



# wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 01:15 PM JST

PDB ID : 3J3W  
EMDB ID : EMD-5643  
Title : Atomic model of the immature 50S subunit from *Bacillus subtilis* (state II-a)  
Authors : Li, N.; Guo, Q.; Zhang, Y.; Yuan, Y.; Ma, C.; Lei, J.; Gao, N.  
Deposited on : 2013-04-28  
Resolution : 10.70 Å (reported)  
Based on initial models : 2AW4, 2J01

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

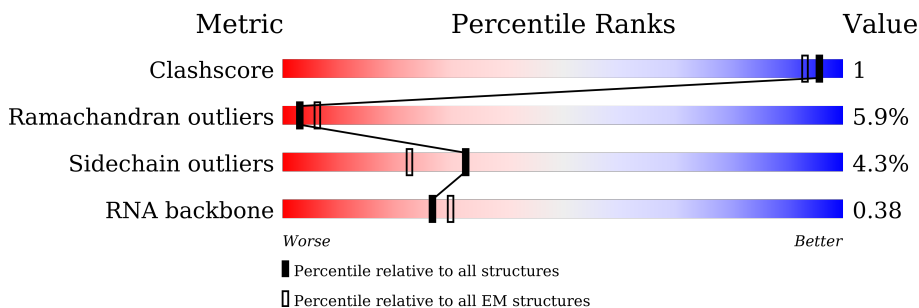
EMDB validation analysis : 0.0.1.dev70  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.70 Å.

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




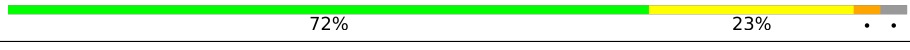
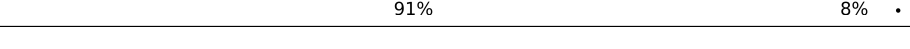

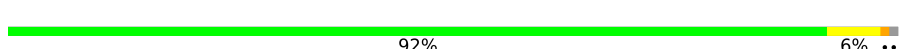


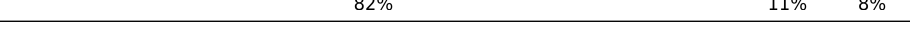

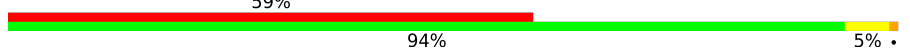



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2927	53% 32% 7% 8%
2	0	59	83% 10% 7%
3	C	277	88% 12%
4	N	120	96% .
5	G	179	84% 7% 9%
6	J	145	87% 10% ..
7	K	122	93% 7%

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Mol	Chain	Length	Quality of chain
8	L	146	 88% 10%
9	P	115	 72% 23%
10	Q	119	 91% 8%
11	D	209	 91% 6%
12	R	102	 88% 11%
13	S	113	 92% 6%
14	T	95	 86% 13%
15	U	103	 83% 17%
16	X	66	 82% 11% 8%
17	2	44	 91% 9%
18	5	232	 48% 48%
19	6	141	 59% 94% 5%
20	E	207	 86% 13%

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 76573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called ribosome RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2685	57639	25720	10638	18600	2681	0	0

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	0	55	433	267	87	72	7	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	277	2129	1323	419	380	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	120	962	588	187	182	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	163	1246	776	226	242	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	143	1134	717	207	204	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	122	921	571	173	173	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	146	1082	671	207	202	2	0	0

- Molecule 9 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	P	112	916	584	178	154	0	0

- Molecule 10 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	117	940	591	189	156	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	206	1568	984	289	290	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	R	102	795	506	140	148	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	S	112	868	541	168	155	4	0	0

- Molecule 14 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	95	Total	C	N	O	S	0	0
			767	480	139	144	4		

- Molecule 15 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	103	Total	C	N	O	S	0	0
			780	488	145	143	4		

- Molecule 16 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	61	Total	C	N	O	S	0	0
			504	312	97	93	2		

- Molecule 17 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 18 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	120	Total	C	N	O	S	0	0
			910	576	156	176	2		

- Molecule 19 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	141	Total	C	N	O	S	0	0
			1044	657	184	196	7		

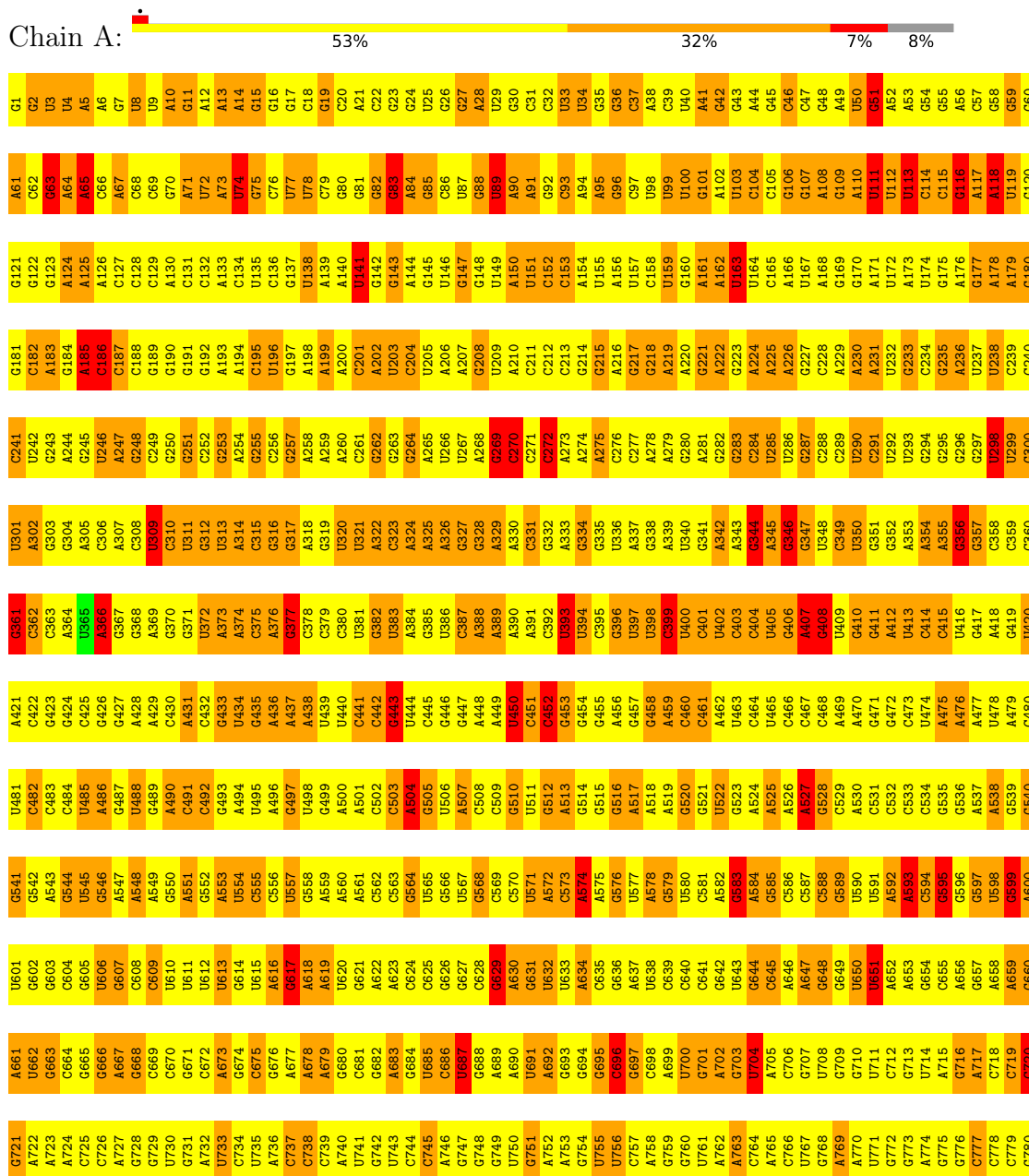
- Molecule 20 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

### 3 Residue-property plots i

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

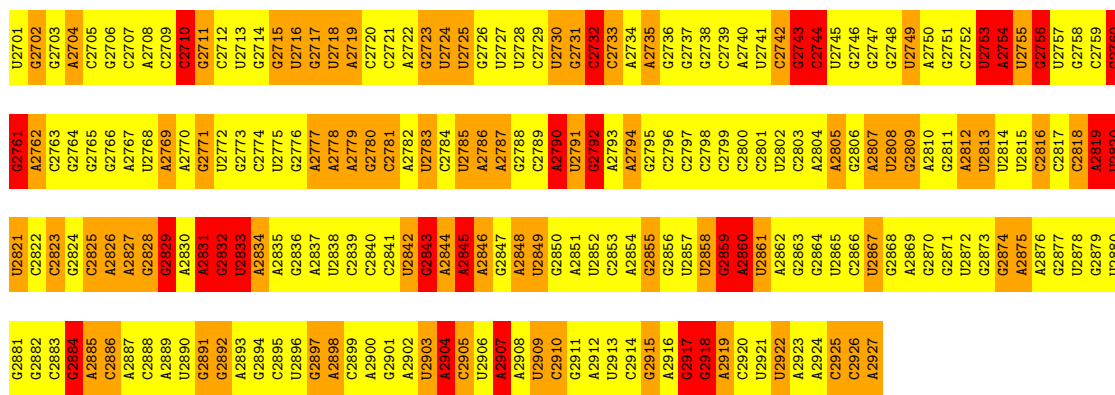
- Molecule 1: ribosome RNA 23S



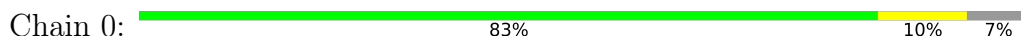
A1681	C1622	G1623	U1621	C1261	A1201	A1141	U1081	A1021	C961	U901	A841	A781
C1662	G1663	U1661	C1262	A1202	A1142	U1082	A1022	C962	G902	A842	C842	C782
C1663	G1664	U1662	G1263	A1203	A1143	U1083	G1023	G963	G903	C843	C783	C784
C1664	G1665	U1663	G1264	A1204	A1144	U1084	G1024	G964	A904	C844	C784	C785
C1665	G1666	U1664	A1265	U1205	G1145	U1085	A1025	A965	G905	C845	C785	C786
C1666	G1667	U1665	G1266	A1206	A1146	U1086	A1026	A966	G906	C846	C786	C787
C1667	G1668	U1666	G1267	C1207	U1147	U1087	A1027	G967	U907	C847	C787	C788
C1668	G1669	U1667	G1268	U1208	A1148	U1088	C1028	C968	A908	C848	C788	C789
C1669	G1670	U1668	G1269	A1209	A1149	U1089	A1029	C969	G909	C849	C789	C790
C1670	G1671	U1669	C1270	C1210	C1150	U1090	A1030	A970	A910	C850	C790	C791
C1671	G1672	U1670	U1271	U1211	C1151	U1091	C1031	A971	G911	C851	C791	C792
C1672	G1673	U1671	G1272	U1212	G1152	A1092	C1032	G972	A912	C852	C792	C793
C1673	G1674	U1672	G1273	C1213	G1153	U1093	C1033	G973	C913	C853	C793	C794
C1674	G1675	U1673	U1274	U1214	U1154	A1094	A1034	A974	C914	C854	C794	C795
C1675	G1676	U1674	G1275	U1215	C1155	C1095	A1035	C975	U915	C855	C795	C796
C1676	G1677	U1675	G1276	C1216	G1156	U1096	A1036	U976	G916	C856	C796	C797
C1677	G1678	U1676	A1277	U1217	A1157	U1097	C1037	U977	A917	C857	C797	C798
C1678	G1679	U1677	G1278	U1218	G1158	U1098	A1038	A978	U918	C858	C798	C799
C1679	G1680	U1678	U1279	C1219	U1159	C1099	G1039	U979	U919	C859	C799	C800
C1680	G1681	U1679	G1280	G1220	A1160	A1100	C1040	C980	G920	U860	C800	C801
C1681	G1682	U1680	U1281	A1221	C1161	G1101	A1041	C981	G921	U861	C801	C802
C1682	G1683	U1681	G1282	A1222	G1162	U1102	A1042	U862	A922	C862	C802	C803
C1683	G1684	U1682	U1283	C1223	U1163	A1103	G1043	U863	C923	C863	C803	C804
C1684	G1685	U1683	A1284	A1224	C1164	U1104	A1044	G984	U924	C864	C804	C805
C1685	G1686	U1684	G1285	U1225	U1165	U1105	U1045	G985	A925	C865	C805	C806
C1686	G1687	U1685	A1286	U1226	G1166	U1106	A1046	G986	G926	A866	C806	C807
C1687	G1688	U1686	G1287	G1227	C1167	U1107	A1047	A987	G927	A867	C807	C808
C1688	G1689	U1687	U1288	G1228	G1168	U1108	G1048	G988	G928	A868	C808	C809
C1689	G1690	U1688	G1289	U1229	C1169	U1109	A1049	U989	G929	A869	C809	C810
C1690	G1691	U1689	U1290	A1230	U1170	G1110	U1050	C990	C930	A870	C810	C811
C1691	G1692	U1690	A1291	U1231	G1171	U1111	C1051	A991	G931	C871	C811	C812
C1692	G1693	U1691	G1292	G1232	A1172	U1112	C1052	G992	C932	C872	C812	C813
C1693	G1694	U1692	U1293	A1233	U1173	U1113	C1053	A993	C933	C873	C813	C814
C1694	G1695	U1693	A1294	G1234	A1174	G1114	A1054	C994	C934	C874	C814	C815
C1695	G1696	U1694	U1295	A1235	U1175	A1115	A1055	U995	U935	C875	C815	C816
C1696	G1697	U1695	G1296	G1236	U1176	U1116	A1056	G996	A936	A876	C816	C817
C1697	G1698	U1696	U1297	C1237	G1177	U1117	C1057	C997	C936	C877	C817	C818
C1698	G1699	U1697	G1298	U1238	U1178	C1118	U1058	G998	C937	C878	C818	C819
C1699	G1700	U1698	U1299	G1239	A1179	U1119	A1059	A999	G937	C879	C819	C820
C1700	G1701	U1699	G1300	U1240	C1180	U1120	C1060	G1000	G938	C880	C820	C821
C1701	G1702	U1700	U1301	A1241	C1181	G1121	A1061	U1001	G939	C881	C821	C822
C1702	G1703	U1701	G1302	U1242	U1182	C1122	C1062	G1002	G940	C882	C822	C823
C1703	G1704	U1702	U1303	A1243	G1183	A1123	G1063	U1003	U941	C883	C823	C824
C1704	G1705	U1703	G1304	U1244	U1184	C1124	U1064	U1004	A942	C884	C824	C825
C1705	G1706	U1704	A1305	G1245	G1185	C1125	U1065	A1005	A943	C885	C825	C826
C1706	G1707	U1705	G1306	U1246	U1186	U1126	A1066	A1006	C944	C886	C826	C827
C1707	G1708	U1706	U1307	G1247	U1187	U1127	A1067	G1007	C945	C887	C827	C828
C1708	G1709	U1707	A1308	U1248	C1188	U1128	C1068	A1008	G946	C888	C828	C829
C1709	G1710	U1708	G1309	U1249	A1189	U1129	U1069	U1009	A947	C889	C829	C830
C1710	G1711	U1709	C1310	G1250	C1190	A1130	G1070	C1010	A948	C890	C830	C831
C1711	G1712	U1710	G1311	U1251	C1191	A1131	G1071	C1011	U949	C891	C831	C832
C1712	G1713	U1711	A1312	G1252	U1192	A1132	A1072	C1012	U949	C892	C832	C833
C1713	G1714	U1712	U1313	C1253	U1193	G1133	A1073	G1013	U950	C893	C833	C834
C1714	G1715	U1713	A1314	A1254	A1194	A1074	A1074	A1014	C951	C894	C834	C835
C1715	G1716	U1714	G1315	U1255	U1195	A1075	A1075	G1015	A952	C895	C835	C836
C1716	G1717	U1715	A1316	C1256	C1196	U1136	G1076	U1016	U954	C896	C836	C837
C1717	G1718	U1716	G1317	U1257	A1197	G1137	G1077	C1017	C955	C897	C837	C838
C1718	G1719	U1717	U1318	A1258	C1198	U1138	A1078	G1018	A956	C898	C838	C839
C1719	G1720	U1718	G1319	U1259	U1199	C1139	U1079	A1019	C957	C899	C839	C840
C1720	G1721	U1719	U1320	G1260	A1260	U1200	U1080	A1020	A958	C959	C840	C841
C1721	G1722	U1720	C1321	U1261	C1171	U1111	C1081	G981	C959	C960	C841	C842



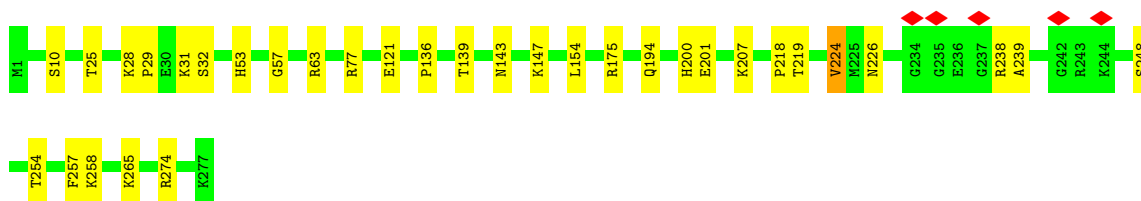
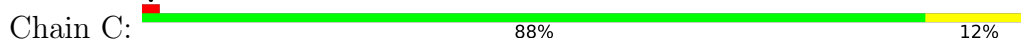




• Molecule 2: 50S ribosomal protein L32



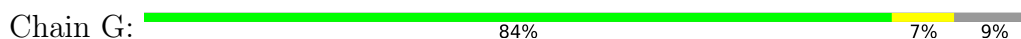
• Molecule 3: 50S ribosomal protein L2



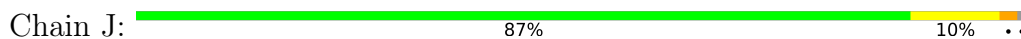
• Molecule 4: 50S ribosomal protein L17



• Molecule 5: 50S ribosomal protein L6



• Molecule 6: 50S ribosomal protein L13




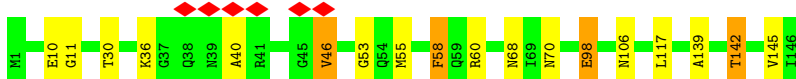
- Molecule 7: 50S ribosomal protein L14

Chain K:  93% 7%



- Molecule 8: 50S ribosomal protein L15

Chain L:  88% 10%



- Molecule 9: 50S ribosomal protein L19

Chain P:  72% 23%



- Molecule 10: 50S ribosomal protein L20

Chain Q:  91% 8%




- Molecule 11: 50S ribosomal protein L3

Chain D:  91% 6%




- Molecule 12: 50S ribosomal protein L21

Chain R:  88% 11%

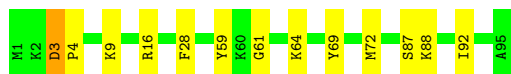
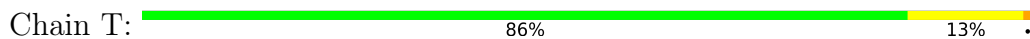


- Molecule 13: 50S ribosomal protein L22

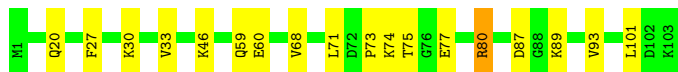
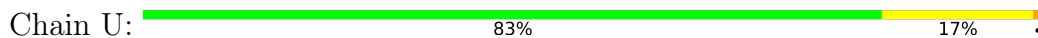
Chain S:  92% 6%



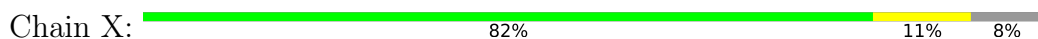
• Molecule 14: 50S ribosomal protein L23



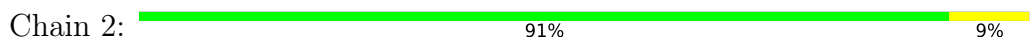
• Molecule 15: 50S ribosomal protein L24



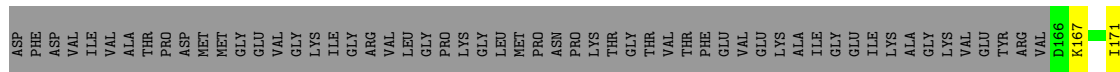
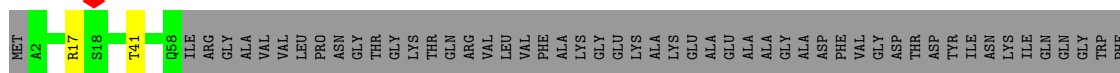
• Molecule 16: 50S ribosomal protein L29



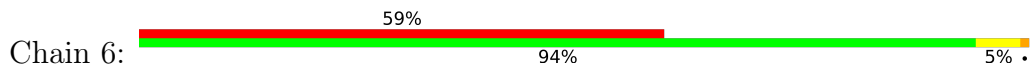
• Molecule 17: 50S ribosomal protein L34

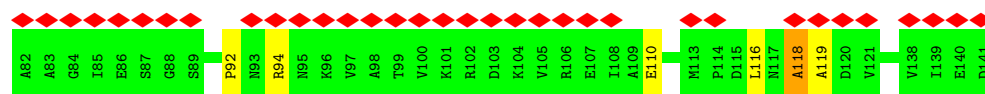


• Molecule 18: 50S ribosomal protein L1



• Molecule 19: 50S ribosomal protein L11





- Molecule 20: 50S ribosomal protein L4

Chain E: 86% 13%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27652	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	10.909	Depositor
Minimum map value	-3.262	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size ( $\text{\AA}$ )	384.0, 384.0, 384.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.5, 1.5, 1.5	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	1.68	83/64560 (0.1%)	2.67	8132/100715 (8.1%)
2	O	1.04	0/440	1.20	2/584 (0.3%)
3	C	1.00	0/2166	1.09	0/2902
4	N	1.09	0/969	1.05	0/1294
5	G	0.97	0/1264	1.04	0/1709
6	J	0.95	0/1157	1.08	2/1557 (0.1%)
7	K	1.02	0/928	1.05	0/1245
8	L	0.97	0/1094	1.10	2/1457 (0.1%)
9	P	1.10	0/929	1.17	2/1243 (0.2%)
10	Q	1.05	0/952	1.06	2/1266 (0.2%)
11	D	0.96	0/1590	1.09	2/2130 (0.1%)
12	R	0.92	0/806	1.13	1/1080 (0.1%)
13	S	1.01	0/877	1.10	0/1179
14	T	1.01	0/774	1.15	2/1030 (0.2%)
15	U	0.87	0/790	1.16	3/1054 (0.3%)
16	X	1.04	0/505	1.01	0/671
17	2	1.26	0/371	1.04	0/483
18	5	0.87	0/921	1.05	2/1239 (0.2%)
19	6	0.92	0/1058	1.06	1/1427 (0.1%)
20	E	0.97	0/1586	1.10	1/2139 (0.0%)
All	All	1.55	83/83737 (0.1%)	2.43	8154/126404 (6.5%)

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	320
4	N	0	1
8	L	0	2
9	P	0	2
14	T	0	2

*Continued on next page...*

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	U	0	1
20	E	0	2
All	All	0	330

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1339	A	O3'-P	-7.12	1.52	1.61
1	A	1831	A	N7-C5	-6.74	1.35	1.39
1	A	52	A	N7-C5	-6.72	1.35	1.39
1	A	653	A	N7-C5	-6.68	1.35	1.39
1	A	1839	A	N7-C5	-6.64	1.35	1.39

The worst 5 of 8154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1339	A	P-O3'-C3'	34.26	160.81	119.70
1	A	313	U	P-O3'-C3'	20.76	144.62	119.70
1	A	178	A	P-O3'-C3'	20.05	143.75	119.70
1	A	74	U	P-O3'-C3'	19.98	143.68	119.70
1	A	375	C	P-O3'-C3'	19.92	143.60	119.70

There are no chirality outliers.

5 of 330 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	G	Sidechain
1	A	27	G	Sidechain
1	A	28	A	Sidechain
1	A	33	U	Sidechain
1	A	5	A	Sidechain

## 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	57639	0	29016	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	433	0	454	0	0
3	C	2129	0	2225	4	0
4	N	962	0	995	0	0
5	G	1246	0	1273	2	0
6	J	1134	0	1178	0	0
7	K	921	0	977	0	0
8	L	1082	0	1132	0	0
9	P	916	0	987	5	0
10	Q	940	0	1005	0	0
11	D	1568	0	1635	0	0
12	R	795	0	838	0	0
13	S	868	0	930	0	0
14	T	767	0	813	2	0
15	U	780	0	838	0	0
16	X	504	0	541	1	0
17	2	368	0	410	1	0
18	5	910	0	944	0	0
19	6	1044	0	1098	1	0
20	E	1567	0	1652	1	0
All	All	76573	0	48941	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 116 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1245:G:H1	1:A:1281:C:H41	1.25	0.84
1:A:898:U:H3	1:A:973:G:H1	1.41	0.68
1:A:2557:U:H3	1:A:2564:A:H61	1.41	0.68
1:A:1799:G:H1	1:A:2011:U:H3	1.46	0.63
1:A:2543:U:H3	1:A:2599:G:H1	1.48	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0	53/59 (90%)	43 (81%)	6 (11%)	4 (8%)	1	13
3	C	275/277 (99%)	217 (79%)	40 (14%)	18 (6%)	1	16
4	N	118/120 (98%)	101 (86%)	14 (12%)	3 (2%)	5	32
5	G	161/179 (90%)	148 (92%)	7 (4%)	6 (4%)	3	24
6	J	141/145 (97%)	124 (88%)	9 (6%)	8 (6%)	1	18
7	K	120/122 (98%)	106 (88%)	9 (8%)	5 (4%)	3	22
8	L	144/146 (99%)	100 (69%)	30 (21%)	14 (10%)	0	10
9	P	110/115 (96%)	76 (69%)	20 (18%)	14 (13%)	0	5
10	Q	115/119 (97%)	101 (88%)	9 (8%)	5 (4%)	2	22
11	D	204/209 (98%)	175 (86%)	21 (10%)	8 (4%)	3	23
12	R	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	1	17
13	S	110/113 (97%)	97 (88%)	10 (9%)	3 (3%)	5	31
14	T	93/95 (98%)	77 (83%)	11 (12%)	5 (5%)	2	19
15	U	101/103 (98%)	70 (69%)	20 (20%)	11 (11%)	0	8
16	X	59/66 (89%)	55 (93%)	2 (3%)	2 (3%)	3	26
17	2	42/44 (96%)	37 (88%)	4 (10%)	1 (2%)	6	33
18	5	116/232 (50%)	97 (84%)	13 (11%)	6 (5%)	2	19
19	6	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3	25
20	E	204/207 (99%)	161 (79%)	25 (12%)	18 (9%)	1	11
All	All	2405/2594 (93%)	1981 (82%)	282 (12%)	142 (6%)	3	17

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	0	19	HIS
3	C	219	THR

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Mol	Chain	Res	Type
7	K	30	ARG
7	K	73	ASP
8	L	117	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	0	49/53 (92%)	48 (98%)	1 (2%)	55	74
3	C	225/225 (100%)	215 (96%)	10 (4%)	28	53
4	N	100/100 (100%)	99 (99%)	1 (1%)	76	86
5	G	138/151 (91%)	135 (98%)	3 (2%)	52	71
6	J	122/123 (99%)	111 (91%)	11 (9%)	9	30
7	K	101/101 (100%)	98 (97%)	3 (3%)	41	63
8	L	110/110 (100%)	105 (96%)	5 (4%)	27	52
9	P	97/100 (97%)	90 (93%)	7 (7%)	14	39
10	Q	96/98 (98%)	93 (97%)	3 (3%)	40	62
11	D	167/170 (98%)	159 (95%)	8 (5%)	25	51
12	R	84/84 (100%)	78 (93%)	6 (7%)	14	39
13	S	93/93 (100%)	87 (94%)	6 (6%)	17	42
14	T	85/85 (100%)	82 (96%)	3 (4%)	36	59
15	U	87/87 (100%)	82 (94%)	5 (6%)	20	45
16	X	54/57 (95%)	50 (93%)	4 (7%)	13	38
17	2	39/39 (100%)	37 (95%)	2 (5%)	24	48
18	5	98/185 (53%)	97 (99%)	1 (1%)	76	86
19	6	110/110 (100%)	109 (99%)	1 (1%)	78	87
20	E	169/170 (99%)	162 (96%)	7 (4%)	30	55
All	All	2024/2141 (94%)	1937 (96%)	87 (4%)	33	53

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	R	98	GLU
15	U	101	LEU
13	S	20	VAL
14	T	64	LYS
16	X	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
20	E	169	ASN
19	6	34	ASN
13	S	57	ASN
18	5	172	HIS
12	R	90	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2681/2927 (91%)	823 (30%)	200 (7%)

5 of 823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	8	U
1	A	10	A

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1590	C
1	A	2050	G
1	A	2918	G
1	A	1606	A
1	A	1711	G

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

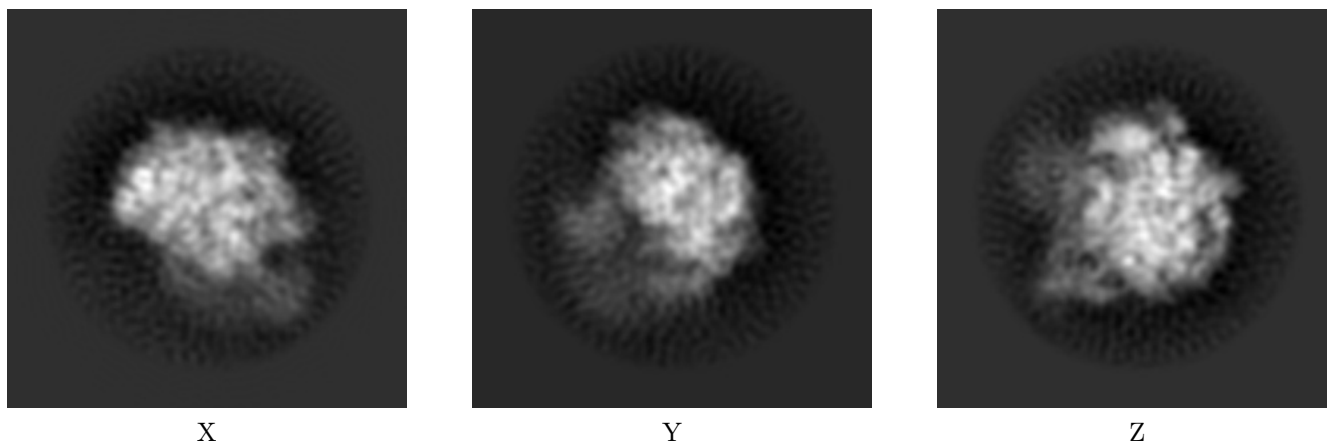
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5643. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

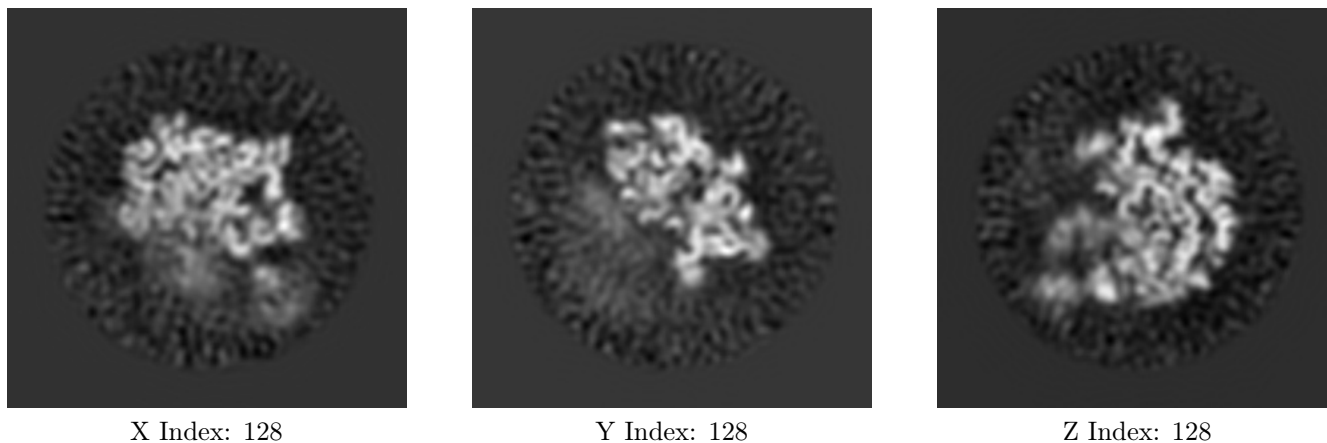
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

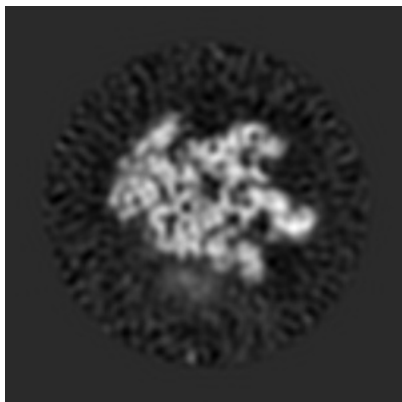
#### 6.2.1 Primary map



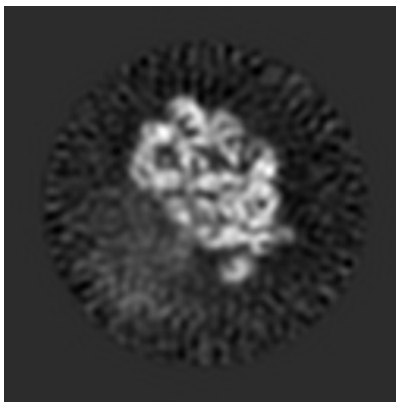
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

### 6.3.1 Primary map



X Index: 140



Y Index: 139

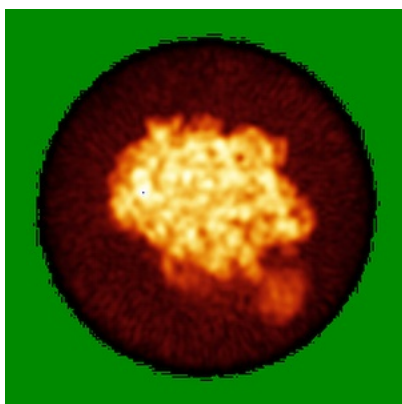


Z Index: 148

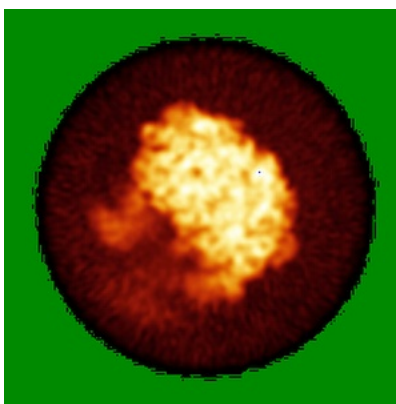
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

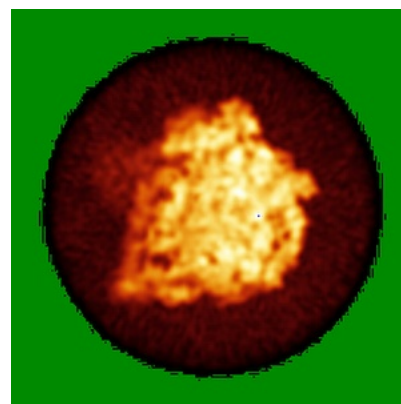
### 6.4.1 Primary map



X



Y

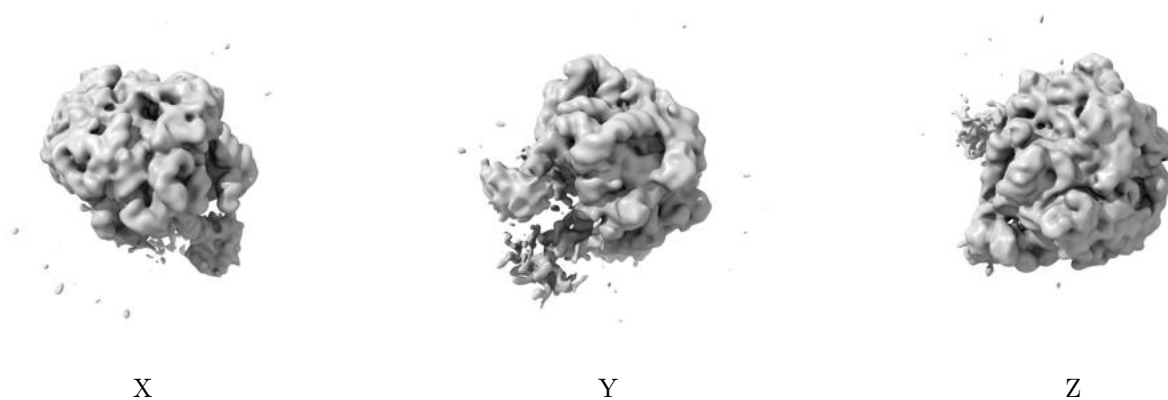


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

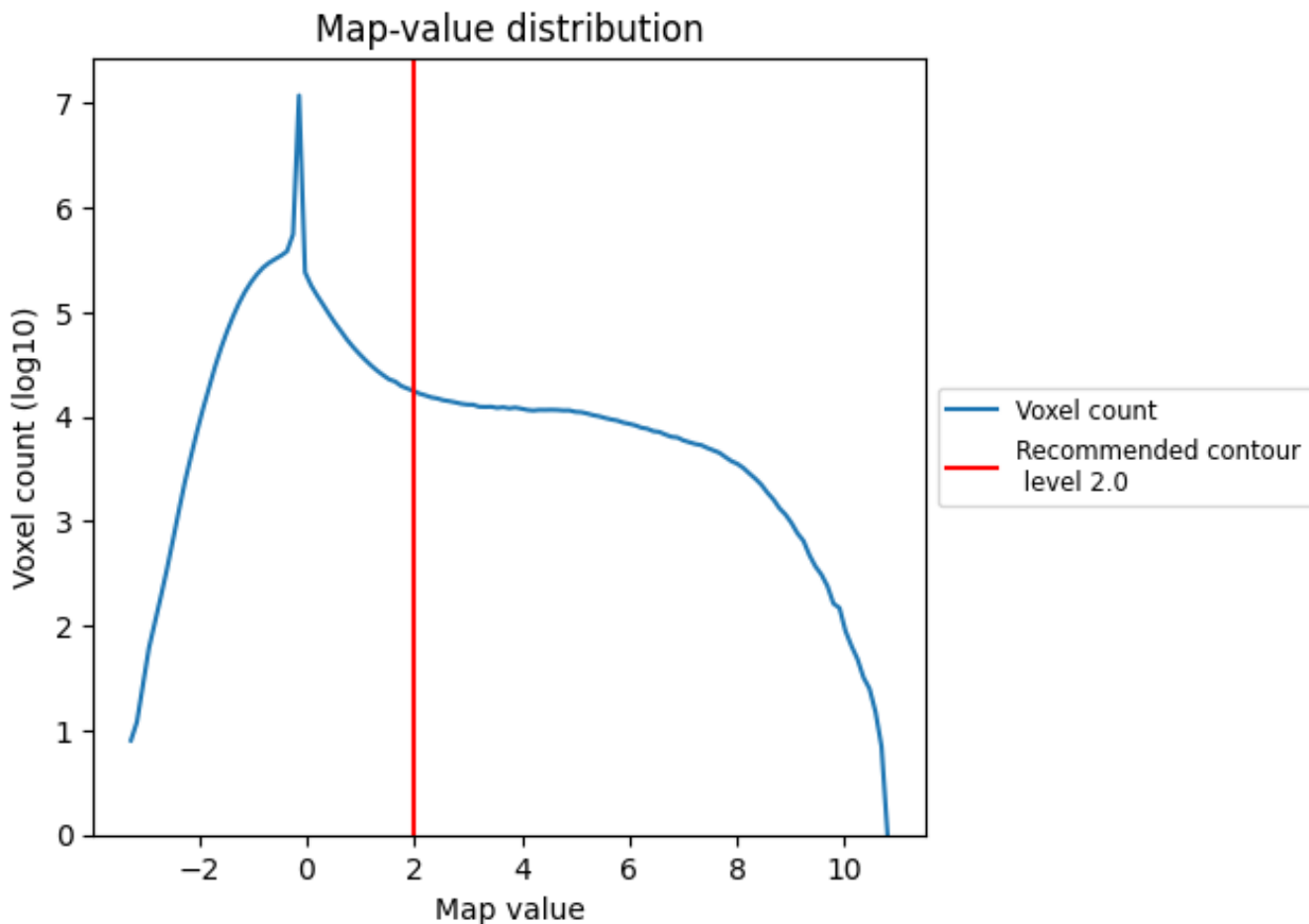
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

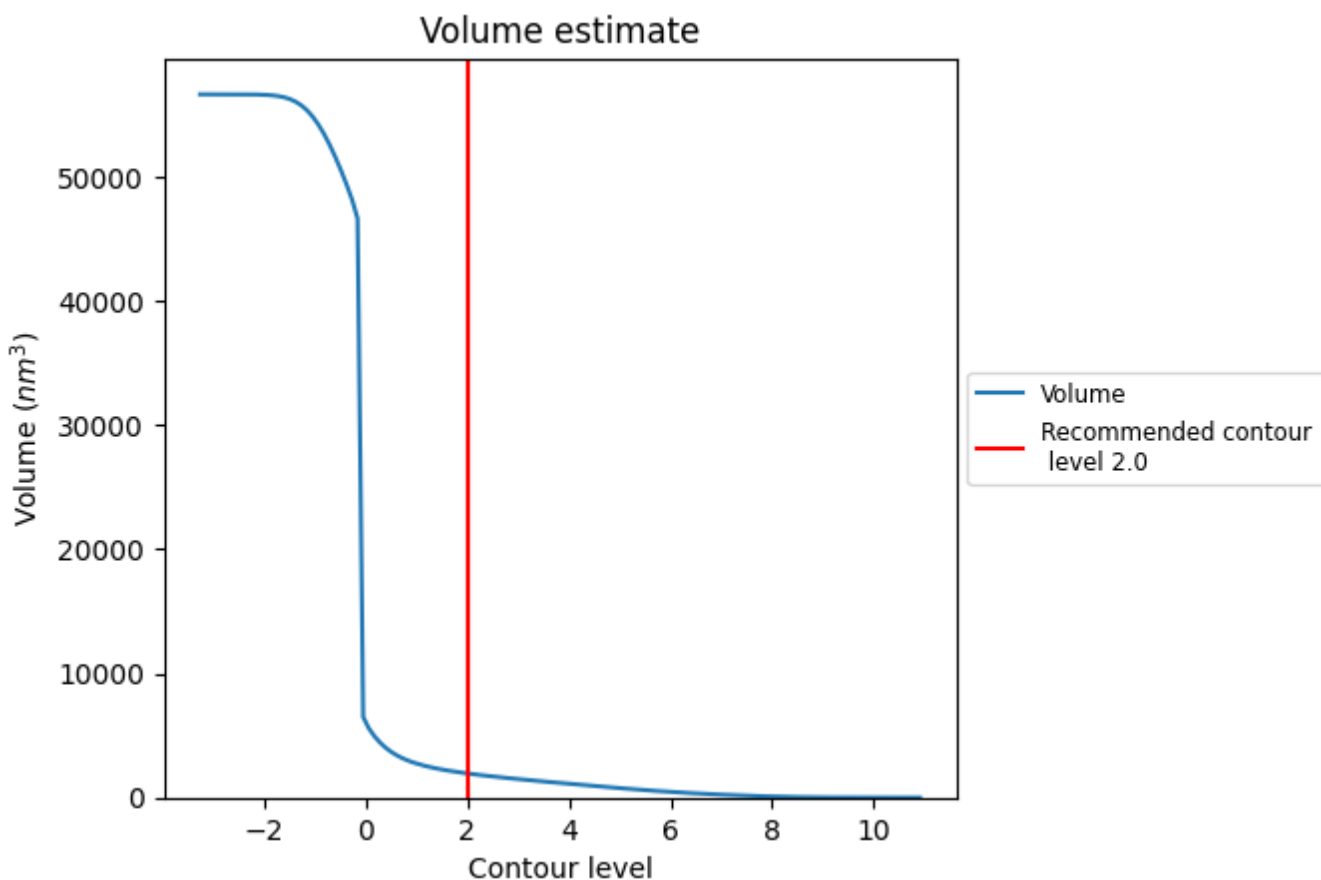
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

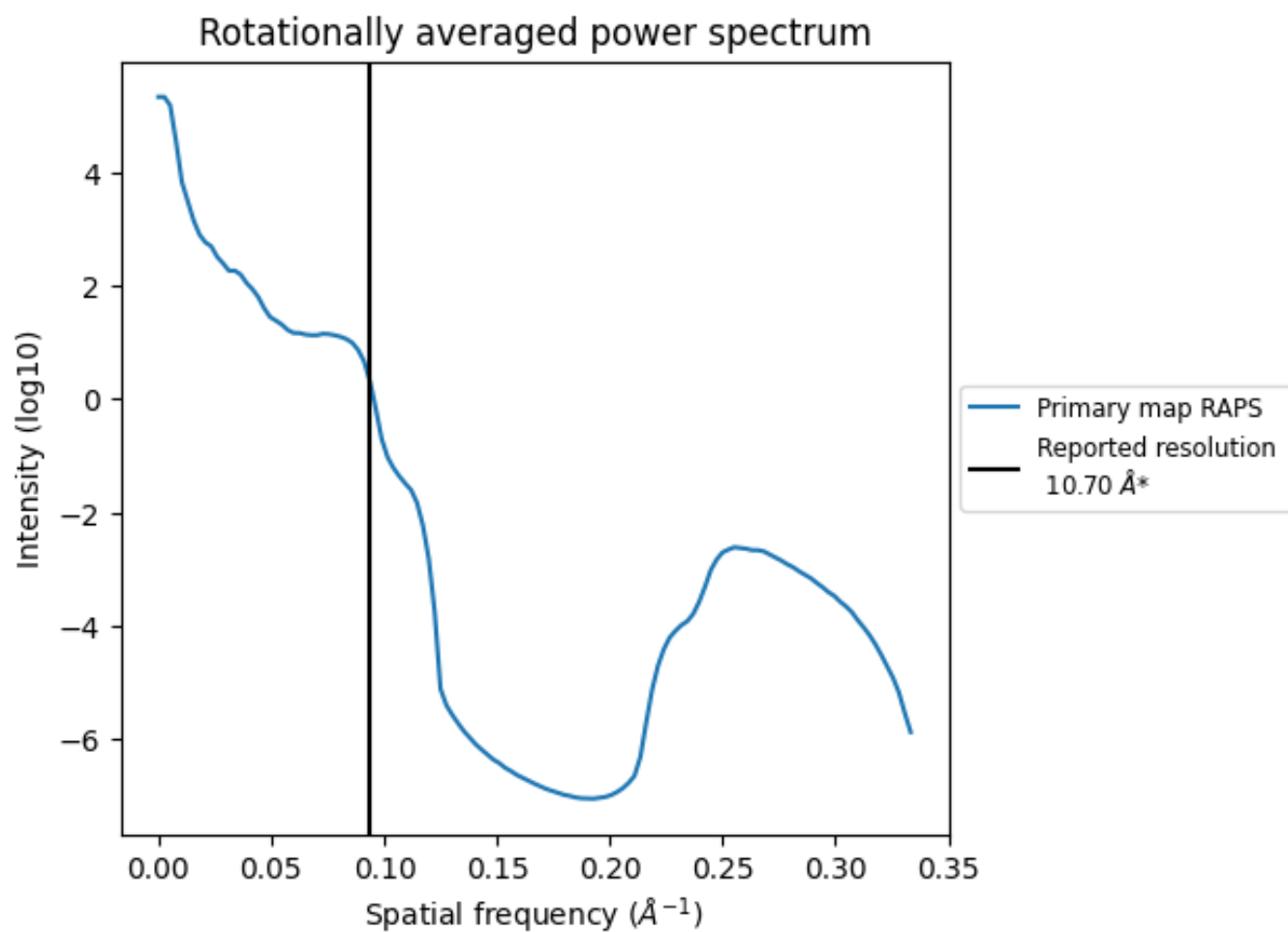
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1942 nm<sup>3</sup>; this corresponds to an approximate mass of 1754 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.093 Å<sup>-1</sup>

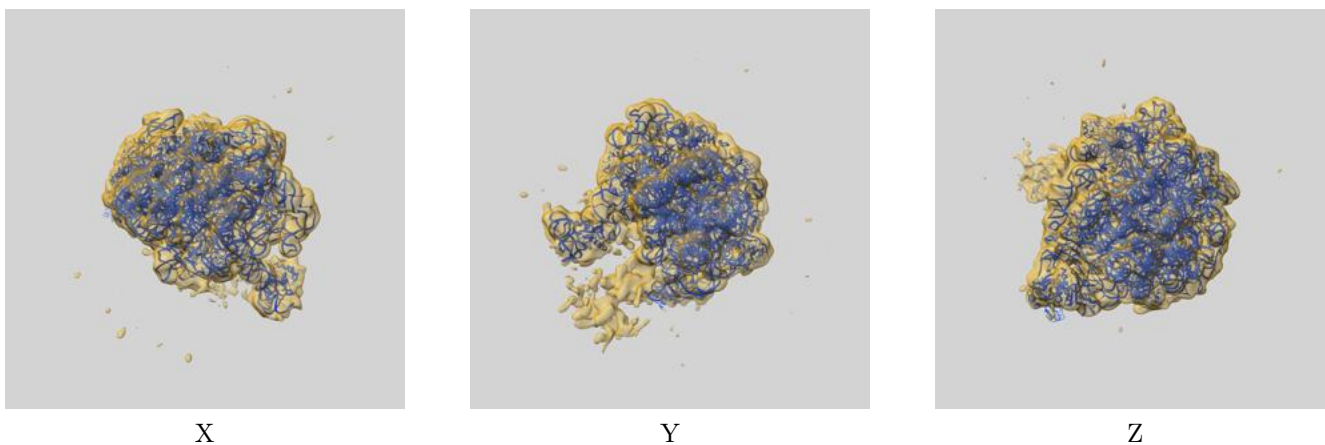
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

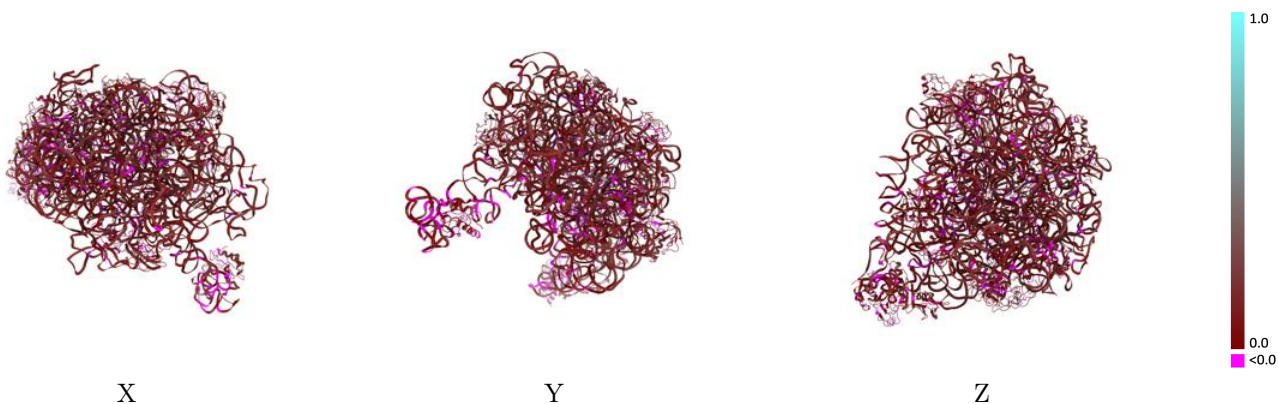
This section contains information regarding the fit between EMDB map EMD-5643 and PDB model 3J3W. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlay [i](#)



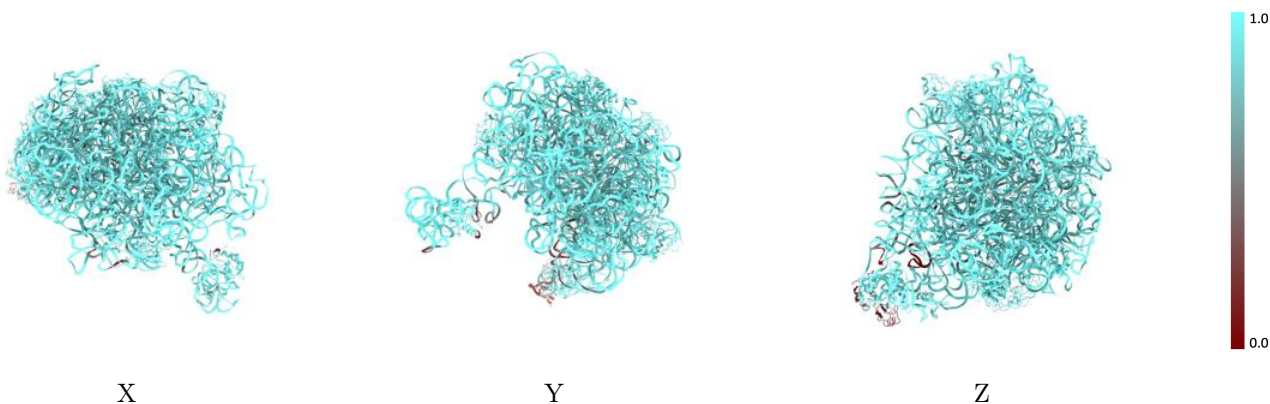
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



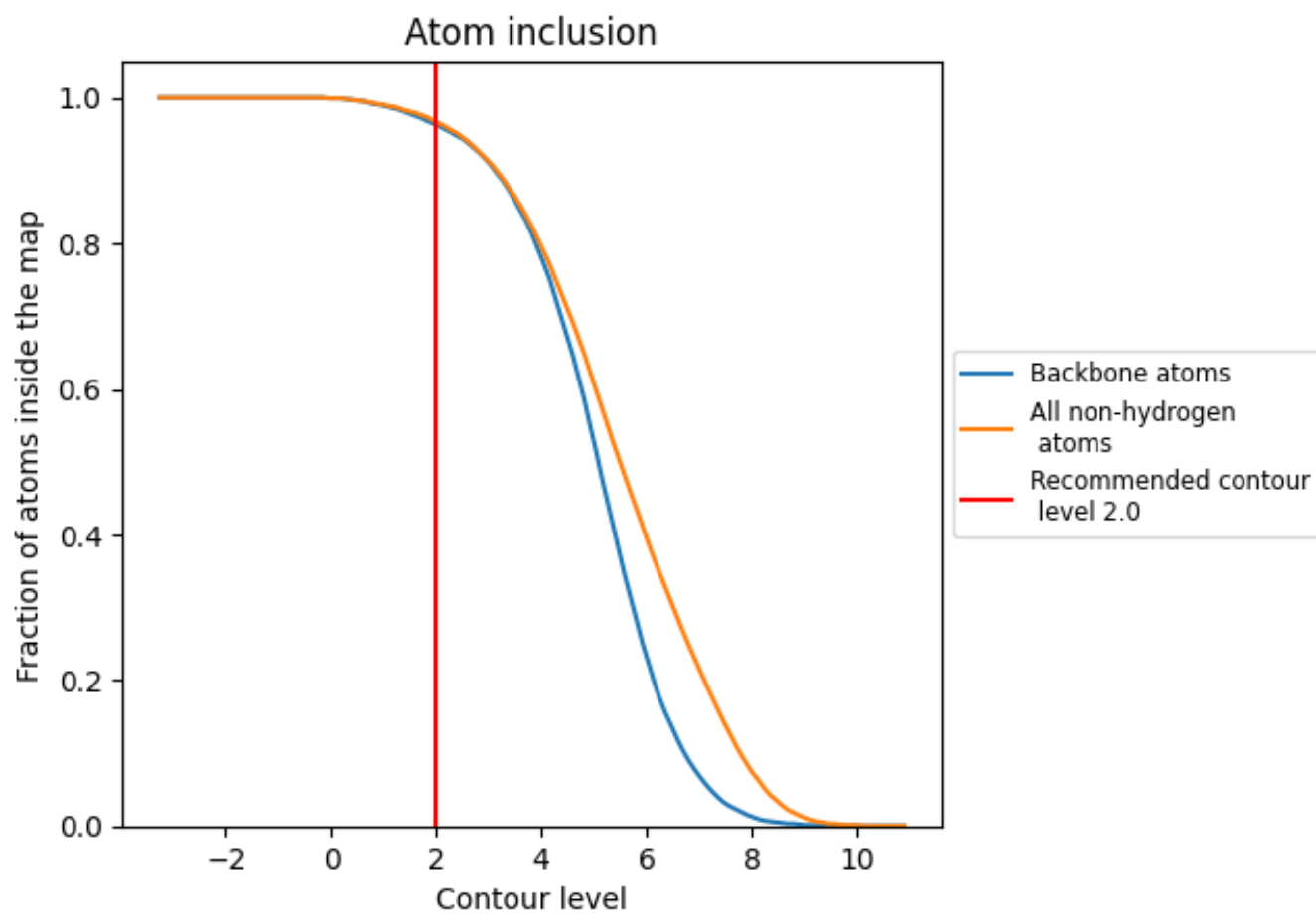
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.0).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9670	 0.1190
0	 0.9950	 0.0450
2	 0.9940	 0.0670
5	 0.9410	 0.0570
6	 0.3720	 0.0390
A	 0.9730	 0.1310
C	 0.9740	 0.0650
D	 0.9890	 0.0800
E	 0.9770	 0.0850
G	 0.9850	 0.1250
J	 0.9940	 0.0970
K	 0.9960	 0.1000
L	 0.9470	 0.0560
N	 0.9940	 0.0700
P	 0.9890	 0.1030
Q	 0.9920	 0.0770
R	 0.9960	 0.0960
S	 0.9790	 0.0910
T	 0.9840	 0.0830
U	 0.9990	 0.0700
X	 0.9980	 0.1510

