
21	BCR	B	6010	-	-	X	-
21	BCR	B	6017	-	-	X	X
21	BCR	B	6020	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	BCR	F	6014	-	-	X	-
21	BCR	F	6016	-	-	X	-
21	BCR	I	6021	-	-	X	-
21	BCR	J	6012	-	-	X	-
21	BCR	L	6019	-	-	X	-
22	LMU	3	7005	-	-	X	-
22	LMU	4	7034	-	-	X	-
22	LMU	4	7052	-	-	X	-
22	LMU	D	7050	-	-	X	-
24	SF4	A	8001	-	-	X	-
24	SF4	C	8002	-	-	X	-
24	SF4	C	8003	-	-	X	-

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 36370 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	730	Total	C	N	O	S	0	0	0
			5739	3762	974	985	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5844	3841	997	993	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1097	704	191	199	3			

- Molecule 5 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	64	Total	C	N	O	0	0	0
			513	327	90	96			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	95	Total	C	N	O	0	0	0
			738	481	120	137			

- Molecule 8 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	69	Total	C	N	O	0	0	0
			517	334	80	103			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			334	228	51	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	84	Total	C	N	O	S	0	0	0
			592	377	102	110	3			

- Molecule 12 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	161	Total	C	N	O	S	0	0	0
			1209	797	192	219	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 14 is a protein called CHAIN R.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 15 is a protein called AT3g54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	165	Total	C	N	O	S	0	0	0
			1257	816	208	229	4			

- Molecule 16 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	2	176	Total	C	N	O	S	0	0	0
			1367	895	223	245	4			

- Molecule 17 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	3	156	Total	C	N	O	S	0	0	0
			1197	784	199	209	5			

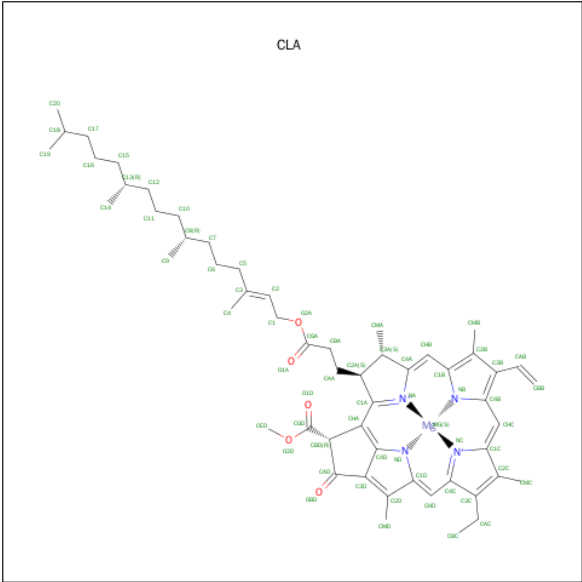
- Molecule 18 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	4	166	Total	C	N	O	S	0	0	0
			1309	856	216	234	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	SEE REMARK 999	UNP Q9SQL2

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	1	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	1	1	Total 25	C 20	Mg 1	N 4	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 57	C 47	Mg 1	N 4 O 5	0	0
19	A	1	Total 46	C 36	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 55	C 45	Mg 1	N 4 O 5	0	0
19	A	1	Total 45	C 35	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 54	C 44	Mg 1	N 4 O 5	0	0
19	A	1	Total 54	C 44	Mg 1	N 4 O 5	0	0
19	A	1	Total 45	C 35	Mg 1	N 4 O 5	0	0
19	A	1	Total 50	C 40	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 52	C 42	Mg 1	N 4 O 5	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	3	1	Total 36	C 30	Mg 1	N 4 O 1	0	0
19	A	1	Total 65	C 55	Mg 1	N 4 O 5	0	0
19	A	1	Total 51	C 41	Mg 1	N 4 O 5	0	0
19	A	1	Total 42	C 34	Mg 1	N 4 O 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	B	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
19	B	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 54	C 44	Mg 1	N 4	O 5	0	0
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
19	B	1	Total 51	C 41	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
19	1	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	A	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	1	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
19	2	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	3	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		

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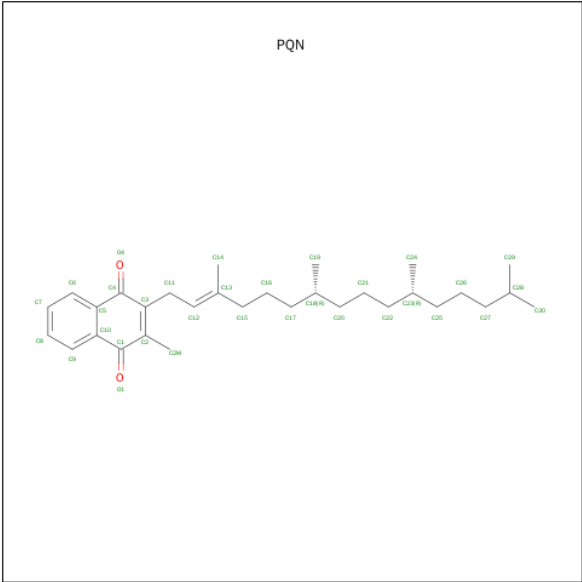
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	0	0
			25	20	1	4		
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	0
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	0
19	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
19	3	1	Total	C	Mg	N		0
			25	20	1	4		0
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
19	3	1	Total	C	Mg	N		0
			25	20	1	4		0
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
19	3	1	Total	C	Mg	N		0
			25	20	1	4		0
19	3	1	Total	C	Mg	N		0
			25	20	1	4		0
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	0
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	0
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	0
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	0
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	0
19	4	1	Total	C	Mg	N		0
			25	20	1	4		0
19	4	1	Total	C	Mg	N		0
			25	20	1	4		0
19	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	0
19	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	0

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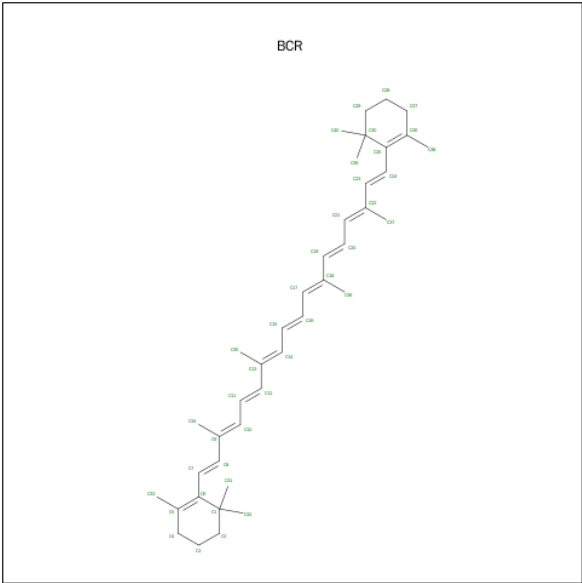
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
19	4	1	Total	C	Mg	N		0	0
			25	20	1	4			
19	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
19	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
19	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
19	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



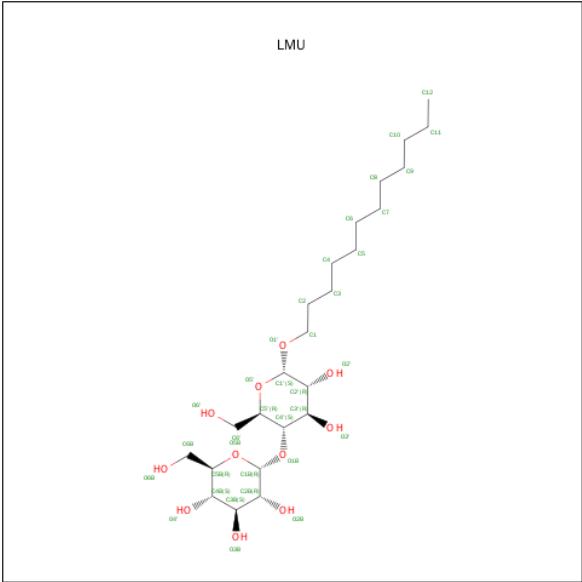
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	C		0
			40	40		
21	A	1	Total	C		0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	1	1	Total C 40 40	0	0

- Molecule 22 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	K	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	3	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			25	14	11		
22	1	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		

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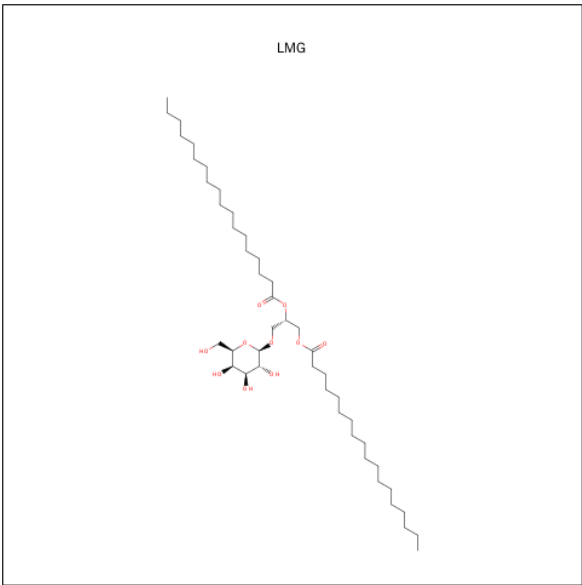
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	R	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	L	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		

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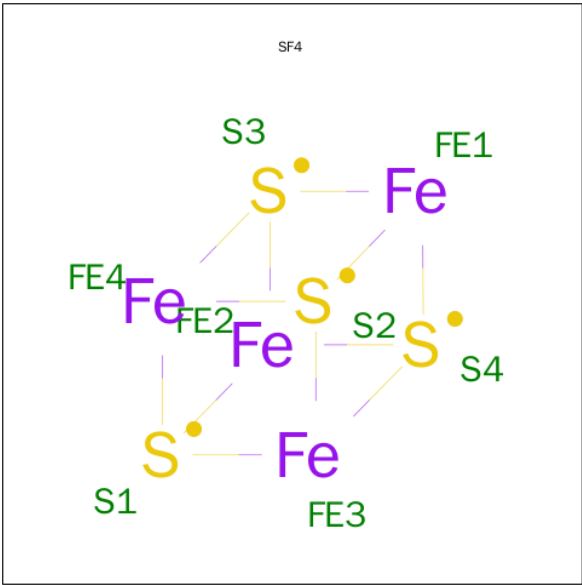
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	F	1	Total	C	O	0	0
			34	23	11		
22	E	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	B	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	H	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	A	1	Total	C	O	0	0
			35	24	11		
22	2	1	Total	C	O	0	0
			35	24	11		
22	K	1	Total	C	O	0	0
			35	24	11		
22	E	1	Total	C	O	0	0
			35	24	11		
22	N	1	Total	C	O	0	0
			35	24	11		
22	D	1	Total	C	O	0	0
			35	24	11		
22	G	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			35	24	11		
22	4	1	Total	C	O	0	0
			34	23	11		

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

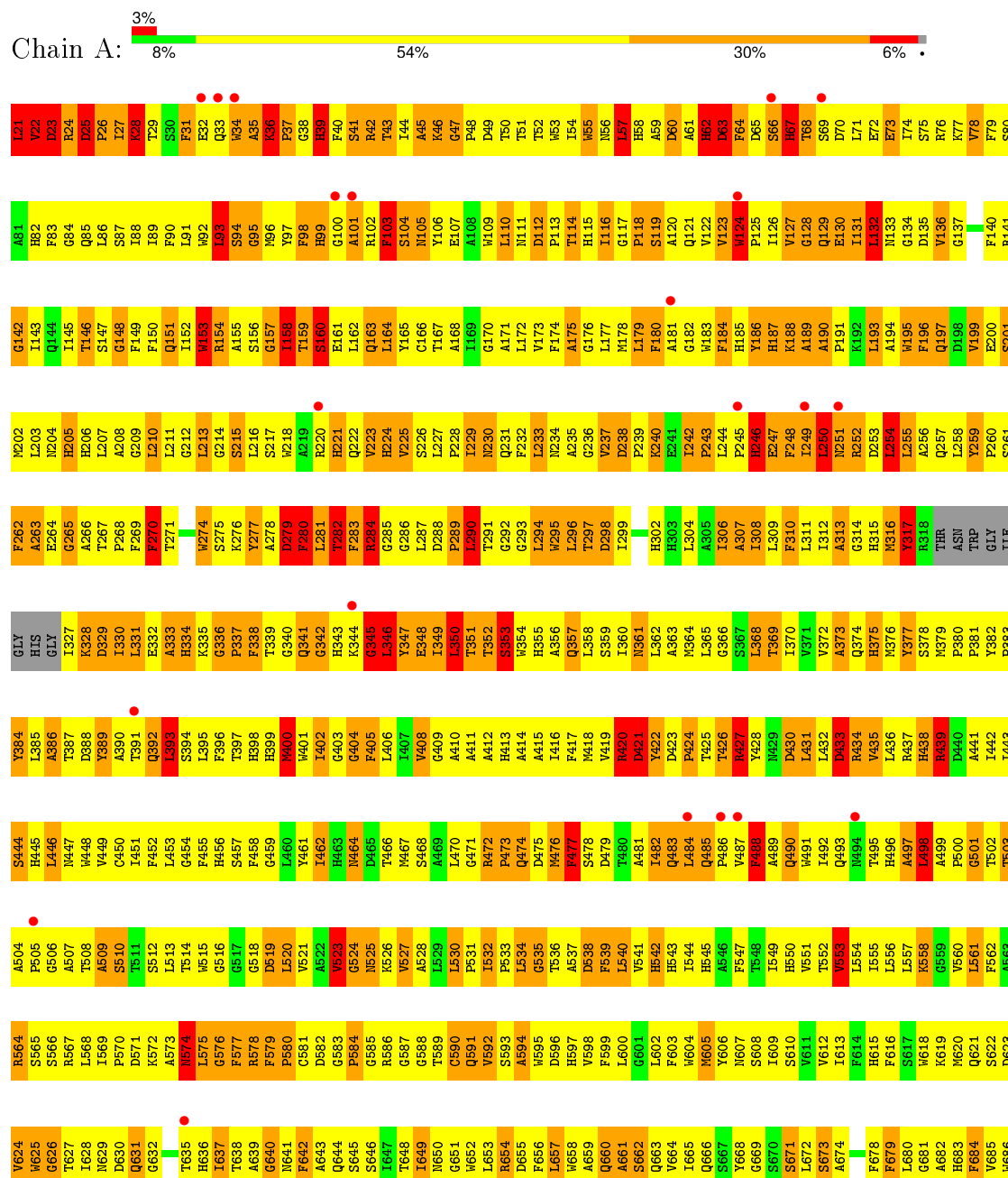


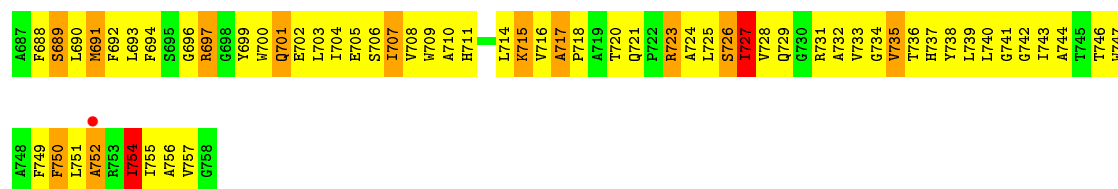
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	Fe	S	0	0
			8	4	4		
24	C	1	Total	Fe	S	0	0
			8	4	4		
24	C	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

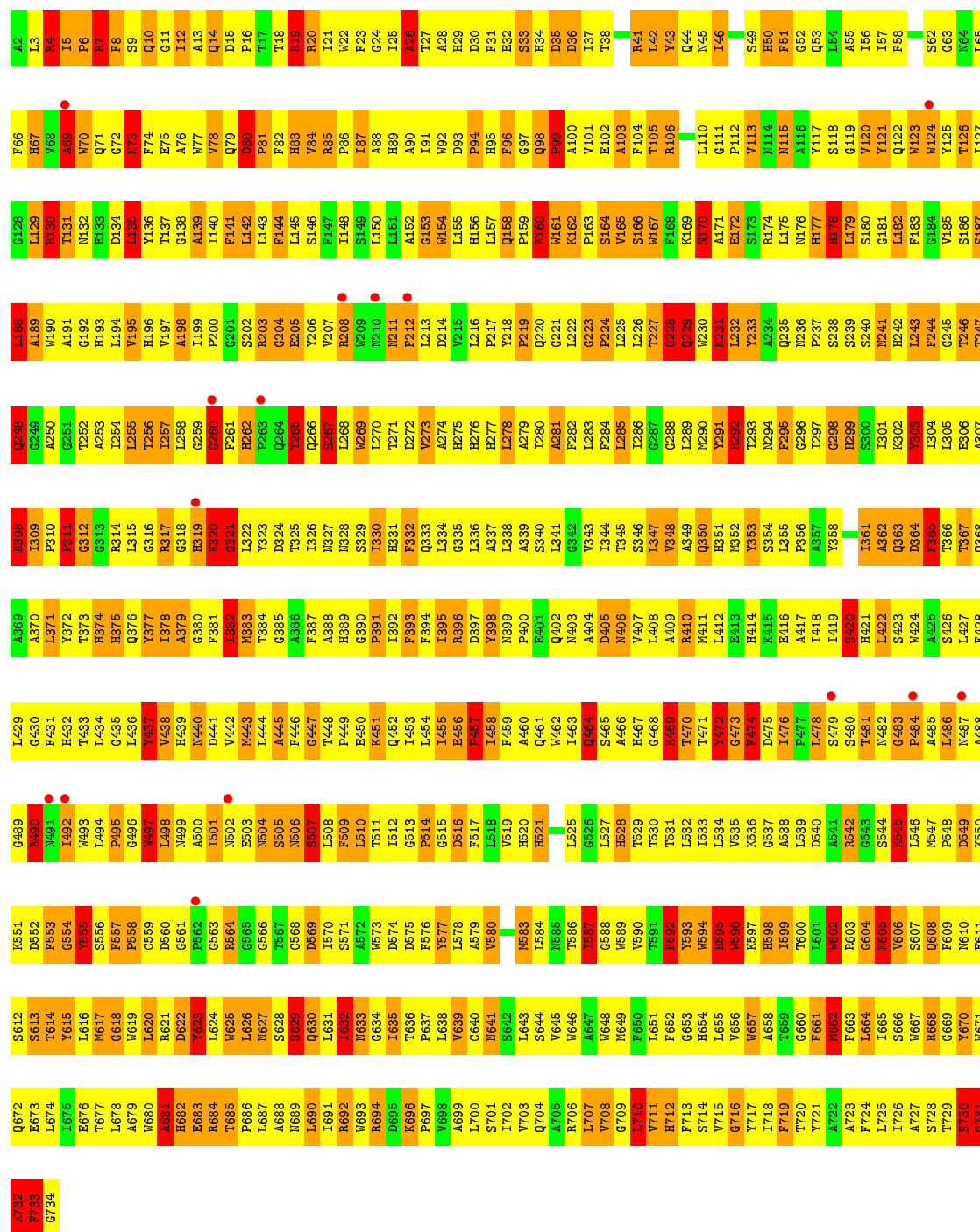
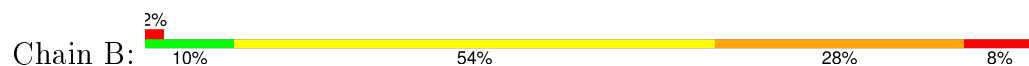
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

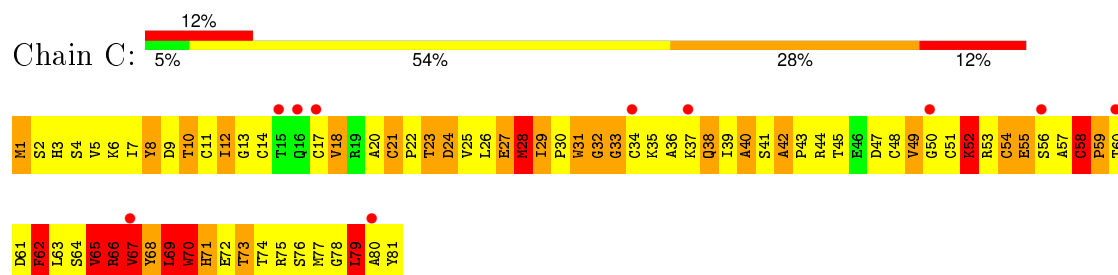




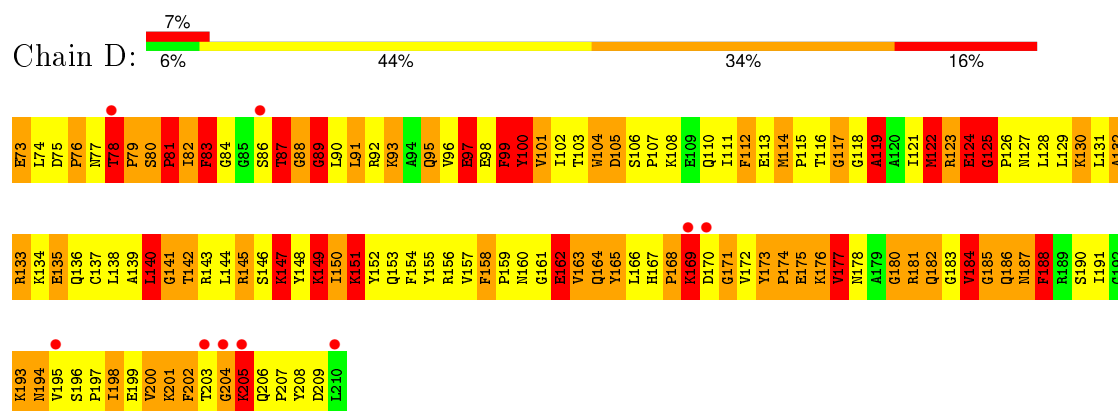
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



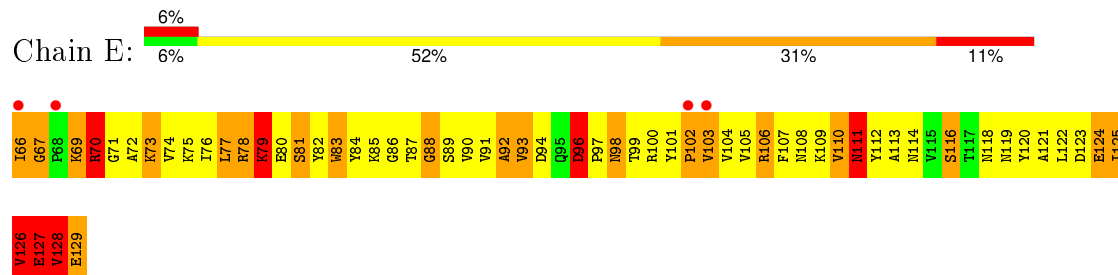
- Molecule 3: Photosystem I iron-sulfur center



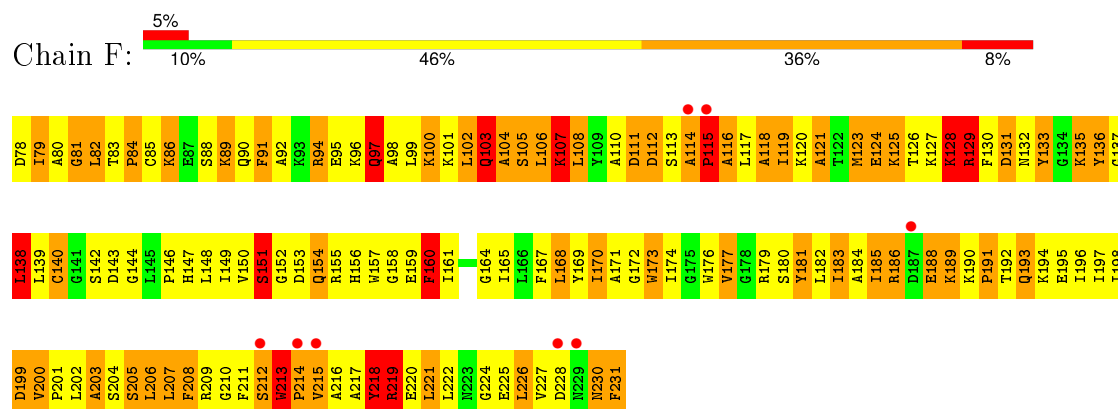
- Molecule 4: Putative uncharacterized protein



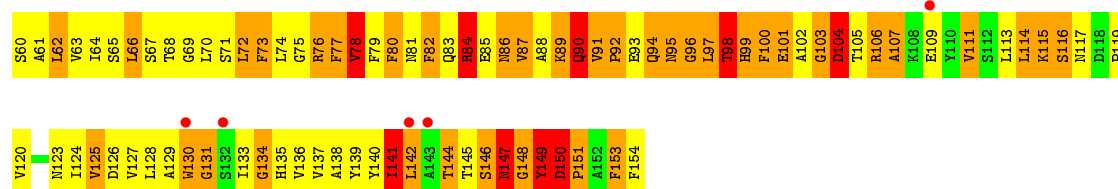
- Molecule 5: Putative uncharacterized protein



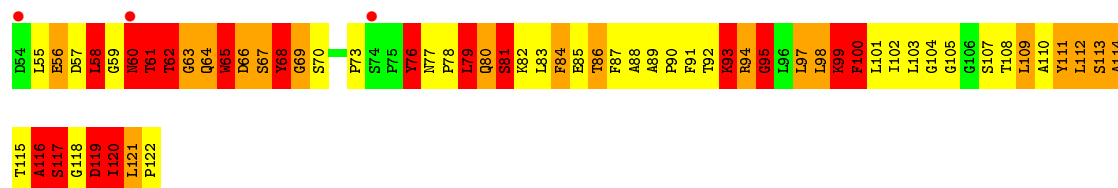
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



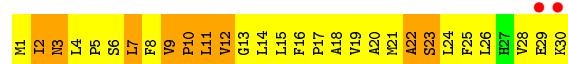
- Molecule 7: Putative uncharacterized protein



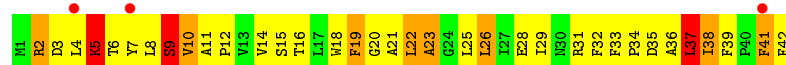
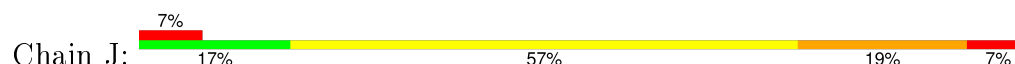
• Molecule 8: Putative uncharacterized protein



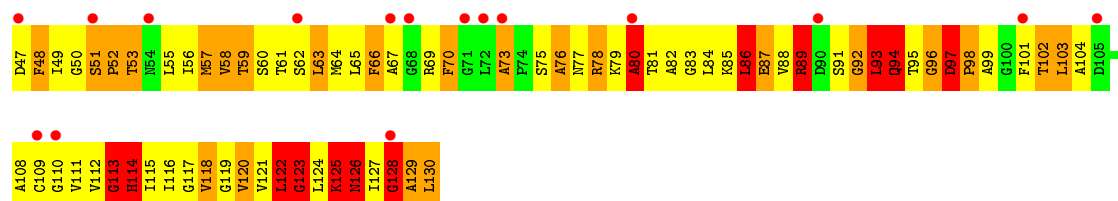
• Molecule 9: Photosystem I reaction center subunit VIII



• Molecule 10: Photosystem I reaction center subunit IX

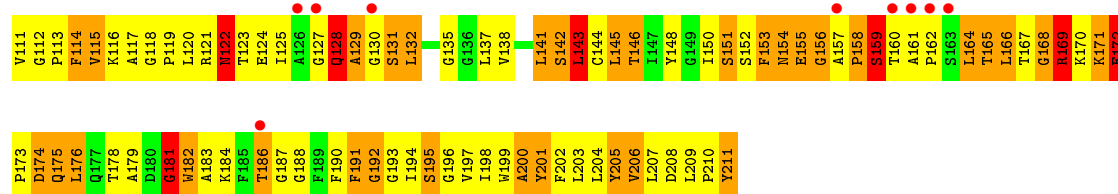


• Molecule 11: Photosystem I reaction center subunit X psaK

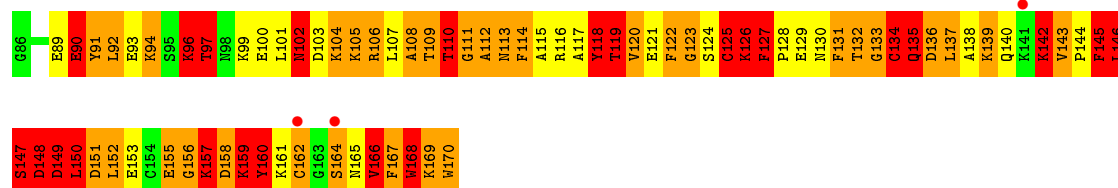


• Molecule 12: Putative uncharacterized protein

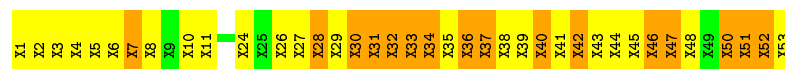




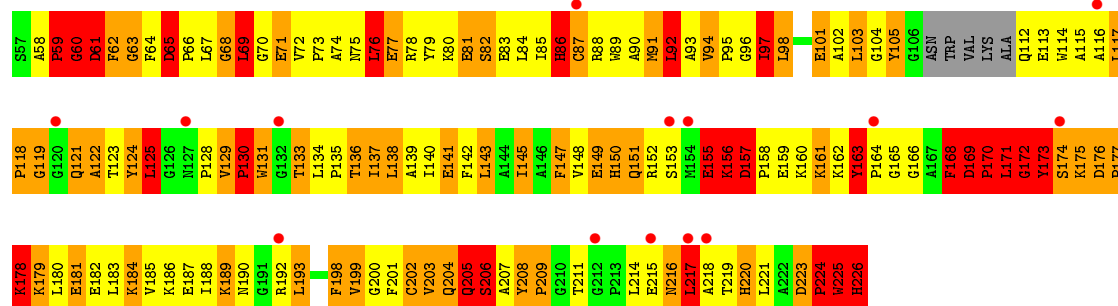
• Molecule 13: Photosystem I-N subunit



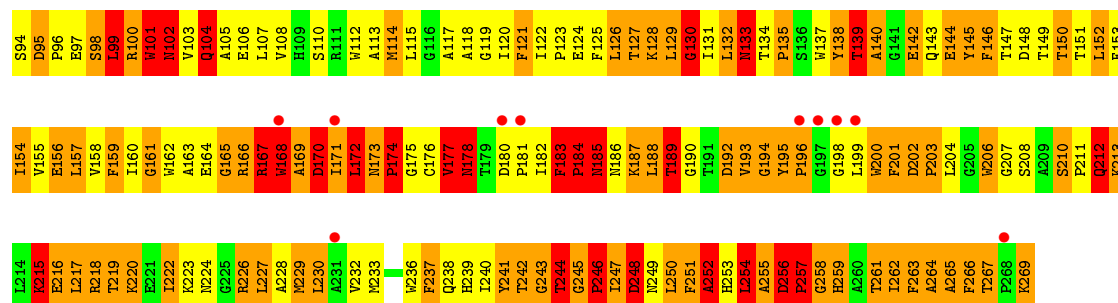
• Molecule 14: CHAIN R



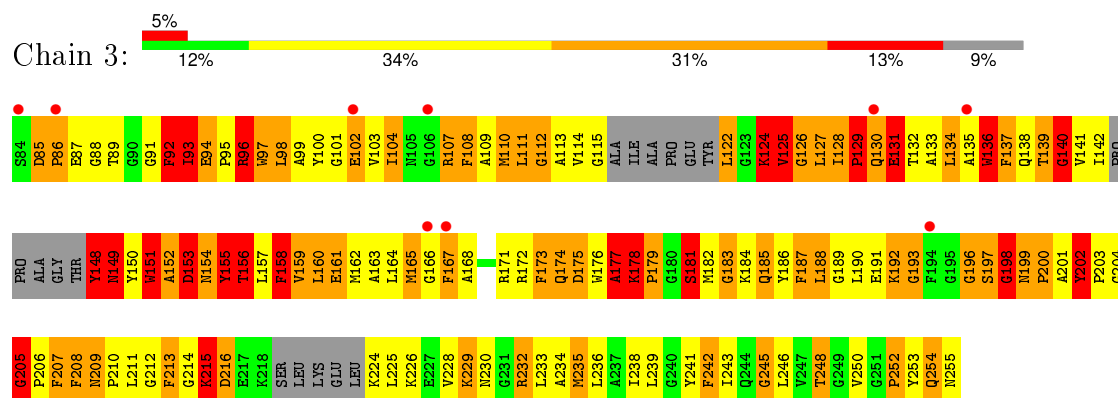
• Molecule 15: AT3g54890



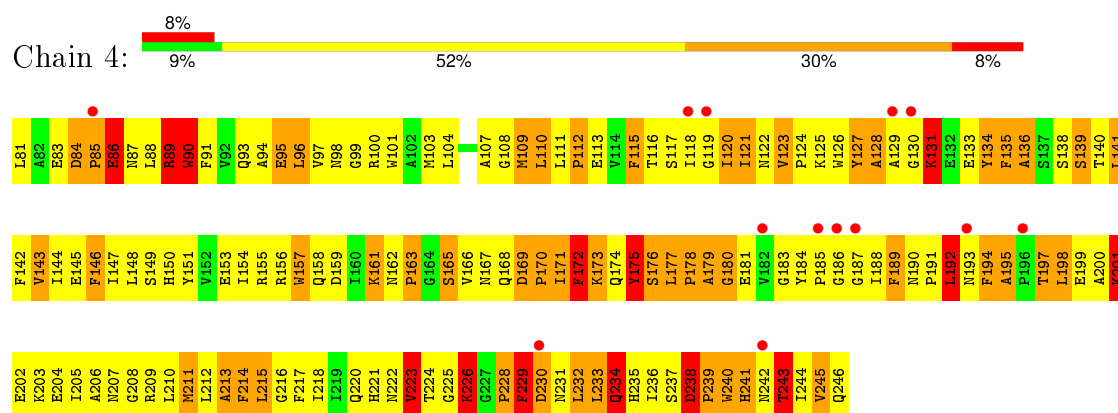
• Molecule 16: Type II chlorophyll a/b binding protein from photosystem I



• Molecule 17: Chlorophyll a-b binding protein 3, chloroplastic



• Molecule 18: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 49.14 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.0 (49.14-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.349 , 0.383 0.352 , 0.375	Depositor DCC
R_{free} test set	4349 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 93.8	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 93858 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	36370	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, CLA, PQN, LMU, 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	A	0.88	5/5932 (0.1%)	1.20	49/8096 (0.6%)
2	B	0.96	8/6054 (0.1%)	1.16	35/8273 (0.4%)
3	C	1.10	1/632 (0.2%)	1.35	5/856 (0.6%)
4	D	1.13	2/1124 (0.2%)	1.49	15/1516 (1.0%)
5	E	1.26	2/523 (0.4%)	1.38	7/710 (1.0%)
6	F	0.98	0/1250	1.29	10/1687 (0.6%)
7	G	1.00	3/757 (0.4%)	1.41	5/1031 (0.5%)
8	H	1.12	3/530 (0.6%)	1.58	11/722 (1.5%)
9	I	0.82	0/235	0.88	0/320
10	J	0.83	0/344	0.99	0/469
11	K	1.14	4/599 (0.7%)	1.50	8/811 (1.0%)
12	L	1.07	3/1244 (0.2%)	1.32	10/1703 (0.6%)
13	N	1.11	3/699 (0.4%)	1.51	10/936 (1.1%)
15	1	1.50	20/1295 (1.5%)	1.51	21/1763 (1.2%)
16	2	1.16	9/1413 (0.6%)	1.51	30/1934 (1.6%)
17	3	1.09	9/1231 (0.7%)	1.37	18/1658 (1.1%)
18	4	1.13	6/1349 (0.4%)	1.56	13/1839 (0.7%)
All	All	1.04	78/25211 (0.3%)	1.32	247/34324 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	81
2	B	0	83
3	C	0	14
4	D	0	37
5	E	0	10
6	F	0	27

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	1	24
8	H	2	22
11	K	0	21
12	L	0	23
13	N	0	40
14	R	0	17
15	1	0	37
16	2	0	45
17	3	0	35
18	4	0	28
All	All	3	544

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	119	GLY	N-CA	13.83	1.66	1.46
15	1	172	GLY	C-O	12.76	1.44	1.23
15	1	63	GLY	C-O	11.60	1.42	1.23
15	1	225	TRP	C-N	10.48	1.58	1.34
2	B	94	PRO	N-CD	-10.34	1.33	1.47

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	84	ASP	C-N-CD	-31.95	50.30	120.60
16	2	184	PRO	O-C-N	11.36	140.88	122.70
16	2	258	GLY	N-CA-C	10.50	139.35	113.10
4	D	123	ARG	NE-CZ-NH2	-10.44	115.08	120.30
18	4	186	GLY	N-CA-C	10.00	138.11	113.10

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	77	PHE	CA
8	H	60	ASN	CA
8	H	68	TYR	CA

5 of 544 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	LEU	Peptide
1	A	22	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	23	ASP	Peptide
1	A	25	ASP	Peptide
1	A	26	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5739	0	5574	1922	6
2	B	5844	0	5648	1926	14
3	C	619	0	605	325	0
4	D	1097	0	1101	436	4
5	E	513	0	514	252	0
6	F	1221	0	1247	373	28
7	G	738	0	709	337	6
8	H	517	0	503	208	2
9	I	229	0	252	53	1
10	J	334	0	344	84	0
11	K	592	0	618	270	5
12	L	1209	0	1220	435	64
13	N	685	0	667	344	0
14	R	265	0	67	79	0
15	1	1257	0	1220	592	37
16	2	1367	0	1312	644	35
17	3	1197	0	1137	516	2
18	4	1309	0	1264	532	45
19	1	665	0	453	123	1
19	2	663	0	494	142	0
19	3	736	0	453	158	0
19	4	729	0	496	154	0
19	A	2676	0	2544	1037	0
19	B	2177	0	2072	680	0
19	F	130	0	85	21	0
19	G	51	0	40	9	0
19	H	240	0	237	61	0
19	I	60	0	58	7	0
19	J	116	0	107	51	0
19	K	210	0	179	40	8

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	322	0	275	118	0
19	R	122	0	123	13	0
20	A	33	0	45	9	0
20	B	33	0	46	22	0
21	1	40	0	54	6	0
21	3	40	0	54	6	0
21	A	200	0	271	162	0
21	B	240	0	323	116	0
21	F	80	0	107	61	0
21	I	80	0	111	46	0
21	J	40	0	52	32	0
21	L	40	0	53	34	0
22	1	70	0	92	10	0
22	2	140	0	184	14	0
22	3	70	0	90	38	0
22	4	278	0	357	69	0
22	A	210	0	275	27	0
22	B	95	0	115	11	0
22	C	35	0	46	0	0
22	D	35	0	45	21	0
22	E	70	0	92	24	0
22	F	34	0	41	12	0
22	G	105	0	138	14	0
22	H	245	0	322	40	0
22	K	140	0	184	37	2
22	L	35	0	46	11	0
22	N	35	0	46	9	0
22	R	245	0	322	34	0
23	B	49	0	71	19	0
24	A	8	0	0	2	0
24	C	16	0	0	9	0
All	All	36370	0	35200	10756	130

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 150.

The worst 5 of 10756 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)
22:4:7034:LMU:C9	22:4:7052:LMU:H1'	1.24	1.64
2:B:459:PHE:CE2	19:B:1235:CLA:C2D	1.76	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:1125:CLA:HBB2	19:A:1133:CLA:CMA	1.18	1.60
1:A:244:LEU:CB	1:A:247:GLU:HG3	1.25	1.60
16:2:130:GLY:CA	16:2:131:ILE:HG13	1.29	1.60

The worst 5 of 130 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1:173:TYR:OH	16:2:132:LEU:C[2_646]	0.71	1.49
6:F:130:PHE:CG	12:L:170:LYS:NZ[2_556]	0.72	1.48
2:B:205:GLU:OE2	11:K:69:ARG:NH1[1_554]	0.79	1.41
12:L:123:THR:O	18:4:180:GLY:CA[1_455]	0.88	1.32
15:1:171:LEU:N	16:2:132:LEU:N[2_646]	0.98	1.22

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	726/738 (98%)	483 (66%)	139 (19%)	104 (14%)	0	1
2	B	731/733 (100%)	527 (72%)	111 (15%)	93 (13%)	0	2
3	C	79/81 (98%)	42 (53%)	18 (23%)	19 (24%)	0	0
4	D	136/138 (99%)	94 (69%)	24 (18%)	18 (13%)	0	2
5	E	62/64 (97%)	44 (71%)	11 (18%)	7 (11%)	0	3
6	F	152/154 (99%)	105 (69%)	27 (18%)	20 (13%)	0	2
7	G	93/95 (98%)	60 (64%)	22 (24%)	11 (12%)	0	3
8	H	67/69 (97%)	49 (73%)	9 (13%)	9 (13%)	0	2
9	I	28/30 (93%)	11 (39%)	9 (32%)	8 (29%)	0	0
10	J	40/42 (95%)	19 (48%)	11 (28%)	10 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	82/84 (98%)	66 (80%)	9 (11%)	7 (8%)	1	7
12	L	159/161 (99%)	110 (69%)	23 (14%)	26 (16%)	0	1
13	N	83/85 (98%)	50 (60%)	19 (23%)	14 (17%)	0	1
15	1	161/170 (95%)	119 (74%)	28 (17%)	14 (9%)	1	7
16	2	174/176 (99%)	129 (74%)	26 (15%)	19 (11%)	0	4
17	3	148/172 (86%)	111 (75%)	20 (14%)	17 (12%)	0	3
18	4	164/166 (99%)	129 (79%)	21 (13%)	14 (8%)	1	7
All	All	3085/3158 (98%)	2148 (70%)	527 (17%)	410 (13%)	0	2

5 of 410 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LYS
1	A	41	SER
1	A	98	PHE
1	A	99	HIS
1	A	158	ILE

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	A	590/599 (98%)	475 (80%)	115 (20%)	2	7
2	B	597/599 (100%)	468 (78%)	129 (22%)	1	5
3	C	70/70 (100%)	60 (86%)	10 (14%)	4	19
4	D	117/117 (100%)	83 (71%)	34 (29%)	0	1
5	E	56/56 (100%)	42 (75%)	14 (25%)	1	3
6	F	127/127 (100%)	91 (72%)	36 (28%)	0	2
7	G	78/79 (99%)	60 (77%)	18 (23%)	1	4
8	H	55/55 (100%)	42 (76%)	13 (24%)	1	3
9	I	26/26 (100%)	23 (88%)	3 (12%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	35/36 (97%)	26 (74%)	9 (26%)	0	2
11	K	62/62 (100%)	45 (73%)	17 (27%)	0	2
12	L	127/127 (100%)	105 (83%)	22 (17%)	2	11
13	N	74/74 (100%)	49 (66%)	25 (34%)	0	1
15	1	126/134 (94%)	76 (60%)	50 (40%)	0	0
16	2	139/142 (98%)	91 (66%)	48 (34%)	0	1
17	3	113/129 (88%)	74 (66%)	39 (34%)	0	1
18	4	136/140 (97%)	107 (79%)	29 (21%)	1	5
All	All	2528/2572 (98%)	1917 (76%)	611 (24%)	1	3

5 of 611 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	152	TYR
7	G	87	VAL
17	3	167	PHE
4	D	198	ILE
6	F	106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	375	HIS
2	B	610	ASN
17	3	149	ASN
2	B	403	ASN
2	B	502	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

252 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	$\# Z > 2$
19	CLA	1	1001	-	36,54,73	2.57	13 (36%)	41,90,113	5.06	22 (53%)
19	CLA	1	1002	-	37,55,73	2.37	10 (27%)	42,91,113	4.01	19 (45%)
19	CLA	1	1003	-	37,55,73	2.36	10 (27%)	42,91,113	5.21	19 (45%)
19	CLA	1	1005	-	36,54,73	2.80	11 (30%)	41,90,113	4.64	16 (39%)
19	CLA	1	1006	-	24,44,73	2.93	8 (33%)	28,78,113	4.61	13 (46%)
19	CLA	1	1007	-	51,69,73	2.11	10 (19%)	56,108,113	3.86	17 (30%)
19	CLA	1	1008	-	41,59,73	2.43	14 (34%)	44,96,113	4.94	20 (45%)
19	CLA	1	1010	-	36,54,73	2.46	12 (33%)	41,90,113	5.24	20 (48%)
19	CLA	1	1011	-	24,44,73	2.90	9 (37%)	28,78,113	5.29	14 (50%)
19	CLA	1	1012	-	24,44,73	2.74	8 (33%)	28,78,113	4.32	12 (42%)
19	CLA	1	1013	-	41,59,73	2.67	16 (39%)	44,96,113	4.85	20 (45%)
19	CLA	1	1014	-	51,69,73	2.12	11 (21%)	56,108,113	4.06	15 (26%)
19	CLA	1	1015	-	16,32,73	1.75	4 (25%)	21,54,113	3.13	11 (52%)
19	CLA	1	1303	-	41,59,73	2.47	13 (31%)	44,96,113	5.78	18 (40%)
19	CLA	1	1310	-	16,32,73	1.71	2 (12%)	21,54,113	3.48	12 (57%)
21	BCR	1	6023	-	41,41,41	1.72	3 (7%)	56,56,56	6.27	31 (55%)
22	LMU	1	7004	-	36,36,36	0.64	1 (2%)	47,47,47	0.85	1 (2%)
22	LMU	1	7013	-	36,36,36	0.69	0	47,47,47	1.06	1 (2%)
19	CLA	2	1307	-	16,32,73	1.76	3 (18%)	21,54,113	3.26	11 (52%)
19	CLA	2	2001	-	41,59,73	2.26	10 (24%)	44,96,113	4.63	17 (38%)
19	CLA	2	2002	-	46,64,73	2.18	11 (23%)	50,102,113	4.27	20 (40%)
19	CLA	2	2003	-	16,32,73	1.73	3 (18%)	21,54,113	3.13	11 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	2004	-	40,58,73	2.25	10 (25%)	44,95,113	4.64	16 (36%)
19	CLA	2	2005	-	16,32,73	1.72	3 (18%)	21,54,113	3.21	11 (52%)
19	CLA	2	2006	-	55,73,73	2.02	11 (20%)	61,113,113	4.28	15 (24%)
19	CLA	2	2007	-	55,73,73	1.97	10 (18%)	61,113,113	3.70	19 (31%)
19	CLA	2	2008	-	16,32,73	1.69	3 (18%)	21,54,113	3.13	11 (52%)
19	CLA	2	2010	-	16,32,73	1.75	4 (25%)	21,54,113	2.85	8 (38%)
19	CLA	2	2011	-	16,32,73	1.73	3 (18%)	21,54,113	3.19	12 (57%)
19	CLA	2	2012	16	40,58,73	2.30	9 (22%)	44,95,113	4.11	18 (40%)
19	CLA	2	2013	-	40,58,73	2.31	10 (25%)	44,95,113	4.91	18 (40%)
19	CLA	2	2014	-	51,69,73	1.99	11 (21%)	56,108,113	4.35	21 (37%)
19	CLA	2	4009	-	55,73,73	1.98	11 (20%)	61,113,113	4.47	20 (32%)
22	LMU	2	7006	-	36,36,36	0.62	0	47,47,47	0.76	0
22	LMU	2	7027	-	36,36,36	0.79	1 (2%)	47,47,47	1.76	11 (23%)
22	LMU	2	7031	-	36,36,36	1.19	2 (5%)	47,47,47	1.42	6 (12%)
22	LMU	2	7046	-	36,36,36	0.69	1 (2%)	47,47,47	0.90	3 (6%)
19	CLA	3	1118	-	24,44,73	2.78	8 (33%)	28,78,113	4.68	13 (46%)
19	CLA	3	1147	-	36,54,73	2.50	12 (33%)	41,90,113	5.07	23 (56%)
19	CLA	3	2009	-	46,64,73	2.23	13 (28%)	50,102,113	4.62	19 (38%)
19	CLA	3	3001	-	16,32,73	1.83	4 (25%)	21,54,113	3.27	12 (57%)
19	CLA	3	3002	-	16,32,73	1.77	3 (18%)	21,54,113	2.94	11 (52%)
19	CLA	3	3003	-	24,44,73	2.73	8 (33%)	28,78,113	4.21	13 (46%)
19	CLA	3	3004	-	16,32,73	1.75	5 (31%)	21,54,113	3.14	11 (52%)
19	CLA	3	3005	-	16,32,73	1.79	3 (18%)	21,54,113	3.18	12 (57%)
19	CLA	3	3006	-	16,32,73	1.83	5 (31%)	21,54,113	3.23	12 (57%)
19	CLA	3	3007	-	32,50,73	2.36	8 (25%)	36,85,113	5.51	17 (47%)
19	CLA	3	3008	-	40,58,73	2.28	11 (27%)	44,95,113	5.19	18 (40%)
19	CLA	3	3010	-	16,32,73	1.60	3 (18%)	21,54,113	3.04	11 (52%)
19	CLA	3	3011	-	55,73,73	1.91	10 (18%)	61,113,113	3.96	19 (31%)
19	CLA	3	3012	-	16,32,73	1.82	4 (25%)	21,54,113	3.43	12 (57%)
19	CLA	3	3013	-	55,73,73	2.04	12 (21%)	61,113,113	4.68	17 (27%)
19	CLA	3	3014	-	16,32,73	1.77	4 (25%)	21,54,113	3.49	12 (57%)
19	CLA	3	3015	-	16,32,73	1.76	4 (25%)	21,54,113	2.93	11 (52%)
19	CLA	3	3016	-	55,73,73	1.97	10 (18%)	61,113,113	4.11	20 (32%)
19	CLA	3	3017	-	40,58,73	2.27	10 (25%)	44,95,113	4.76	23 (52%)
21	BCR	3	6022	-	41,41,41	1.33	4 (9%)	56,56,56	4.91	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	3	7003	-	36,36,36	0.78	0	47,47,47	1.48	7 (14%)
22	LMU	3	7005	-	36,36,36	0.70	0	47,47,47	2.17	14 (29%)
19	CLA	4	1004	-	45,63,73	2.30	15 (33%)	49,101,113	4.82	19 (38%)
19	CLA	4	1009	-	24,44,73	2.88	9 (37%)	28,78,113	4.66	14 (50%)
19	CLA	4	1304	-	55,73,73	2.07	11 (20%)	61,113,113	4.34	22 (36%)
19	CLA	4	1306	-	45,63,73	2.17	9 (20%)	49,101,113	4.17	17 (34%)
19	CLA	4	4001	-	40,58,73	2.37	10 (25%)	44,95,113	4.83	15 (34%)
19	CLA	4	4002	18	42,60,73	2.32	14 (33%)	45,97,113	5.27	26 (57%)
19	CLA	4	4003	-	45,63,73	2.21	10 (22%)	49,101,113	4.36	18 (36%)
19	CLA	4	4004	-	16,32,73	1.78	3 (18%)	21,54,113	3.31	12 (57%)
19	CLA	4	4005	-	16,32,73	1.81	4 (25%)	21,54,113	3.14	11 (52%)
19	CLA	4	4006	-	45,63,73	2.22	9 (20%)	49,101,113	4.27	17 (34%)
19	CLA	4	4007	-	42,60,73	2.29	10 (23%)	45,97,113	4.11	20 (44%)
19	CLA	4	4010	-	16,32,73	1.72	3 (18%)	21,54,113	3.11	11 (52%)
19	CLA	4	4011	-	16,32,73	1.69	3 (18%)	21,54,113	3.21	12 (57%)
19	CLA	4	4012	-	24,44,73	2.74	7 (29%)	28,78,113	5.01	15 (53%)
19	CLA	4	4013	18	16,32,73	1.70	4 (25%)	21,54,113	2.71	11 (52%)
19	CLA	4	4014	-	37,55,73	2.26	12 (32%)	42,91,113	5.52	19 (45%)
19	CLA	4	4015	-	36,54,73	2.41	12 (33%)	41,90,113	5.01	14 (34%)
22	LMU	4	7008	-	36,36,36	0.56	0	47,47,47	0.92	2 (4%)
22	LMU	4	7009	-	35,35,36	1.31	2 (5%)	46,46,47	1.34	3 (6%)
22	LMU	4	7018	-	36,36,36	0.72	1 (2%)	47,47,47	1.13	3 (6%)
22	LMU	4	7019	-	36,36,36	0.79	1 (2%)	47,47,47	1.40	9 (19%)
22	LMU	4	7033	-	36,36,36	0.73	0	47,47,47	1.60	9 (19%)
22	LMU	4	7034	-	36,36,36	0.60	0	47,47,47	0.74	0
22	LMU	4	7052	-	36,36,36	1.20	4 (11%)	47,47,47	1.92	8 (17%)
22	LMU	4	7053	-	35,35,36	0.68	1 (2%)	46,46,47	1.31	6 (13%)
19	CLA	A	1101	-	40,58,73	2.30	11 (27%)	44,95,113	4.46	19 (43%)
19	CLA	A	1102	19	45,63,73	2.22	11 (24%)	49,101,113	3.77	19 (38%)
19	CLA	A	1103	-	55,73,73	2.00	12 (21%)	61,113,113	3.83	18 (29%)
19	CLA	A	1104	-	47,65,73	2.10	10 (21%)	50,103,113	4.57	19 (38%)
19	CLA	A	1105	-	36,54,73	2.31	10 (27%)	41,90,113	5.55	18 (43%)
19	CLA	A	1106	-	55,73,73	1.93	12 (21%)	61,113,113	3.30	19 (31%)
19	CLA	A	1107	-	45,63,73	2.10	10 (22%)	49,101,113	3.94	21 (42%)
19	CLA	A	1108	-	32,53,73	2.43	9 (28%)	37,89,113	4.44	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1109	19	55,73,73	2.00	11 (20%)	61,113,113	3.65	21 (34%)
19	CLA	A	1110	-	44,62,73	2.19	10 (22%)	47,99,113	4.12	16 (34%)
19	CLA	A	1111	-	44,62,73	2.12	10 (22%)	47,99,113	4.35	17 (36%)
19	CLA	A	1112	-	32,53,73	2.51	10 (31%)	37,89,113	4.70	15 (40%)
19	CLA	A	1113	-	40,58,73	2.37	10 (25%)	44,95,113	4.57	18 (40%)
19	CLA	A	1115	-	55,73,73	1.97	11 (20%)	61,113,113	4.09	19 (31%)
19	CLA	A	1116	-	42,60,73	2.33	11 (26%)	45,97,113	4.95	16 (35%)
19	CLA	A	1117	-	55,73,73	1.99	11 (20%)	61,113,113	3.63	19 (31%)
19	CLA	A	1119	-	55,73,73	1.99	11 (20%)	61,113,113	4.13	18 (29%)
19	CLA	A	1120	-	41,59,73	2.29	11 (26%)	44,96,113	4.66	18 (40%)
19	CLA	A	1121	1	32,50,73	2.49	10 (31%)	36,85,113	5.14	15 (41%)
19	CLA	A	1122	-	45,63,73	2.20	11 (24%)	49,101,113	4.54	18 (36%)
19	CLA	A	1123	-	55,73,73	1.88	11 (20%)	61,113,113	3.52	19 (31%)
19	CLA	A	1124	-	55,73,73	1.95	11 (20%)	61,113,113	3.94	18 (29%)
19	CLA	A	1125	-	55,73,73	1.95	11 (20%)	61,113,113	3.68	16 (26%)
19	CLA	A	1126	-	55,73,73	1.97	10 (18%)	61,113,113	3.95	17 (27%)
19	CLA	A	1127	-	45,63,73	2.20	11 (24%)	49,101,113	4.23	17 (34%)
19	CLA	A	1128	-	55,73,73	1.97	12 (21%)	61,113,113	3.50	21 (34%)
19	CLA	A	1129	-	40,58,73	2.26	11 (27%)	44,95,113	4.97	21 (47%)
19	CLA	A	1131	-	55,73,73	1.97	11 (20%)	61,113,113	4.14	17 (27%)
19	CLA	A	1132	-	55,73,73	1.96	11 (20%)	61,113,113	4.21	22 (36%)
19	CLA	A	1133	-	40,58,73	2.27	11 (27%)	44,95,113	4.74	17 (38%)
19	CLA	A	1134	1	32,53,73	2.40	10 (31%)	37,89,113	5.53	16 (43%)
19	CLA	A	1135	-	41,59,73	2.29	10 (24%)	44,96,113	4.58	18 (40%)
19	CLA	A	1136	-	55,73,73	1.94	11 (20%)	61,113,113	4.24	18 (29%)
19	CLA	A	1137	-	37,55,73	2.38	12 (32%)	42,91,113	5.12	16 (38%)
19	CLA	A	1138	-	55,73,73	1.98	10 (18%)	61,113,113	4.15	18 (29%)
19	CLA	A	1139	-	41,59,73	2.30	10 (24%)	44,96,113	4.81	18 (40%)
19	CLA	A	1140	-	55,73,73	1.93	10 (18%)	61,113,113	4.16	17 (27%)
19	CLA	A	1141	-	55,73,73	1.97	10 (18%)	61,113,113	4.21	19 (31%)
19	CLA	A	1149	-	36,54,73	2.74	12 (33%)	42,90,113	4.74	26 (61%)
19	CLA	A	1151	-	40,58,73	2.31	10 (25%)	44,95,113	4.74	17 (38%)
19	CLA	A	1237	-	55,73,73	1.96	11 (20%)	61,113,113	4.39	17 (27%)
19	CLA	A	1309	-	16,32,73	1.74	4 (25%)	21,54,113	2.97	11 (52%)
20	PQN	A	5001	-	34,34,34	1.51	2 (5%)	44,45,45	1.34	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	A	6002	-	41,41,41	1.83	5 (12%)	56,56,56	4.63	34 (60%)
21	BCR	A	6003	-	41,41,41	1.47	3 (7%)	56,56,56	4.11	29 (51%)
21	BCR	A	6007	-	41,41,41	1.51	4 (9%)	56,56,56	3.83	32 (57%)
21	BCR	A	6008	-	41,41,41	1.35	4 (9%)	56,56,56	4.09	27 (48%)
21	BCR	A	6011	-	41,41,41	1.33	5 (12%)	56,56,56	4.19	31 (55%)
22	LMU	A	7010	-	36,36,36	1.25	2 (5%)	47,47,47	1.27	5 (10%)
22	LMU	A	7016	-	36,36,36	0.66	0	47,47,47	1.49	6 (12%)
22	LMU	A	7023	-	36,36,36	0.58	0	47,47,47	1.25	4 (8%)
22	LMU	A	7035	-	36,36,36	0.59	0	47,47,47	1.61	10 (21%)
22	LMU	A	7044	-	36,36,36	0.84	1 (2%)	47,47,47	1.71	9 (19%)
22	LMU	A	7045	-	36,36,36	0.73	1 (2%)	47,47,47	1.56	8 (17%)
24	SF4	A	8001	1,2	0,12,12	0.00	-	0,24,24	0.00	-
19	CLA	A	9011	-	55,73,73	2.01	11 (20%)	61,113,113	4.02	19 (31%)
19	CLA	A	9012	-	55,73,73	2.01	12 (21%)	61,113,113	4.13	20 (32%)
19	CLA	A	9013	-	55,73,73	2.09	11 (20%)	61,113,113	4.29	17 (27%)
19	CLA	A	9022	-	55,73,73	2.00	11 (20%)	61,113,113	4.10	20 (32%)
19	CLA	A	9023	-	55,73,73	2.03	10 (18%)	61,113,113	3.95	17 (27%)
19	CLA	B	1201	-	32,53,73	2.42	10 (31%)	37,89,113	4.68	15 (40%)
19	CLA	B	1202	-	55,73,73	1.98	10 (18%)	61,113,113	4.36	20 (32%)
19	CLA	B	1203	-	55,73,73	1.98	11 (20%)	61,113,113	4.27	25 (40%)
19	CLA	B	1205	-	55,73,73	2.03	11 (20%)	61,113,113	4.23	18 (29%)
19	CLA	B	1206	2	55,73,73	1.89	11 (20%)	61,113,113	3.90	18 (29%)
19	CLA	B	1208	-	44,62,73	2.44	10 (22%)	49,100,113	3.22	18 (36%)
19	CLA	B	1209	-	45,63,73	2.11	11 (24%)	49,101,113	4.10	19 (38%)
19	CLA	B	1210	-	55,73,73	2.00	10 (18%)	61,113,113	4.00	19 (31%)
19	CLA	B	1211	-	55,73,73	2.04	11 (20%)	61,113,113	3.58	17 (27%)
19	CLA	B	1212	-	50,68,73	2.03	10 (20%)	55,107,113	3.93	18 (32%)
19	CLA	B	1213	-	36,54,73	2.42	10 (27%)	41,90,113	4.42	15 (36%)
19	CLA	B	1214	-	49,67,73	2.12	10 (20%)	53,105,113	3.98	17 (32%)
19	CLA	B	1215	-	50,68,73	2.02	11 (22%)	55,107,113	4.46	19 (34%)
19	CLA	B	1216	-	51,69,73	1.97	11 (21%)	56,108,113	4.54	19 (33%)
19	CLA	B	1217	-	40,58,73	2.25	11 (27%)	44,95,113	4.75	18 (40%)
19	CLA	B	1218	-	36,54,73	2.38	11 (30%)	41,90,113	4.88	14 (34%)
19	CLA	B	1219	-	45,63,73	2.30	10 (22%)	49,101,113	4.75	17 (34%)
19	CLA	B	1220	-	55,73,73	2.12	13 (23%)	61,113,113	4.42	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1221	-	44,62,73	2.29	13 (29%)	47,99,113	4.45	20 (42%)
19	CLA	B	1222	-	48,66,73	2.13	12 (25%)	52,104,113	4.58	18 (34%)
19	CLA	B	1223	-	55,73,73	1.95	11 (20%)	61,113,113	3.84	16 (26%)
19	CLA	B	1224	-	55,73,73	2.04	11 (20%)	61,113,113	4.18	19 (31%)
19	CLA	B	1225	-	55,73,73	1.96	12 (21%)	61,113,113	3.85	20 (32%)
19	CLA	B	1226	-	55,73,73	1.90	11 (20%)	61,113,113	3.37	18 (29%)
19	CLA	B	1227	-	40,58,73	2.33	10 (25%)	44,95,113	4.44	17 (38%)
19	CLA	B	1228	-	40,58,73	2.26	11 (27%)	44,95,113	5.03	18 (40%)
19	CLA	B	1229	-	55,73,73	2.05	11 (20%)	61,113,113	4.28	17 (27%)
19	CLA	B	1230	-	40,58,73	2.31	12 (30%)	44,95,113	4.13	18 (40%)
19	CLA	B	1231	19	32,53,73	2.55	9 (28%)	37,89,113	4.73	14 (37%)
19	CLA	B	1232	19	32,53,73	2.46	10 (31%)	37,89,113	5.31	15 (40%)
19	CLA	B	1233	-	41,59,73	2.38	9 (21%)	44,96,113	4.92	17 (38%)
19	CLA	B	1234	-	50,68,73	2.06	11 (22%)	55,107,113	4.49	14 (25%)
19	CLA	B	1235	-	55,73,73	1.88	10 (18%)	61,113,113	3.40	17 (27%)
19	CLA	B	1236	-	37,55,73	2.33	11 (29%)	42,91,113	4.41	17 (40%)
19	CLA	B	1238	-	55,73,73	1.95	10 (18%)	61,113,113	3.72	20 (32%)
19	CLA	B	1239	-	55,73,73	1.90	12 (21%)	61,113,113	3.87	18 (29%)
19	CLA	B	1301	-	24,44,73	2.80	9 (37%)	28,78,113	4.82	16 (57%)
20	PQN	B	5002	-	34,34,34	1.40	2 (5%)	44,45,45	1.44	6 (13%)
21	BCR	B	6004	-	41,41,41	1.25	3 (7%)	56,56,56	4.29	30 (53%)
21	BCR	B	6005	-	41,41,41	1.34	4 (9%)	56,56,56	4.75	31 (55%)
21	BCR	B	6006	-	41,41,41	1.49	6 (14%)	56,56,56	4.50	25 (44%)
21	BCR	B	6010	-	41,41,41	1.36	3 (7%)	56,56,56	4.28	30 (53%)
21	BCR	B	6017	-	41,41,41	1.49	5 (12%)	56,56,56	3.97	26 (46%)
21	BCR	B	6020	-	41,41,41	2.17	10 (24%)	56,56,56	4.43	26 (46%)
22	LMU	B	7012	-	26,26,36	0.76	1 (3%)	37,37,47	1.49	8 (21%)
22	LMU	B	7038	-	36,36,36	0.73	0	47,47,47	1.71	11 (23%)
22	LMU	B	7040	-	36,36,36	0.72	1 (2%)	47,47,47	1.66	11 (23%)
23	LMG	B	7101	-	49,49,55	1.00	3 (6%)	57,57,63	1.02	2 (3%)
19	CLA	B	9010	-	55,73,73	1.92	11 (20%)	61,113,113	3.62	18 (29%)
22	LMU	C	7015	-	36,36,36	0.67	1 (2%)	47,47,47	1.35	6 (12%)
24	SF4	C	8002	3	0,12,12	0.00	-	0,24,24	0.00	-
24	SF4	C	8003	3	0,12,12	0.00	-	0,24,24	0.00	-
22	LMU	D	7050	-	36,36,36	0.60	0	47,47,47	0.85	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	E	7037	-	36,36,36	0.71	1 (2%)	47,47,47	1.75	11 (23%)
22	LMU	E	7048	-	36,36,36	0.81	1 (2%)	47,47,47	2.09	10 (21%)
19	CLA	F	1240	-	24,44,73	2.63	8 (33%)	28,78,113	3.65	15 (53%)
19	CLA	F	1302	-	30,49,73	2.52	11 (36%)	34,84,113	5.45	16 (47%)
19	CLA	F	1305	-	43,61,73	2.45	15 (34%)	46,98,113	4.15	20 (43%)
21	BCR	F	6014	-	41,41,41	1.29	6 (14%)	56,56,56	4.83	27 (48%)
21	BCR	F	6016	-	41,41,41	1.61	10 (24%)	56,56,56	3.66	27 (48%)
22	LMU	F	7036	-	35,35,36	0.74	1 (2%)	46,46,47	1.55	6 (13%)
19	CLA	G	1242	-	41,59,73	2.33	9 (21%)	44,96,113	4.76	20 (45%)
22	LMU	G	7026	-	36,36,36	0.86	2 (5%)	47,47,47	1.51	6 (12%)
22	LMU	G	7039	-	36,36,36	0.66	0	47,47,47	1.41	4 (8%)
22	LMU	G	7051	-	36,36,36	0.85	1 (2%)	47,47,47	2.16	12 (25%)
19	CLA	H	1145	-	55,73,73	1.91	10 (18%)	61,113,113	4.39	19 (31%)
19	CLA	H	1207	-	55,73,73	2.00	11 (20%)	61,113,113	4.17	18 (29%)
19	CLA	H	1241	-	45,63,73	2.25	9 (20%)	49,101,113	4.51	19 (38%)
19	CLA	H	1505	-	45,63,73	2.22	11 (24%)	49,101,113	4.67	17 (34%)
22	LMU	H	7002	-	36,36,36	0.59	0	47,47,47	1.56	7 (14%)
22	LMU	H	7011	-	36,36,36	0.76	2 (5%)	47,47,47	1.95	12 (25%)
22	LMU	H	7017	-	36,36,36	0.71	1 (2%)	47,47,47	1.88	11 (23%)
22	LMU	H	7028	-	36,36,36	0.58	0	47,47,47	1.05	2 (4%)
22	LMU	H	7030	-	36,36,36	0.74	2 (5%)	47,47,47	1.24	5 (10%)
22	LMU	H	7032	-	36,36,36	0.70	1 (2%)	47,47,47	1.47	8 (17%)
22	LMU	H	7043	-	36,36,36	0.81	1 (2%)	47,47,47	1.67	10 (21%)
19	CLA	I	1204	-	50,68,73	2.03	11 (22%)	55,107,113	4.80	14 (25%)
21	BCR	I	6018	-	41,41,41	1.44	4 (9%)	56,56,56	4.73	31 (55%)
21	BCR	I	6021	-	41,41,41	2.01	8 (19%)	56,56,56	4.74	31 (55%)
19	CLA	J	1308	-	45,63,73	2.23	12 (26%)	49,101,113	4.81	20 (40%)
19	CLA	J	1311	-	51,69,73	2.03	11 (21%)	56,108,113	4.49	17 (30%)
21	BCR	J	6012	-	41,41,41	1.44	5 (12%)	56,56,56	5.41	24 (42%)
19	CLA	K	1142	-	32,53,73	2.33	9 (28%)	37,89,113	5.18	14 (37%)
19	CLA	K	1143	-	40,58,73	2.27	10 (25%)	44,95,113	4.51	18 (40%)
19	CLA	K	1146	-	40,58,73	2.36	11 (27%)	44,95,113	4.96	21 (47%)
19	CLA	K	3009	-	55,73,73	2.01	9 (16%)	61,113,113	4.24	18 (29%)
22	LMU	K	7001	-	36,36,36	0.80	2 (5%)	47,47,47	1.44	8 (17%)
22	LMU	K	7041	-	36,36,36	0.55	0	47,47,47	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LMU	K	7042	-	36,36,36	0.61	0	47,47,47	1.18	6 (12%)
22	LMU	K	7047	-	36,36,36	0.77	1 (2%)	47,47,47	1.09	5 (10%)
19	CLA	L	1130	-	55,73,73	2.05	11 (20%)	61,113,113	4.09	19 (31%)
19	CLA	L	1148	-	45,63,73	2.26	14 (31%)	49,101,113	4.70	21 (42%)
19	CLA	L	1501	12	40,58,73	2.31	10 (25%)	44,95,113	5.09	14 (31%)
19	CLA	L	1502	-	37,55,73	2.41	10 (27%)	42,91,113	5.12	19 (45%)
19	CLA	L	1503	-	40,58,73	2.47	14 (35%)	44,95,113	5.56	18 (40%)
19	CLA	L	1504	-	45,63,73	2.26	9 (20%)	49,101,113	4.06	19 (38%)
21	BCR	L	6019	-	41,41,41	1.71	10 (24%)	56,56,56	4.30	25 (44%)
22	LMU	L	7029	-	36,36,36	0.66	1 (2%)	47,47,47	0.77	1 (2%)
22	LMU	N	7049	-	36,36,36	0.56	1 (2%)	47,47,47	1.38	4 (8%)
19	CLA	R	1144	-	47,65,73	2.14	11 (23%)	50,103,113	4.62	17 (34%)
19	CLA	R	1150	-	55,73,73	2.15	11 (20%)	61,113,113	4.05	20 (32%)
22	LMU	R	7007	-	36,36,36	0.56	0	47,47,47	0.86	2 (4%)
22	LMU	R	7014	-	36,36,36	0.89	2 (5%)	47,47,47	2.09	9 (19%)
22	LMU	R	7020	-	36,36,36	0.66	0	47,47,47	1.48	7 (14%)
22	LMU	R	7021	-	36,36,36	0.73	0	47,47,47	1.40	4 (8%)
22	LMU	R	7022	-	36,36,36	0.70	0	47,47,47	1.35	6 (12%)
22	LMU	R	7024	-	36,36,36	0.74	1 (2%)	47,47,47	1.53	8 (17%)
22	LMU	R	7025	-	36,36,36	0.74	1 (2%)	47,47,47	1.22	5 (10%)

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
19	CLA	1	1001	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1002	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1003	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	1	1005	-	3/3/16/25	1/15/113/135	0/0/9/9
19	CLA	1	1006	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1007	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1008	-	4/4/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1010	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	1	1011	-	3/3/14/25	0/0/96/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	1012	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	1	1013	-	4/4/17/25	1/21/119/135	0/0/9/9
19	CLA	1	1014	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	1	1015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	1	1303	-	5/5/17/25	0/21/119/135	0/0/9/9
19	CLA	1	1310	-	3/3/7/25	0/0/66/135	0/0/8/9
21	BCR	1	6023	-	-	2/29/63/63	0/2/2/2
22	LMU	1	7004	-	-	0/21/61/61	0/2/2/2
22	LMU	1	7013	-	-	0/21/61/61	0/2/2/2
19	CLA	2	1307	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2001	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	2	2002	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	2	2003	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2004	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	2005	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2006	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	2007	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	2	2008	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2011	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	2	2012	16	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	2013	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	2	2014	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	2	4009	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	2	7006	-	-	0/21/61/61	0/2/2/2
22	LMU	2	7027	-	-	0/21/61/61	0/2/2/2
22	LMU	2	7031	-	-	0/21/61/61	0/2/2/2
22	LMU	2	7046	-	-	0/21/61/61	0/2/2/2
19	CLA	3	1118	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	1147	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	3	2009	-	4/4/18/25	0/27/125/135	0/0/9/9
19	CLA	3	3001	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3002	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3003	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	3	3004	-	3/3/7/25	0/0/66/135	0/0/8/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	3005	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3006	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3007	-	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	3	3008	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	3	3010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3012	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3013	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3014	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3015	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	3	3016	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	3	3017	-	3/3/17/25	0/19/117/135	0/0/9/9
21	BCR	3	6022	-	-	1/29/63/63	0/2/2/2
22	LMU	3	7003	-	-	0/21/61/61	0/2/2/2
22	LMU	3	7005	-	-	0/21/61/61	0/2/2/2
19	CLA	4	1004	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	1009	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	1304	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	4	1306	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	4001	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	4	4002	18	4/4/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4003	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	4004	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4005	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4006	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	4	4007	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	4	4010	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4011	-	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4012	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	4	4013	18	3/3/7/25	0/0/66/135	0/0/8/9
19	CLA	4	4014	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	4	4015	-	3/3/16/25	0/15/113/135	0/0/9/9
22	LMU	4	7008	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7009	-	-	0/20/60/61	0/2/2/2
22	LMU	4	7018	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LMU	4	7019	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7033	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7034	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7052	-	-	0/21/61/61	0/2/2/2
22	LMU	4	7053	-	-	0/20/60/61	0/2/2/2
19	CLA	A	1101	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1102	19	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1103	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1104	-	4/4/18/25	0/28/126/135	0/0/9/9
19	CLA	A	1105	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	A	1106	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1107	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1108	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1109	19	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1110	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1111	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	A	1112	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1113	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1115	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1116	-	3/3/17/25	0/22/120/135	0/0/9/9
19	CLA	A	1117	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1119	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1120	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1121	1	3/3/15/25	0/10/108/135	0/0/9/9
19	CLA	A	1122	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1123	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1124	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	1125	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1126	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1127	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	A	1128	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1129	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1131	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1132	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1133	-	3/3/17/25	0/19/117/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1134	1	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	A	1135	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1136	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1137	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	A	1138	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1139	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	A	1140	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1141	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1149	-	5/5/16/25	0/16/112/135	0/0/9/9
19	CLA	A	1151	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	A	1237	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	1309	-	3/3/7/25	0/0/66/135	0/0/8/9
20	PQN	A	5001	-	1/1/8/9	0/23/43/43	0/2/2/2
21	BCR	A	6002	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6003	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6007	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6008	-	-	0/29/63/63	0/2/2/2
21	BCR	A	6011	-	-	0/29/63/63	0/2/2/2
22	LMU	A	7010	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7016	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7023	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7035	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7044	-	-	0/21/61/61	0/2/2/2
22	LMU	A	7045	-	-	0/21/61/61	0/2/2/2
24	SF4	A	8001	1,2	-	0/0/48/48	0/6/5/5
19	CLA	A	9011	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	9012	-	4/4/20/25	1/37/135/135	0/0/9/9
19	CLA	A	9013	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	9022	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	A	9023	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1201	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1202	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1203	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1205	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1206	2	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1208	-	4/4/18/25	0/25/121/135	0/0/9/9
19	CLA	B	1209	-	4/4/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1210	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1211	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1212	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1213	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1214	-	4/4/18/25	0/30/128/135	0/0/9/9
19	CLA	B	1215	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1216	-	4/4/19/25	0/33/131/135	0/0/9/9
19	CLA	B	1217	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1218	-	3/3/16/25	0/15/113/135	0/0/9/9
19	CLA	B	1219	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	B	1220	-	3/3/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
19	CLA	B	1222	-	4/4/18/25	1/29/127/135	0/0/9/9
19	CLA	B	1223	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1224	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1225	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1226	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1227	-	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	B	1228	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1229	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1230	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	B	1231	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1232	19	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	B	1233	-	3/3/17/25	0/21/119/135	0/0/9/9
19	CLA	B	1234	-	4/4/19/25	0/31/129/135	0/0/9/9
19	CLA	B	1235	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1236	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	B	1238	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1239	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	B	1301	-	3/3/14/25	0/0/96/135	0/0/9/9
20	PQN	B	5002	-	1/1/8/9	0/23/43/43	0/2/2/2
21	BCR	B	6004	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6005	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6006	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6010	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	B	6017	-	-	0/29/63/63	0/2/2/2
21	BCR	B	6020	-	-	0/29/63/63	0/2/2/2
22	LMU	B	7012	-	-	0/11/51/61	0/2/2/2
22	LMU	B	7038	-	-	0/21/61/61	0/2/2/2
22	LMU	B	7040	-	-	0/21/61/61	0/2/2/2
23	LMG	B	7101	-	-	0/44/64/70	0/1/1/1
19	CLA	B	9010	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	C	7015	-	-	0/21/61/61	0/2/2/2
24	SF4	C	8002	3	-	0/0/48/48	0/6/5/5
24	SF4	C	8003	3	-	0/0/48/48	0/6/5/5
22	LMU	D	7050	-	-	0/21/61/61	0/2/2/2
22	LMU	E	7037	-	-	0/21/61/61	0/2/2/2
22	LMU	E	7048	-	-	0/21/61/61	0/2/2/2
19	CLA	F	1240	-	3/3/14/25	0/0/96/135	0/0/9/9
19	CLA	F	1302	-	3/3/15/25	0/8/106/135	0/0/9/9
19	CLA	F	1305	-	6/6/17/25	1/23/121/135	0/0/9/9
21	BCR	F	6014	-	-	1/29/63/63	0/2/2/2
21	BCR	F	6016	-	-	0/29/63/63	0/2/2/2
22	LMU	F	7036	-	-	1/20/60/61	0/2/2/2
19	CLA	G	1242	-	3/3/17/25	0/21/119/135	0/0/9/9
22	LMU	G	7026	-	-	0/21/61/61	0/2/2/2
22	LMU	G	7039	-	-	0/21/61/61	0/2/2/2
22	LMU	G	7051	-	-	0/21/61/61	0/2/2/2
19	CLA	H	1145	-	5/5/20/25	0/37/135/135	0/0/9/9
19	CLA	H	1207	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	H	1241	-	4/4/18/25	0/25/123/135	0/0/9/9
19	CLA	H	1505	-	4/4/18/25	0/25/123/135	0/0/9/9
22	LMU	H	7002	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7011	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7017	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7028	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7030	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7032	-	-	0/21/61/61	0/2/2/2
22	LMU	H	7043	-	-	0/21/61/61	0/2/2/2
19	CLA	I	1204	-	4/4/19/25	0/31/129/135	0/0/9/9
21	BCR	I	6018	-	-	0/29/63/63	0/2/2/2
21	BCR	I	6021	-	-	0/29/63/63	0/2/2/2
19	CLA	J	1308	-	4/4/18/25	1/25/123/135	0/0/9/9
19	CLA	J	1311	-	4/4/19/25	1/33/131/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	J	6012	-	-	0/29/63/63	0/2/2/2
19	CLA	K	1142	-	3/3/16/25	0/11/111/135	0/0/9/9
19	CLA	K	1143	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	1146	-	3/3/17/25	0/19/117/135	0/0/9/9
19	CLA	K	3009	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	K	7001	-	-	0/21/61/61	0/2/2/2
22	LMU	K	7041	-	-	0/21/61/61	0/2/2/2
22	LMU	K	7042	-	-	0/21/61/61	0/2/2/2
22	LMU	K	7047	-	-	0/21/61/61	0/2/2/2
19	CLA	L	1130	-	4/4/20/25	0/37/135/135	0/0/9/9
19	CLA	L	1148	-	5/5/18/25	0/25/123/135	0/0/9/9
19	CLA	L	1501	12	3/3/17/25	1/19/117/135	0/0/9/9
19	CLA	L	1502	-	3/3/16/25	0/16/114/135	0/0/9/9
19	CLA	L	1503	-	4/4/17/25	0/19/117/135	0/0/9/9
19	CLA	L	1504	-	4/4/18/25	1/25/123/135	0/0/9/9
21	BCR	L	6019	-	-	0/29/63/63	0/2/2/2
22	LMU	L	7029	-	-	1/21/61/61	0/2/2/2
22	LMU	N	7049	-	-	0/21/61/61	0/2/2/2
19	CLA	R	1144	-	4/4/18/25	0/28/126/135	0/0/9/9
19	CLA	R	1150	-	4/4/20/25	0/37/135/135	0/0/9/9
22	LMU	R	7007	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7014	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7020	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7021	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7022	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7024	-	-	0/21/61/61	0/2/2/2
22	LMU	R	7025	-	-	0/21/61/61	0/2/2/2

The worst 5 of 1849 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	1011	CLA	CAB-C3B	-9.04	1.33	1.51
19	1	1006	CLA	CAB-C3B	-9.03	1.33	1.51
19	4	1009	CLA	CAB-C3B	-8.69	1.33	1.51
19	B	1208	CLA	CAB-C3B	-8.41	1.34	1.51
19	4	4012	CLA	CAB-C3B	-8.40	1.34	1.51

The worst 5 of 3857 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	1303	CLA	OBD-CAD-CBD	-20.54	94.95	125.94
21	1	6023	BCR	C2-C1-C6	-19.89	78.87	110.36
19	A	1105	CLA	OBD-CAD-CBD	-17.66	99.29	125.94
19	A	1126	CLA	OBD-CAD-CBD	-15.67	102.29	125.94
19	B	1215	CLA	OBD-CAD-CBD	-15.33	102.81	125.94

5 of 619 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1105	CLA	NC
19	A	1105	CLA	ND
19	A	1105	CLA	NA
19	A	9012	CLA	C8
19	A	9012	CLA	NC

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	F	6014	BCR	C21-C20-C19-C18
21	1	6023	BCR	C11-C10-C9-C34
21	1	6023	BCR	C11-C10-C9-C8
22	L	7029	LMU	C1-O1'-C1'-O5'
21	3	6022	BCR	C21-C20-C19-C18

There are no ring outliers.

234 monomers are involved in 3097 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	1	1001	CLA	11	0
19	1	1002	CLA	10	0
19	1	1003	CLA	5	0
19	1	1005	CLA	5	0
19	1	1006	CLA	15	0
19	1	1007	CLA	19	0
19	1	1008	CLA	8	1
19	1	1010	CLA	8	0
19	1	1011	CLA	6	0
19	1	1012	CLA	2	0
19	1	1013	CLA	13	0
19	1	1014	CLA	17	0
19	1	1015	CLA	3	0
19	1	1303	CLA	10	0
21	1	6023	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	7004	LMU	6	0
22	1	7013	LMU	4	0
19	2	2001	CLA	13	0
19	2	2002	CLA	19	0
19	2	2003	CLA	1	0
19	2	2004	CLA	18	0
19	2	2006	CLA	7	0
19	2	2007	CLA	18	0
19	2	2011	CLA	1	0
19	2	2012	CLA	20	0
19	2	2013	CLA	5	0
19	2	2014	CLA	35	0
19	2	4009	CLA	6	0
22	2	7006	LMU	8	0
22	2	7027	LMU	3	0
22	2	7031	LMU	2	0
22	2	7046	LMU	1	0
19	3	1147	CLA	15	0
19	3	2009	CLA	37	0
19	3	3003	CLA	7	0
19	3	3004	CLA	7	0
19	3	3005	CLA	9	0
19	3	3006	CLA	9	0
19	3	3007	CLA	2	0
19	3	3008	CLA	15	0
19	3	3010	CLA	5	0
19	3	3011	CLA	12	0
19	3	3012	CLA	11	0
19	3	3013	CLA	18	0
19	3	3016	CLA	14	0
19	3	3017	CLA	4	0
21	3	6022	BCR	6	0
22	3	7003	LMU	20	0
22	3	7005	LMU	38	0
19	4	1004	CLA	33	0
19	4	1009	CLA	3	0
19	4	1304	CLA	23	0
19	4	1306	CLA	19	0
19	4	4001	CLA	4	0
19	4	4002	CLA	23	0
19	4	4003	CLA	2	0
19	4	4004	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	4006	CLA	11	0
19	4	4010	CLA	2	0
19	4	4011	CLA	2	0
19	4	4012	CLA	7	0
19	4	4013	CLA	11	0
19	4	4014	CLA	8	0
19	4	4015	CLA	4	0
22	4	7008	LMU	3	0
22	4	7009	LMU	3	0
22	4	7019	LMU	1	0
22	4	7033	LMU	7	0
22	4	7034	LMU	36	0
22	4	7052	LMU	36	0
22	4	7053	LMU	13	0
19	A	1101	CLA	15	0
19	A	1102	CLA	19	0
19	A	1103	CLA	19	0
19	A	1104	CLA	15	0
19	A	1105	CLA	26	0
19	A	1106	CLA	27	0
19	A	1107	CLA	40	0
19	A	1108	CLA	7	0
19	A	1109	CLA	18	0
19	A	1110	CLA	3	0
19	A	1111	CLA	21	0
19	A	1112	CLA	31	0
19	A	1113	CLA	9	0
19	A	1115	CLA	76	0
19	A	1116	CLA	9	0
19	A	1117	CLA	27	0
19	A	1119	CLA	43	0
19	A	1120	CLA	10	0
19	A	1121	CLA	8	0
19	A	1122	CLA	24	0
19	A	1123	CLA	29	0
19	A	1124	CLA	59	0
19	A	1125	CLA	65	0
19	A	1126	CLA	43	0
19	A	1127	CLA	16	0
19	A	1128	CLA	21	0
19	A	1129	CLA	8	0
19	A	1131	CLA	36	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1132	CLA	18	0
19	A	1133	CLA	31	0
19	A	1134	CLA	20	0
19	A	1135	CLA	23	0
19	A	1136	CLA	24	0
19	A	1137	CLA	8	0
19	A	1138	CLA	29	0
19	A	1139	CLA	31	0
19	A	1140	CLA	47	0
19	A	1141	CLA	29	0
19	A	1149	CLA	7	0
19	A	1151	CLA	18	0
19	A	1237	CLA	31	0
20	A	5001	PQN	9	0
21	A	6002	BCR	43	0
21	A	6003	BCR	14	0
21	A	6007	BCR	32	0
21	A	6008	BCR	27	0
21	A	6011	BCR	46	0
22	A	7010	LMU	6	0
22	A	7016	LMU	12	0
22	A	7023	LMU	6	0
22	A	7044	LMU	1	0
22	A	7045	LMU	2	0
24	A	8001	SF4	2	0
19	A	9011	CLA	13	0
19	A	9012	CLA	39	0
19	A	9013	CLA	29	0
19	A	9022	CLA	39	0
19	A	9023	CLA	53	0
19	B	1201	CLA	11	0
19	B	1202	CLA	31	0
19	B	1203	CLA	19	0
19	B	1205	CLA	25	0
19	B	1206	CLA	20	0
19	B	1208	CLA	6	0
19	B	1209	CLA	14	0
19	B	1210	CLA	21	0
19	B	1211	CLA	19	0
19	B	1212	CLA	14	0
19	B	1213	CLA	19	0
19	B	1214	CLA	23	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1215	CLA	10	0
19	B	1216	CLA	15	0
19	B	1217	CLA	9	0
19	B	1218	CLA	20	0
19	B	1219	CLA	13	0
19	B	1220	CLA	44	0
19	B	1221	CLA	21	0
19	B	1222	CLA	43	0
19	B	1223	CLA	38	0
19	B	1224	CLA	19	0
19	B	1225	CLA	28	0
19	B	1226	CLA	21	0
19	B	1227	CLA	11	0
19	B	1228	CLA	14	0
19	B	1229	CLA	20	0
19	B	1230	CLA	21	0
19	B	1231	CLA	16	0
19	B	1232	CLA	18	0
19	B	1233	CLA	6	0
19	B	1234	CLA	11	0
19	B	1235	CLA	62	0
19	B	1236	CLA	24	0
19	B	1238	CLA	24	0
19	B	1239	CLA	22	0
19	B	1301	CLA	6	0
20	B	5002	PQN	22	0
21	B	6004	BCR	6	0
21	B	6005	BCR	7	0
21	B	6006	BCR	14	0
21	B	6010	BCR	23	0
21	B	6017	BCR	42	0
21	B	6020	BCR	24	0
22	B	7012	LMU	1	0
22	B	7038	LMU	7	0
22	B	7040	LMU	3	0
23	B	7101	LMG	19	0
19	B	9010	CLA	17	0
24	C	8002	SF4	6	0
24	C	8003	SF4	3	0
22	D	7050	LMU	21	0
22	E	7037	LMU	7	0
22	E	7048	LMU	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	1302	CLA	10	0
19	F	1305	CLA	13	0
21	F	6014	BCR	24	0
21	F	6016	BCR	37	0
22	F	7036	LMU	12	0
19	G	1242	CLA	9	0
22	G	7026	LMU	9	0
22	G	7039	LMU	4	0
22	G	7051	LMU	1	0
19	H	1145	CLA	22	0
19	H	1207	CLA	25	0
19	H	1241	CLA	11	0
19	H	1505	CLA	3	0
22	H	7002	LMU	3	0
22	H	7011	LMU	15	0
22	H	7017	LMU	2	0
22	H	7028	LMU	2	0
22	H	7030	LMU	4	0
22	H	7032	LMU	11	0
22	H	7043	LMU	3	0
19	I	1204	CLA	7	0
21	I	6018	BCR	15	0
21	I	6021	BCR	32	0
19	J	1308	CLA	31	0
19	J	1311	CLA	20	0
21	J	6012	BCR	32	0
19	K	1142	CLA	15	1
19	K	1143	CLA	29	0
19	K	1146	CLA	7	0
19	K	3009	CLA	3	7
22	K	7001	LMU	11	0
22	K	7041	LMU	6	0
22	K	7042	LMU	16	0
22	K	7047	LMU	5	2
19	L	1130	CLA	29	0
19	L	1148	CLA	21	0
19	L	1501	CLA	17	0
19	L	1502	CLA	27	0
19	L	1503	CLA	9	0
19	L	1504	CLA	21	0
21	L	6019	BCR	34	0
22	L	7029	LMU	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	N	7049	LMU	9	0
19	R	1144	CLA	10	0
19	R	1150	CLA	3	0
22	R	7007	LMU	5	0
22	R	7014	LMU	4	0
22	R	7020	LMU	10	0
22	R	7021	LMU	9	0
22	R	7022	LMU	5	0
22	R	7025	LMU	1	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	A	730/738 (98%)	0.18	22 (3%) 54 47	12, 19, 25, 27	0
2	B	733/733 (100%)	0.11	15 (2%) 68 62	8, 18, 26, 28	0
3	C	81/81 (100%)	0.73	10 (12%) 5 4	17, 21, 23, 24	0
4	D	138/138 (100%)	0.27	9 (6%) 22 18	18, 22, 25, 27	0
5	E	64/64 (100%)	0.18	4 (6%) 23 19	17, 21, 24, 25	0
6	F	154/154 (100%)	0.14	8 (5%) 31 25	17, 22, 25, 26	0
7	G	95/95 (100%)	0.44	5 (5%) 30 24	20, 25, 28, 29	0
8	H	69/69 (100%)	0.27	3 (4%) 39 32	22, 24, 29, 30	0
9	I	30/30 (100%)	0.05	2 (6%) 21 17	17, 19, 22, 22	0
10	J	42/42 (100%)	0.28	3 (7%) 19 15	17, 21, 25, 26	0
11	K	84/84 (100%)	1.06	16 (19%) 2 1	24, 27, 29, 30	0
12	L	161/161 (100%)	0.22	9 (5%) 28 22	16, 20, 26, 27	0
13	N	85/85 (100%)	0.15	3 (3%) 48 40	22, 25, 28, 29	0
14	R	0/53	-	-	-	-
15	1	165/170 (97%)	0.40	14 (8%) 13 10	32, 59, 69, 70	0
16	2	176/176 (100%)	0.23	10 (5%) 27 22	32, 52, 63, 66	0
17	3	156/172 (90%)	0.30	9 (5%) 26 21	25, 28, 32, 33	0
18	4	166/166 (100%)	0.30	13 (7%) 16 13	20, 44, 56, 57	0
All	All	3129/3211 (97%)	0.24	155 (4%) 32 26	8, 22, 57, 70	0

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	62	SER	9.1
16	2	181	PRO	8.7
15	1	132	GLY	8.5

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Mol	Chain	Res	Type	RSRZ
2	B	491	ASN	6.8
18	4	118	ILE	5.3

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
19	CLA	L	1504	55/65	0.57	0.42	5.65	18,25,27,27	0
21	BCR	A	6002	40/40	0.65	0.40	4.95	23,27,32,33	0
19	CLA	1	1006	36/65	0.63	0.43	3.88	29,30,30,31	0
21	BCR	A	6007	40/40	0.74	0.38	3.26	19,23,28,28	0
19	CLA	4	4004	25/65	0.68	0.35	3.06	29,30,30,30	0
21	BCR	B	6017	40/40	0.81	0.34	2.91	15,18,20,20	0
19	CLA	B	1213	46/65	0.69	0.37	2.73	19,21,24,25	0
21	BCR	A	6008	40/40	0.81	0.35	2.72	21,24,27,27	0
19	CLA	B	1201	45/65	0.80	0.28	2.64	19,21,22,22	0
19	CLA	A	1119	65/65	0.81	0.35	2.30	13,18,19,20	0
23	LMG	B	7101	49/55	0.75	0.36	1.91	14,18,26,27	0
19	CLA	B	1301	36/65	0.77	0.30	1.87	27,28,29,29	0
21	BCR	B	6010	40/40	0.82	0.34	1.68	13,15,16,16	0
19	CLA	B	1216	61/65	0.84	0.28	1.64	12,18,19,20	0
21	BCR	J	6012	40/40	0.76	0.33	1.64	19,24,26,26	0
19	CLA	L	1130	65/65	0.81	0.28	1.60	13,18,19,20	0
19	CLA	A	1136	65/65	0.89	0.27	1.57	14,15,16,17	0
21	BCR	A	6003	40/40	0.76	0.35	1.56	21,24,26,26	0
21	BCR	F	6016	40/40	0.84	0.28	1.56	13,16,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	4	4001	50/65	0.68	0.43	1.55	21,23,25,25	0
21	BCR	I	6018	40/40	0.81	0.31	1.52	14,15,18,18	0
19	CLA	A	1120	51/65	0.85	0.37	1.49	22,24,24,26	0
19	CLA	4	4003	55/65	0.63	0.29	1.46	15,34,47,50	0
19	CLA	L	1502	47/65	0.83	0.25	1.45	17,19,20,20	0
21	BCR	F	6014	40/40	0.83	0.31	1.44	9,11,15,15	0
21	BCR	I	6021	40/40	0.76	0.30	1.42	16,20,22,22	0
19	CLA	A	1102	55/65	0.79	0.30	1.40	13,19,20,20	0
19	CLA	B	1231	45/65	0.81	0.28	1.35	19,20,21,21	0
22	LMU	K	7047	35/35	0.71	0.27	1.30	14,33,46,49	0
19	CLA	A	1124	65/65	0.84	0.28	1.25	18,21,23,24	0
19	CLA	B	1226	65/65	0.88	0.31	1.21	11,12,19,19	0
19	CLA	A	1112	45/65	0.69	0.41	1.19	23,26,26,27	0
19	CLA	A	1138	65/65	0.85	0.29	1.16	15,18,19,20	0
19	CLA	B	1239	65/65	0.87	0.30	1.15	8,11,13,14	0
21	BCR	L	6019	40/40	0.79	0.34	1.11	15,17,19,19	0
19	CLA	K	3009	65/65	0.70	0.37	1.03	22,25,27,28	0
19	CLA	H	1207	65/65	0.81	0.28	1.02	15,17,19,20	0
21	BCR	B	6006	40/40	0.80	0.38	1.01	15,19,20,21	0
21	BCR	B	6005	40/40	0.87	0.29	0.99	14,16,17,17	0
19	CLA	A	1237	65/65	0.86	0.28	0.91	8,17,18,18	0
19	CLA	1	1015	25/65	0.71	0.24	0.89	27,28,28,28	0
19	CLA	B	1211	65/65	0.82	0.31	0.88	17,20,21,21	0
19	CLA	B	1232	45/65	0.69	0.42	0.85	23,26,27,27	0
19	CLA	B	1230	50/65	0.83	0.28	0.84	17,18,19,20	0
20	PQN	A	5001	33/33	0.88	0.29	0.82	12,13,14,15	0
21	BCR	B	6020	40/40	0.89	0.25	0.82	8,11,12,13	0
19	CLA	A	1126	65/65	0.88	0.29	0.78	12,14,15,15	0
19	CLA	3	3003	36/65	0.74	0.34	0.77	29,30,31,31	0
19	CLA	A	1117	65/65	0.84	0.31	0.76	10,20,21,22	0
19	CLA	A	1104	57/65	0.89	0.27	0.75	13,15,18,18	0
19	CLA	B	1205	65/65	0.89	0.26	0.74	9,13,14,14	0
19	CLA	A	1106	65/65	0.91	0.29	0.73	10,12,13,14	0
19	CLA	G	1242	51/65	0.68	0.34	0.72	26,28,29,29	0
21	BCR	B	6004	40/40	0.80	0.33	0.71	18,20,22,22	0
19	CLA	A	1103	65/65	0.85	0.28	0.70	13,14,21,22	0
19	CLA	F	1240	36/65	0.87	0.23	0.70	15,16,17,17	0
19	CLA	B	1202	65/65	0.89	0.25	0.69	7,16,16,18	0
19	CLA	A	1105	46/65	0.77	0.37	0.68	22,23,24,24	0
19	CLA	A	1128	65/65	0.86	0.27	0.67	14,16,17,18	0
19	CLA	A	1123	65/65	0.83	0.30	0.64	12,18,19,20	0
19	CLA	B	1223	65/65	0.82	0.32	0.61	13,18,19,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	A	1139	51/65	0.88	0.23	0.59	16,16,17,18	0
19	CLA	A	9022	65/65	0.90	0.28	0.57	2,12,26,31	0
19	CLA	B	1225	65/65	0.88	0.29	0.57	9,12,13,14	0
19	CLA	B	1224	65/65	0.88	0.27	0.57	9,13,14,15	0
19	CLA	4	4006	55/65	0.78	0.23	0.56	16,23,24,24	0
19	CLA	A	1116	52/65	0.78	0.28	0.55	24,25,26,26	0
19	CLA	B	1212	60/65	0.74	0.32	0.53	20,23,25,26	0
19	CLA	B	1222	58/65	0.79	0.34	0.53	18,21,23,24	0
19	CLA	L	1501	50/65	0.86	0.24	0.51	20,20,21,21	0
19	CLA	A	1135	51/65	0.84	0.27	0.51	16,19,19,21	0
19	CLA	A	1125	65/65	0.86	0.24	0.46	15,17,19,20	0
21	BCR	A	6011	40/40	0.86	0.30	0.45	10,15,16,16	0
19	CLA	A	1132	65/65	0.86	0.27	0.44	13,17,18,19	0
19	CLA	B	1229	65/65	0.82	0.27	0.42	8,12,14,15	0
22	LMU	L	7029	35/35	0.63	0.31	0.40	30,44,53,55	0
19	CLA	B	1215	60/65	0.88	0.27	0.39	11,13,15,16	0
19	CLA	B	1218	46/65	0.78	0.30	0.38	20,20,22,23	0
19	CLA	A	9023	65/65	0.89	0.27	0.37	2,14,29,38	0
19	CLA	I	1204	60/65	0.84	0.24	0.37	13,17,18,18	0
19	CLA	3	3005	25/65	0.59	0.28	0.36	31,31,31,31	0
19	CLA	L	1503	50/65	0.81	0.25	0.36	19,21,23,24	0
19	CLA	A	1111	54/65	0.84	0.26	0.29	20,24,24,24	0
19	CLA	B	1206	65/65	0.87	0.27	0.25	10,12,17,18	0
19	CLA	B	1234	60/65	0.85	0.28	0.24	13,14,21,21	0
19	CLA	4	1306	55/65	0.71	0.32	0.23	20,26,27,27	0
19	CLA	3	3002	25/65	0.75	0.27	0.21	28,28,28,28	0
19	CLA	B	1219	55/65	0.85	0.24	0.21	18,18,21,21	0
19	CLA	A	1131	65/65	0.88	0.25	0.18	12,14,16,16	0
19	CLA	B	1217	50/65	0.84	0.26	0.17	19,21,22,23	0
19	CLA	2	2012	50/65	0.81	0.26	0.15	20,22,23,23	0
19	CLA	B	1208	54/65	0.85	0.26	0.13	18,18,21,22	0
19	CLA	B	1236	47/65	0.88	0.28	0.12	14,15,17,17	0
19	CLA	B	1209	55/65	0.83	0.26	0.12	18,19,20,21	0
19	CLA	B	1238	65/65	0.86	0.27	0.11	10,14,15,16	0
19	CLA	B	1235	65/65	0.88	0.26	0.08	14,15,16,17	0
19	CLA	4	4012	36/65	0.86	0.21	0.08	14,15,16,16	0
19	CLA	A	1122	55/65	0.88	0.22	0.01	13,14,18,18	0
19	CLA	A	1101	50/65	0.87	0.23	-0.01	17,18,18,19	0
19	CLA	A	1109	65/65	0.84	0.28	-0.02	13,20,22,23	0
20	PQN	B	5002	33/33	0.90	0.26	-0.05	7,8,14,14	0
19	CLA	1	1003	47/65	0.74	0.24	-0.08	17,19,19,20	0
19	CLA	B	1214	59/65	0.87	0.24	-0.09	18,20,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	4	1004	55/65	0.73	0.26	-0.10	22,25,26,27	0
19	CLA	B	1220	65/65	0.87	0.24	-0.11	13,15,20,21	0
19	CLA	B	1228	50/65	0.86	0.23	-0.12	12,14,14,15	0
19	CLA	B	1203	65/65	0.91	0.24	-0.15	10,13,14,15	0
19	CLA	A	1115	65/65	0.81	0.24	-0.16	10,28,41,42	0
19	CLA	A	1127	55/65	0.89	0.25	-0.17	13,16,17,18	0
19	CLA	A	1140	65/65	0.85	0.28	-0.17	15,18,19,21	0
19	CLA	3	1147	46/65	0.73	0.29	-0.19	25,27,28,28	0
19	CLA	A	1108	45/65	0.78	0.29	-0.21	19,22,23,24	0
19	CLA	A	1107	55/65	0.87	0.26	-0.23	15,16,24,24	0
19	CLA	A	1133	50/65	0.85	0.23	-0.24	17,19,19,20	0
19	CLA	B	1221	54/65	0.91	0.22	-0.24	13,13,16,16	0
19	CLA	B	9010	65/65	0.89	0.25	-0.26	2,12,34,40	0
19	CLA	F	1302	41/65	0.73	0.25	-0.26	24,26,26,26	0
19	CLA	3	3013	65/65	0.77	0.26	-0.27	20,21,24,25	0
19	CLA	A	9011	65/65	0.91	0.26	-0.28	2,11,30,40	0
19	CLA	B	1210	65/65	0.90	0.23	-0.30	16,20,21,22	0
19	CLA	A	1113	50/65	0.75	0.31	-0.31	19,22,23,24	0
22	LMU	A	7044	35/35	0.78	0.18	-0.35	8,20,39,40	0
19	CLA	2	2004	50/65	0.74	0.26	-0.36	23,25,25,25	0
19	CLA	A	1129	50/65	0.88	0.20	-0.38	17,19,20,20	0
19	CLA	1	1012	36/65	0.86	0.22	-0.40	23,24,25,25	0
19	CLA	A	9012	65/65	0.89	0.25	-0.43	2,14,28,36	0
19	CLA	A	1137	47/65	0.90	0.24	-0.43	13,14,15,17	0
19	CLA	B	1227	50/65	0.89	0.23	-0.46	13,15,16,17	0
19	CLA	A	9013	65/65	0.89	0.25	-0.46	2,10,29,32	0
22	LMU	A	7045	35/35	0.77	0.19	-0.65	11,23,41,43	0
19	CLA	1	1011	36/65	0.82	0.22	-0.66	27,27,28,28	0
19	CLA	A	1121	42/65	0.75	0.24	-0.88	26,28,28,28	0
19	CLA	3	3010	25/65	0.70	0.23	-0.89	32,32,33,33	0
19	CLA	4	4011	25/65	0.86	0.18	-1.55	10,11,12,12	0
24	SF4	A	8001	8/8	0.99	0.09	-1.75	12,17,19,21	0
24	SF4	C	8002	8/8	0.97	0.08	-2.11	14,16,24,28	0
24	SF4	C	8003	8/8	0.98	0.07	-3.24	14,19,21,22	0
19	CLA	3	3017	50/65	0.76	0.23	-	26,37,49,52	0
21	BCR	3	6022	40/40	0.71	0.25	-	21,22,23,23	0
19	CLA	H	1505	55/65	0.64	0.39	-	18,27,28,29	0
22	LMU	B	7012	25/35	0.82	0.18	-	22,32,44,49	0
22	LMU	H	7043	35/35	0.68	0.19	-	12,31,46,47	0
22	LMU	A	7035	35/35	0.85	0.27	-	6,18,32,40	0
22	LMU	2	7027	35/35	0.76	0.22	-	6,17,40,40	0
22	LMU	R	7022	35/35	0.79	0.18	-	5,21,33,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	H	1145	65/65	0.76	0.24	-	12,24,33,39	0
22	LMU	1	7004	35/35	0.61	0.49	-	17,44,50,52	0
22	LMU	A	7016	35/35	0.76	0.26	-	10,30,46,46	0
19	CLA	R	1150	65/65	0.75	0.29	-	22,24,25,25	0
22	LMU	4	7018	35/35	0.73	0.30	-	9,23,41,42	0
19	CLA	K	1146	50/65	0.77	0.27	-	25,28,30,30	0
19	CLA	3	3007	42/65	0.73	0.32	-	27,30,30,30	0
22	LMU	G	7039	35/35	0.87	0.15	-	15,30,47,47	0
19	CLA	2	2014	61/65	0.64	0.33	-	24,26,28,28	0
22	LMU	R	7021	35/35	0.75	0.25	-	17,28,45,46	0
22	LMU	H	7002	35/35	0.76	0.17	-	16,29,41,43	0
19	CLA	3	3004	25/65	0.77	0.20	-	27,28,28,28	0
19	CLA	4	1304	65/65	0.72	0.26	-	21,23,25,25	0
19	CLA	A	1151	50/65	0.72	0.37	-	24,27,29,29	0
19	CLA	1	1002	47/65	0.81	0.23	-	22,23,24,24	0
22	LMU	H	7028	35/35	0.77	0.17	-	7,21,40,40	0
19	CLA	1	1008	51/65	0.75	0.35	-	24,26,27,27	0
22	LMU	4	7033	35/35	0.80	0.19	-	12,26,40,41	0
19	CLA	4	4005	25/65	0.77	0.28	-	20,21,22,22	0
19	CLA	1	1303	51/65	0.77	0.32	-	23,28,28,29	0
22	LMU	2	7031	35/35	0.74	0.23	-	17,37,45,48	0
19	CLA	4	4010	25/65	0.78	0.23	-	26,27,27,27	0
22	LMU	A	7023	35/35	0.78	0.25	-	6,20,39,41	0
22	LMU	4	7008	35/35	0.70	0.34	-	11,29,41,42	0
22	LMU	3	7005	35/35	0.74	0.25	-	20,32,42,43	0
19	CLA	1	1005	46/65	0.82	0.23	-	19,21,22,22	0
19	CLA	2	2007	65/65	0.66	0.30	-	17,25,26,26	0
19	CLA	J	1311	61/65	0.73	0.27	-	19,26,27,28	0
22	LMU	R	7014	35/35	0.77	0.36	-	9,26,40,44	0
19	CLA	3	3011	65/65	0.74	0.29	-	23,25,26,26	0
22	LMU	H	7030	35/35	0.68	0.36	-	16,29,46,50	0
19	CLA	3	3001	25/65	0.79	0.28	-	24,25,25,25	0
19	CLA	2	1307	25/65	0.72	0.50	-	29,30,31,31	0
22	LMU	K	7001	35/35	0.75	0.20	-	17,34,48,50	0
22	LMU	H	7032	35/35	0.81	0.31	-	8,25,36,45	0
19	CLA	A	1309	25/65	0.57	0.56	-	25,46,54,54	0
19	CLA	R	1144	57/65	0.76	0.25	-	24,27,28,28	0
19	CLA	4	4015	46/65	0.72	0.37	-	24,25,26,27	0
22	LMU	R	7007	35/35	0.85	0.24	-	8,21,40,41	0
19	CLA	K	1142	45/65	0.67	0.25	-	27,29,30,31	0
19	CLA	F	1305	53/65	0.68	0.36	-	22,23,25,25	0
19	CLA	4	1009	36/65	0.85	0.20	-	20,22,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	K	1143	50/65	0.77	0.26	-	24,27,28,28	0
19	CLA	2	2005	25/65	0.66	0.25	-	30,31,32,32	0
19	CLA	L	1148	55/65	0.74	0.31	-	21,25,26,27	0
19	CLA	2	2010	25/65	0.77	0.28	-	23,23,24,24	0
22	LMU	K	7042	35/35	0.73	0.24	-	13,23,42,43	0
19	CLA	1	1007	61/65	0.78	0.26	-	14,20,21,22	0
19	CLA	2	2006	65/65	0.77	0.38	-	18,23,24,25	0
19	CLA	1	1013	51/65	0.75	0.42	-	26,27,29,29	0
19	CLA	4	4007	52/65	0.70	0.29	-	22,26,27,28	0
22	LMU	E	7048	35/35	0.58	0.31	-	19,30,44,46	0
22	LMU	E	7037	35/35	0.69	0.22	-	8,21,40,40	0
19	CLA	2	4009	65/65	0.80	0.23	-	18,23,24,24	0
19	CLA	A	1141	65/65	0.71	0.27	-	28,30,31,32	0
22	LMU	C	7015	35/35	0.72	0.34	-	9,22,37,39	0
22	LMU	2	7046	35/35	0.66	0.29	-	4,27,42,42	0
22	LMU	R	7025	35/35	0.77	0.25	-	5,22,39,42	0
22	LMU	3	7003	35/35	0.75	0.20	-	8,25,41,41	0
19	CLA	1	1001	46/65	0.72	0.27	-	28,29,30,30	0
19	CLA	2	2013	50/65	0.74	0.27	-	20,22,24,26	0
19	CLA	A	1134	45/65	0.73	0.26	-	22,26,27,28	0
19	CLA	2	2011	25/65	0.71	0.31	-	24,25,25,25	0
19	CLA	3	2009	56/65	0.78	0.23	-	13,35,50,50	0
19	CLA	4	4002	52/65	0.82	0.21	-	21,22,24,25	0
22	LMU	4	7034	35/35	0.73	0.28	-	14,30,42,47	0
19	CLA	3	1118	36/65	0.62	0.33	-	28,29,30,30	0
22	LMU	K	7041	35/35	0.72	0.24	-	15,31,45,45	0
22	LMU	4	7052	35/35	0.65	0.26	-	18,30,48,75	0
19	CLA	1	1014	61/65	0.72	0.27	-	3,31,46,46	0
19	CLA	3	3015	25/65	0.72	0.42	-	28,28,29,29	0
22	LMU	1	7013	35/35	0.56	0.33	-	15,34,47,48	0
19	CLA	2	2008	25/65	0.72	0.22	-	24,24,25,25	0
19	CLA	4	4014	47/65	0.65	0.28	-	21,35,46,48	0
19	CLA	A	1110	54/65	0.81	0.25	-	19,22,23,23	0
22	LMU	R	7024	35/35	0.77	0.20	-	6,19,32,40	0
19	CLA	J	1308	55/65	0.80	0.23	-	12,30,44,45	0
22	LMU	D	7050	35/35	0.76	0.23	-	14,31,46,46	0
19	CLA	1	1010	46/65	0.69	0.26	-	24,25,26,27	0
22	LMU	B	7038	35/35	0.66	0.42	-	13,35,48,48	0
22	LMU	A	7010	35/35	0.64	0.32	-	16,38,45,48	0
22	LMU	F	7036	34/35	0.76	0.30	-	19,32,42,45	0
19	CLA	2	2002	56/65	0.78	0.23	-	21,22,25,25	0
22	LMU	4	7053	34/35	0.58	0.30	-	21,41,47,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	CLA	2	2001	51/65	0.66	0.26	-	27,28,29,29	0
21	BCR	1	6023	40/40	0.61	0.40	-	21,28,29,30	0
22	LMU	4	7009	34/35	0.73	0.26	-	22,44,50,50	0
19	CLA	3	3006	25/65	0.75	0.21	-	26,27,28,28	0
19	CLA	3	3014	25/65	0.53	0.52	-	31,31,32,32	0
19	CLA	3	3016	65/65	0.64	0.47	-	23,26,29,31	0
19	CLA	3	3012	25/65	0.57	0.28	-	30,31,31,31	0
19	CLA	2	2003	25/65	0.77	0.38	-	23,24,25,25	0
19	CLA	1	1310	25/65	0.69	0.31	-	27,28,28,28	0
22	LMU	G	7026	35/35	0.75	0.30	-	12,35,46,51	0
19	CLA	3	3008	50/65	0.74	0.35	-	20,26,27,27	0
22	LMU	G	7051	35/35	0.71	0.27	-	20,32,43,44	0
22	LMU	H	7017	35/35	0.74	0.21	-	8,23,39,41	0
22	LMU	H	7011	35/35	0.67	0.27	-	17,32,38,43	0
22	LMU	2	7006	35/35	0.76	0.22	-	22,25,26,27	0
22	LMU	R	7020	35/35	0.77	0.23	-	7,26,40,44	0
22	LMU	4	7019	35/35	0.75	0.22	-	11,25,40,43	0
19	CLA	H	1241	55/65	0.72	0.26	-	23,25,26,26	0
19	CLA	B	1233	51/65	0.66	0.39	-	24,27,27,28	0
22	LMU	N	7049	35/35	0.67	0.29	-	15,28,40,41	0
19	CLA	A	1149	46/65	0.76	0.31	-	22,25,25,25	0
19	CLA	4	4013	25/65	0.83	0.19	-	20,21,21,21	0
22	LMU	B	7040	35/35	0.69	0.22	-	12,26,40,43	0

6.5 Other polymers

There are no such residues in this entry.