



wwPDB EM Validation Summary Report ⓘ

Jul 3, 2024 – 08:32 am BST

PDB ID : 7OE1
EMDB ID : EMD-12857
Title : 30S ribosomal subunit from E. coli
Authors : Maksimova, E.; Korepanov, A.; Baymukhametov, T.; Kravchenko, O.; Stoboushkina, E.
Deposited on : 2021-04-30
Resolution : 3.05 Å(reported)
Based on initial model : 4V4Q

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

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev92
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) : 2.37.1

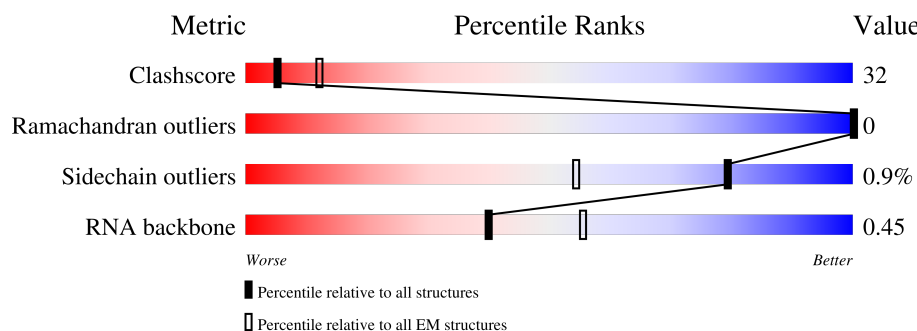
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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 ≥ 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	1542	
2	D	205	
3	E	166	
4	F	135	
5	H	129	
6	K	128	
7	L	123	

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Mol	Chain	Length	Quality of chain
8	O	89	
9	P	82	
10	Q	83	
11	R	74	
12	T	86	
13	B	240	
14	U	71	
15	C	232	
16	G	178	
17	I	129	
18	J	103	
19	M	117	
20	N	100	
21	S	91	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51092 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1530	Total	C	N	O	P	0	0
			32831	14642	6024	10635	1530		

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 4 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 5 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 6 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 7 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 8 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 9 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 10 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 11 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 13 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 14 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	U	18	Total	C	N	O	0	0
			148	94	28	26		

- Molecule 15 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	150	Total	C	N	O	S	0	0
			1174	730	226	214	4		

- Molecule 17 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 18 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 20 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

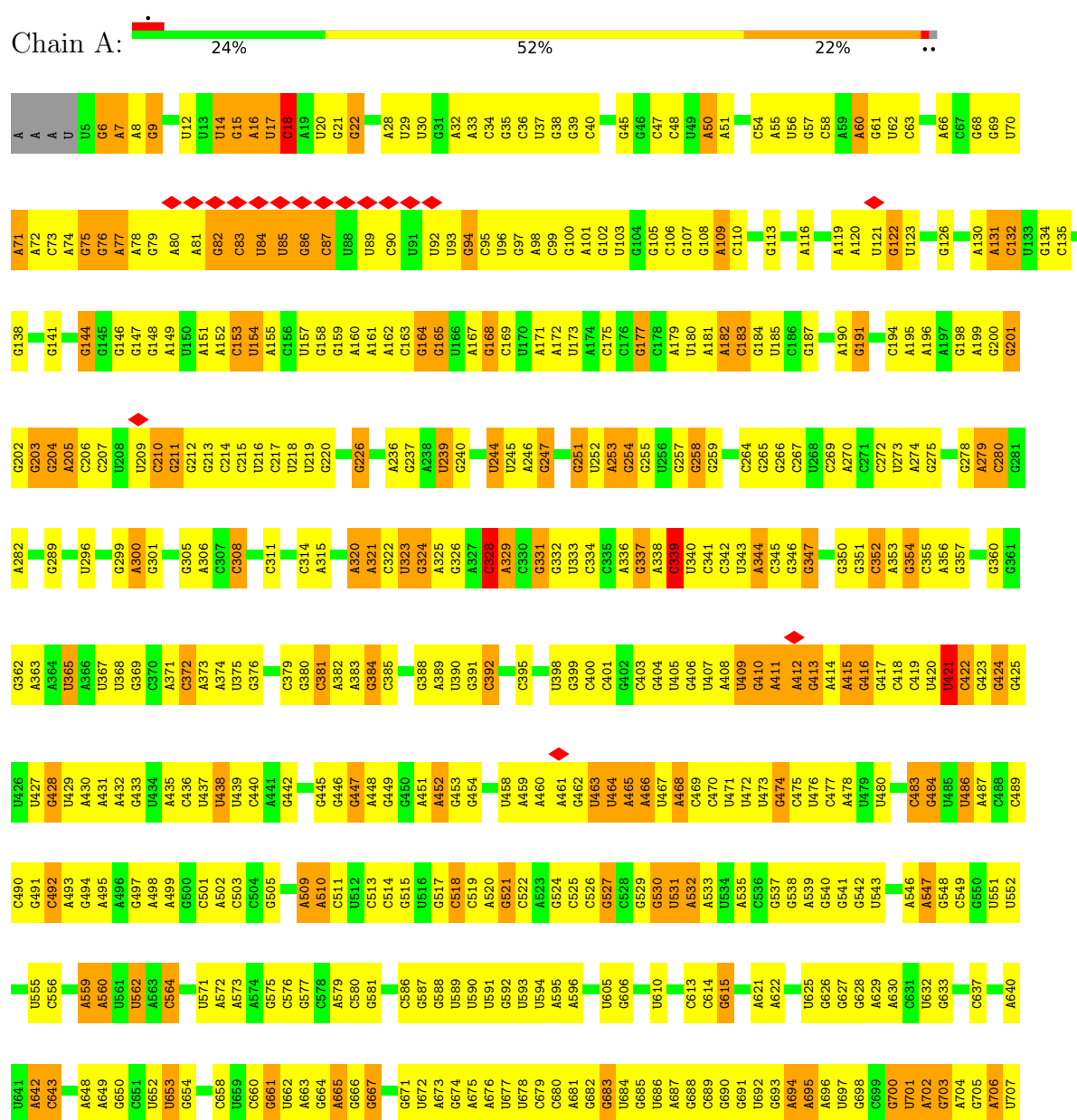
- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	79	637	408	120	107	2	0	0

3 Residue-property plots

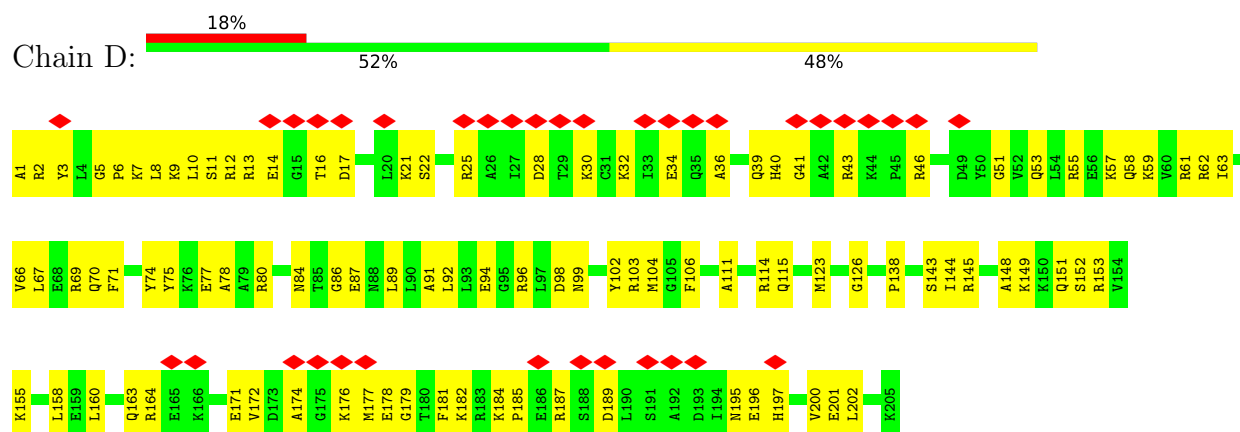
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

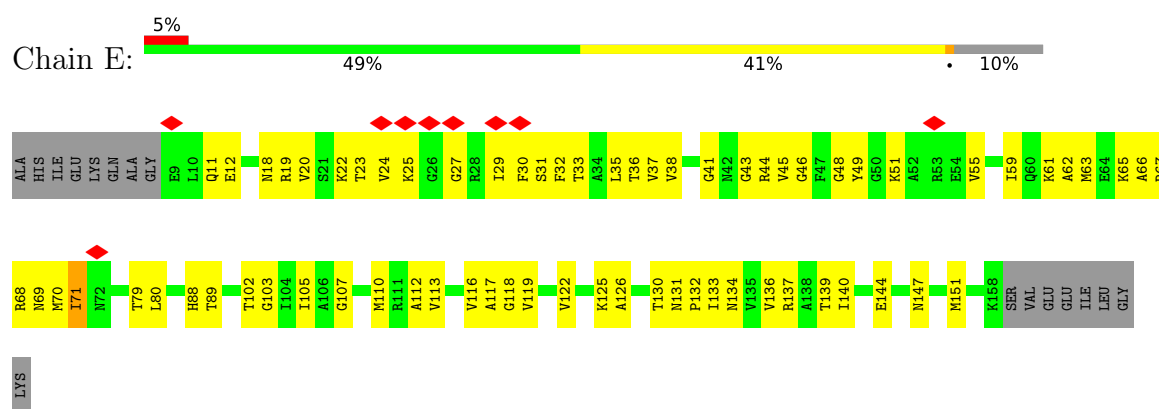


U	G1473	A1410	A1350	G1290	A1229	A1169	C1109	G1047	U986	G926	G849	G774	C708
A	U1474	A1413	U1351	U1291	C1230	A1170	A1110	G1048	G987	G927	U850	G775	U709
	G1476	C1475	C1352	G1292	U1231	A1171	C1112	U1049	G988	G928	G851	A776	G710
	U1413	G1353	G1293	U1232	U1173	C1172	C1113	U1052	U991	C930	C857	G713	G713
	G1416	U1354	G1294	U1233	G1174	U1173	C1114	G1053	U992	C931	C858	G714	G714
	U1478	G1355	U1295	C1234	G1175	C1175	C1115	C1054	G993	C932	G859	G779	A715
	C1479	G1356	U1235	U1235	A1176	G1176	C1116	A1055	A994	G933	A860	A780	A716
	A1418	C1357	G1297	A1236	G1177	U1177	C1117	U1056	C995	C934	A782	A781	
	U1481	U1358	U1298	U1298	G1178	G1178	C1118	G1057	A996	A935	A864	A718	U717
	G1482	A1360	A1239	A1238	A1179	A1179	C1119	G1058	U997	A936	G786	A965	A719
	U1485	G1361	U1240	U1240	G1180	G1180	C1120	U1059	A937	A937	G787	A866	C720
	G1486	A1362	G1241	G1241	G1181	G1181	C1121	U1060	A938	A938	G867	A787	G721
	G1487	C1363	C1242	C1242	G1182	G1182	C1122	G1061	C999	G939	A792	G722	G722
	U1491	G1364	C1243	C1243	U1183	U1183	C1123	U1062	A1000	C940	A873	U723	U723
	A1492	G1365	G1244	G1244	G1184	G1184	C1124	C1063	C1001	G941	A794	G724	G724
	A1493	C1366	C1245	C1245	G1185	G1185	G1125	G1064	G1002	G942	C795	G725	G725
	U1496	A1367	A1246	A1246	G1186	G1186	U1126	U1065	G1003	U943	C796	G726	G726
	U1498	C1368	U1247	U1247	G1187	G1187	G1127	A1004	A878	G944	G727	G727	G727
	A1499	G1369	A1248	A1248	A1188	A1188	C1128	G1006	G881	G945	A728	A728	A728
	A1500	G1370	C1249	C1249	U1189	U1189	C1129	U1007	U1007	A946	A802	A729	A729
	A1501	A1311	A1251	A1251	G1190	G1190	G1131	U1008	U1008	G947	A801	G730	G730
	A1502	G1312	A1252	A1252	C1191	C1191	C1132	U1009	U1009	C948	C883	G731	G731
	A1503	U1313	G1253	G1253	G1192	G1192	C1133	C1010	C1010	A949	C805	G732	G732
	A1504	C1314	A1254	A1254	U1194	U1194	G1134	A1012	G890	U952	C806	G733	G733
	A1505	U1315	G1255	G1255	C1195	C1195	G1135	A1013	U891	G953	A807	G734	G734
	A1506	G1316	A1256	A1256	A1196	A1196	U1136	U1075	A892	G954	G812	C735	C735
	A1507	C1317	A1257	A1257	A1197	A1197	C1137	U1076	C893	U955	G813	C736	C736
	U1511	A1318	G1258	G1258	G1198	G1198	G1138	U1077	A894	U956	A814	C739	C739
	A1512	C1319	C1259	C1259	U1199	U1199	C1139	U1078	C895	G957	A815	U740	U740
	A1513	G1320	A1260	A1260	C1200	C1200	G1140	U1079	G894	U957	A816	G741	G741
	A1514	U1321	G1261	G1261	A1201	A1201	U1141	A1081	A958	C896	A743	A743	A743
	A1515	C1322	A1262	A1262	U1202	U1202	C1142	A1082	A959	U960	G818	G744	G744
	A1516	G1323	U1264	U1264	C1203	C1203	G1143	U1083	A900	U961	A819	G745	G745
	A1517	A1324	C1265	C1265	U1205	U1205	U1144	U1084	A901	C962	U820	A746	A746
	A1518	G1325	G1266	G1266	G1206	G1206	C1145	U1085	G902	G963	G821	A747	A747
	A1519	C1326	C1267	C1267	G1207	G1207	A1146	U1086	G903	U964	C826	G748	G748
	A1520	G1327	A1268	A1268	C1208	C1208	C1147	G1087	A905	U965	U827	U751	U751
	C1524	C1328	A1269	A1269	C1209	C1209	U1148	U1088	U906	G966	U828	G752	G752
	G1525	U1330	G1270	G1270	U1210	U1210	C1149	U1090	A909	C967	G829	A753	A753
	U1526	A1331	A1271	A1271	U1211	U1211	A1150	U1091	C910	U969	G832	C754	C754
	U1527	C1332	C1272	C1272	A1212	A1212	C1151	A1092	U911	C970	U835	C755	C755
	U1528	G1333	C1273	C1273	U1213	U1213	A1152	A1093	C912	G971	G836	C756	C756
	G1529	G1334	A1274	A1274	C1214	C1214	C1153	G1094	A913	C972	U837	A758	A758
	A1531	U1335	G1275	G1275	G1215	G1215	G1154	U1095	A914	G973	G838	G759	G759
	U1532	C1336	C1276	C1276	A1216	A1216	A1155	C1096	A915	C974	C839	G760	G760
	C1534	G1337	G1277	G1277	C1217	C1217	C1156	C1097	U916	A975	C840	G763	G763
	U1533	A1338	G1278	G1278	C1218	C1218	A1157	U1098	A918	G976	C841	C764	C764
	A1534	C1339	A1280	A1280	A1219	A1219	C1158	G1099	A919	A977	U842	G765	G765
	C	U1340	C1281	C1281	G1220	G1220	U1159	C1100	U878	A978	U843	G769	G769
	U	C1342	C1282	C1282	G1221	G1221	C1160	A1101	U920	A979	U844	C770	C770
	U	G1343	U1283	U1283	C1222	C1222	C1161	A1102	C980	C979	G845	G771	G771
	C	U1344	C1284	C1284	C1223	C1223	G1162	G1104	U981	U981	A845	G772	G772
	U	U1345	A1285	A1285	U1224	U1224	A1163	A1105	G922	A982	C924	G773	G773
	U	A1346	C1286	C1286	A1225	A1225	G1164	A1106	C923	C923	C947		
	C	U1347	A1287	A1287	C1226	C1226	U1165	C1107	A983	C924	C947		
	U	A1348	A1287	A1287	A1227	A1227	G1166	A1043	C925	C925	C948		
	U	A1349	A1288	A1288	C1228	C1228	A1167	A1044					
			A1289	A1289			U1169	A1046					

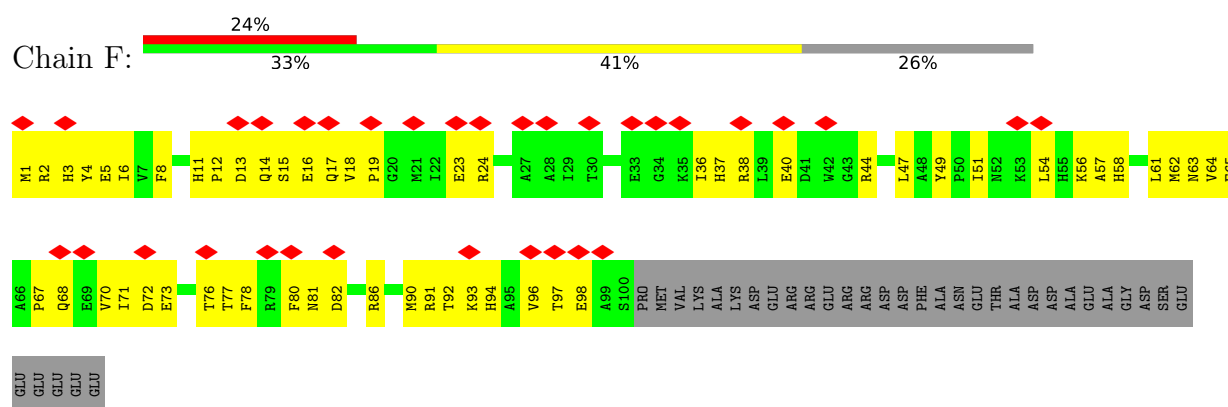
- Molecule 2: 30S ribosomal protein S4



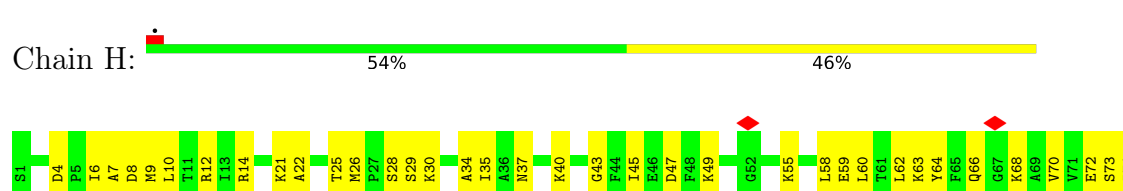
- Molecule 3: 30S ribosomal protein S5



- Molecule 4: 30S ribosomal protein S6, fully modified isoform

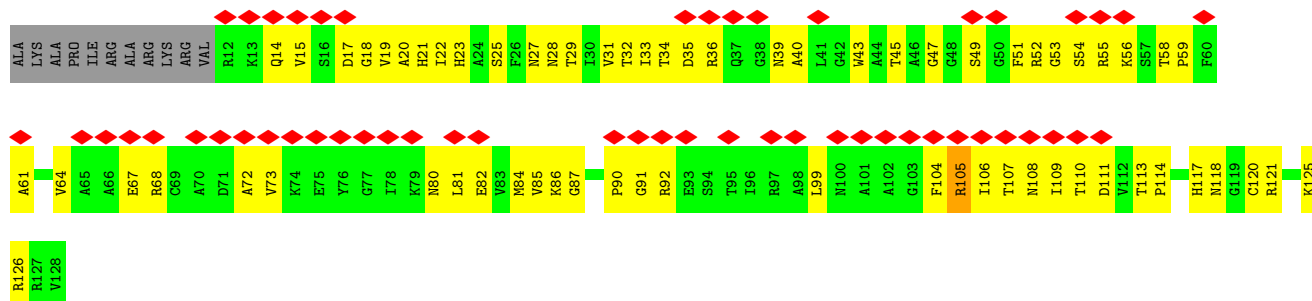


- Molecule 5: 30S ribosomal protein S8

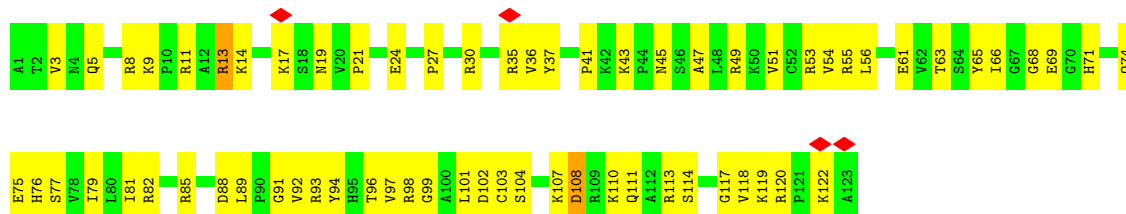




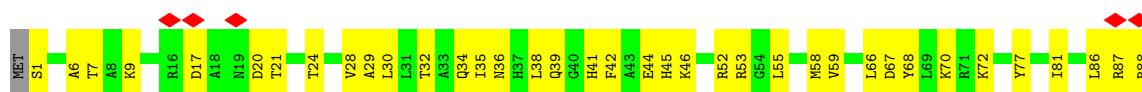
• Molecule 6: 30S ribosomal protein S11



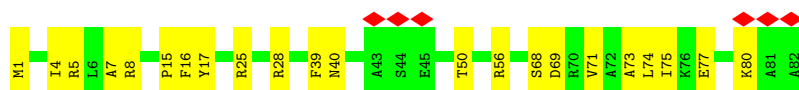
• Molecule 7: 30S ribosomal protein S12



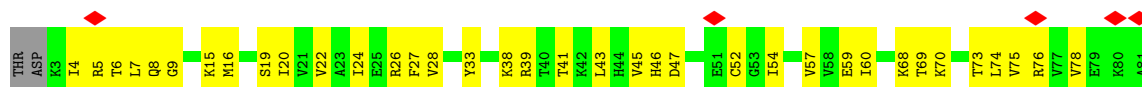
• Molecule 8: 30S ribosomal protein S15



• Molecule 9: 30S ribosomal protein S16

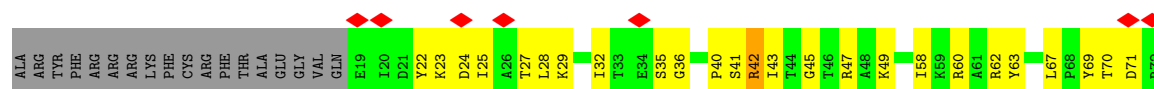


• Molecule 10: 30S ribosomal protein S17

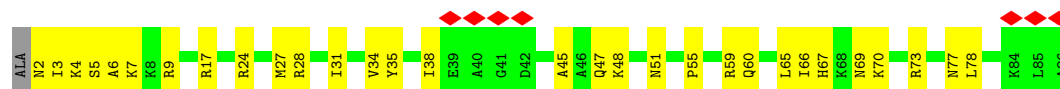




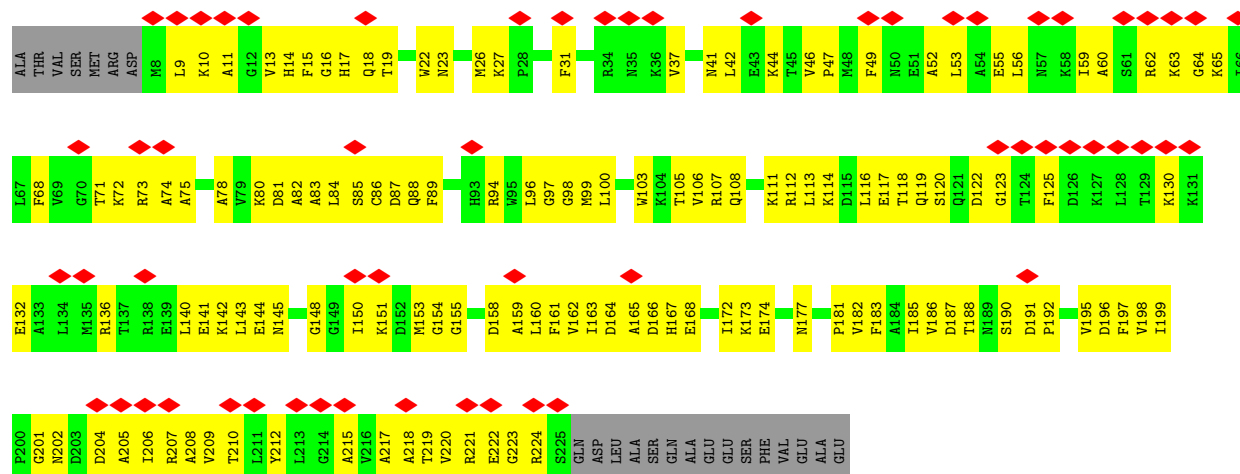
• Molecule 11: 30S ribosomal protein S18



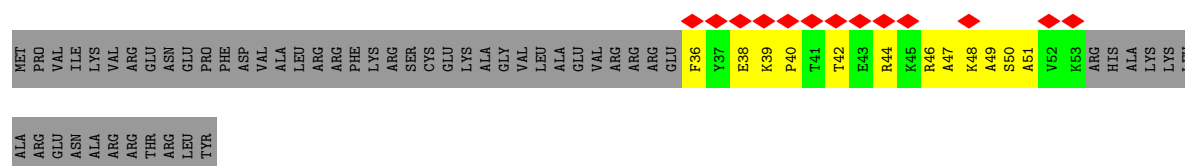
• Molecule 12: 30S ribosomal protein S20



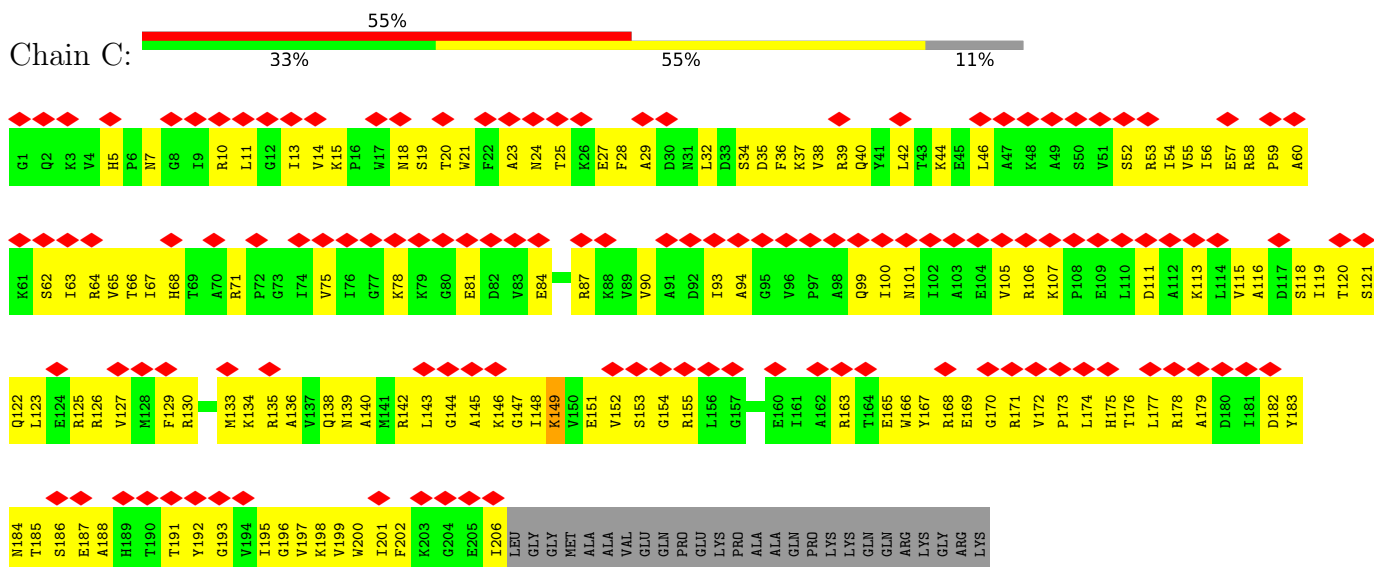
• Molecule 13: 30S ribosomal protein S2



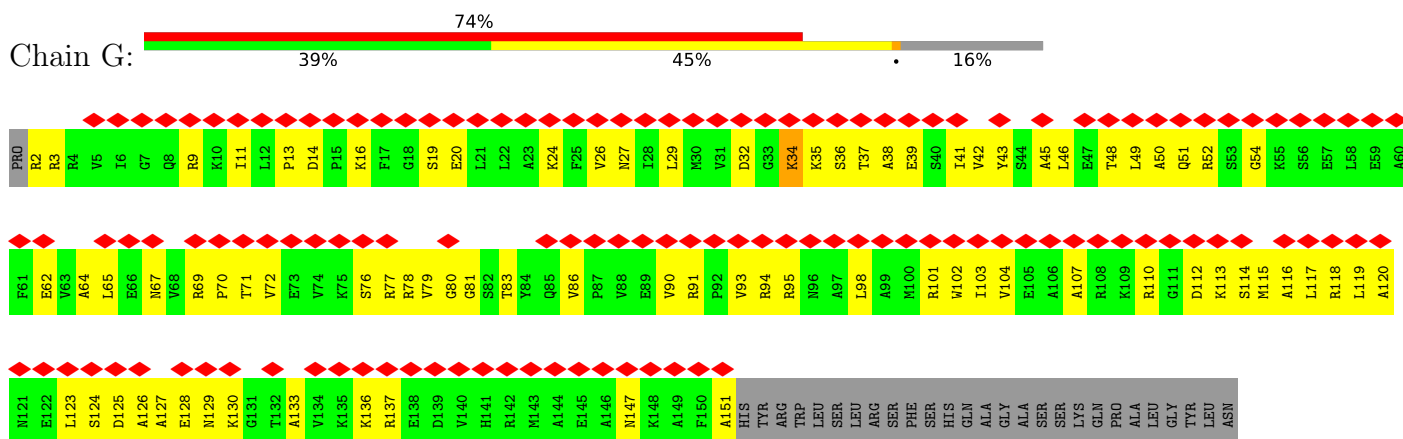
• Molecule 14: 30S ribosomal protein S21



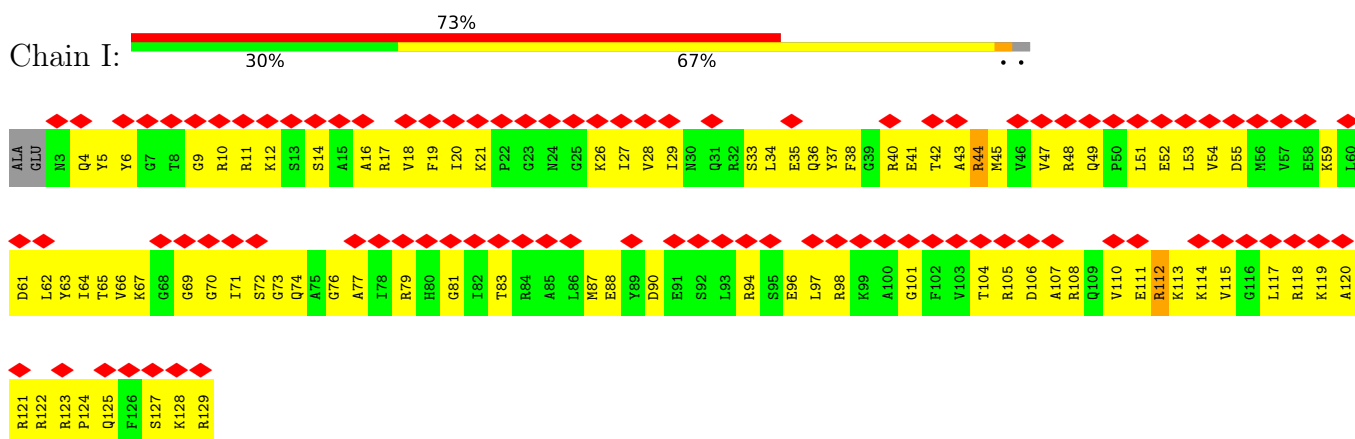
- Molecule 15: 30S ribosomal protein S3



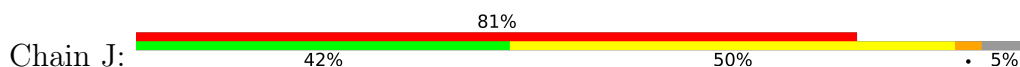
- Molecule 16: 30S ribosomal protein S7



- Molecule 17: 30S ribosomal protein S9

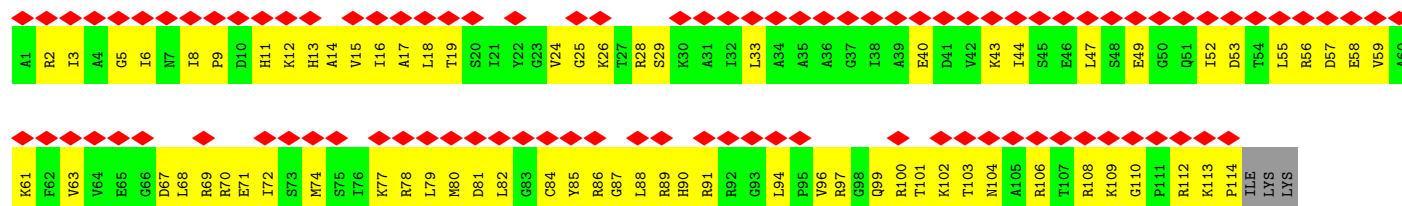
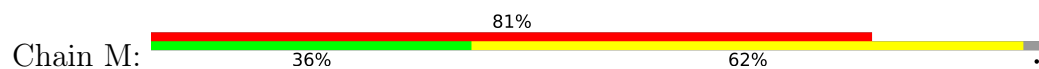


- Molecule 18: 30S ribosomal protein S10

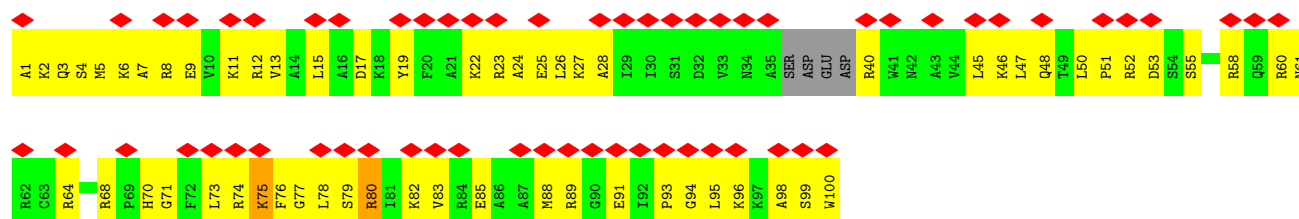




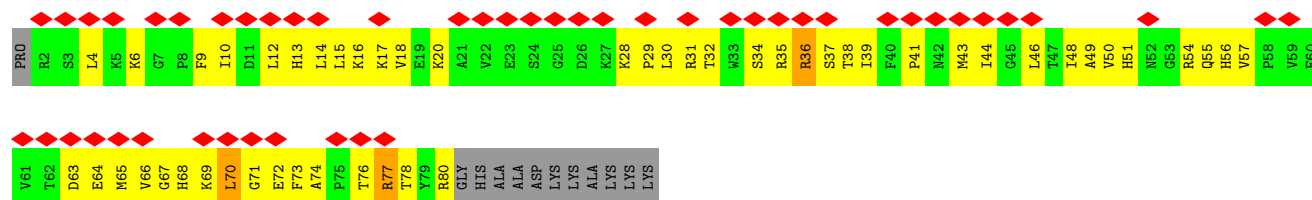
• Molecule 19: 30S ribosomal protein S13



• Molecule 20: 30S ribosomal protein S14



• Molecule 21: 30S ribosomal protein S19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169371	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	8.320	Depositor
Minimum map value	-4.514	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.428	Depositor
Map size (\AA)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

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	1.03	47/36762 (0.1%)	1.07	136/57350 (0.2%)
2	D	0.46	0/1665	0.63	0/2227
3	E	0.59	0/1118	0.71	1/1504 (0.1%)
4	F	0.41	0/835	0.57	0/1128
5	H	0.56	0/989	0.65	0/1326
6	K	0.34	0/893	0.60	0/1205
7	L	0.52	0/969	0.74	1/1300 (0.1%)
8	O	0.49	0/724	0.65	0/966
9	P	0.59	0/659	0.71	0/884
10	Q	0.53	0/657	0.58	0/881
11	R	0.46	0/462	0.70	0/621
12	T	0.38	0/671	0.59	0/888
13	B	0.38	0/1735	0.60	0/2338
14	U	0.34	0/150	0.57	0/198
15	C	0.28	0/1651	0.52	0/2225
16	G	0.27	0/1187	0.50	0/1591
17	I	0.30	0/1034	0.54	0/1375
18	J	0.26	0/796	0.54	0/1077
19	M	0.26	0/892	0.55	0/1193
20	N	0.29	0/785	0.56	0/1043
21	S	0.30	0/652	0.58	1/877 (0.1%)
All	All	0.88	47/55286 (0.1%)	0.95	139/82197 (0.2%)

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	918	A	C6-N1	-14.72	1.25	1.35
1	A	17	U	C2-N3	-11.04	1.30	1.37
1	A	18	C	N1-C6	-10.28	1.30	1.37
1	A	1401	G	N7-C5	-9.99	1.33	1.39
1	A	17	U	C4-O4	-8.87	1.16	1.23

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	A	O5'-P-OP1	-16.03	91.27	105.70
1	A	859	G	N3-C4-C5	-14.60	121.30	128.60
1	A	17	U	N3-C4-C5	12.56	122.14	114.60
1	A	1401	G	C6-C5-N7	-12.11	123.13	130.40
1	A	17	U	C2-N3-C4	-11.84	119.89	127.00

There are no chirality outliers.

There are no planarity outliers.

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	32831	0	16519	1541	0
2	D	1643	0	1710	126	0
3	E	1105	0	1148	66	0
4	F	817	0	808	64	0
5	H	979	0	1034	51	0
6	K	877	0	887	86	0
7	L	955	0	1019	74	0
8	O	716	0	742	35	0
9	P	649	0	666	19	0
10	Q	648	0	691	38	0
11	R	455	0	478	43	0
12	T	665	0	714	25	0
13	B	1704	0	1732	133	0
14	U	148	0	157	13	0
15	C	1624	0	1699	145	0
16	G	1174	0	1230	106	0
17	I	1022	0	1070	106	0
18	J	786	0	828	88	0
19	M	883	0	944	95	0
20	N	774	0	827	88	0
21	S	637	0	665	97	0
All	All	51092	0	35568	2694	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 32.

The worst 5 of 2694 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:1117:A:C2	1:A:1156:G:N1	2.10	1.19
1:A:945:G:H1	1:A:1236:A:N6	1.37	1.19
1:A:1156:G:N2	1:A:1179:A:C2	2.11	1.18
21:S:39:ILE:HG23	21:S:43:MET:HE3	1.30	1.13
2:D:104:MET:HG2	2:D:106:PHE:CE2	1.91	1.06

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	D	203/205 (99%)	174 (86%)	29 (14%)	0	100	100
3	E	148/166 (89%)	119 (80%)	29 (20%)	0	100	100
4	F	98/135 (73%)	80 (82%)	18 (18%)	0	100	100
5	H	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
6	K	115/128 (90%)	94 (82%)	21 (18%)	0	100	100
7	L	121/123 (98%)	96 (79%)	25 (21%)	0	100	100
8	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
9	P	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
10	Q	78/83 (94%)	66 (85%)	12 (15%)	0	100	100
11	R	53/74 (72%)	45 (85%)	8 (15%)	0	100	100
12	T	83/86 (96%)	77 (93%)	6 (7%)	0	100	100
13	B	216/240 (90%)	172 (80%)	44 (20%)	0	100	100
14	U	16/71 (22%)	10 (62%)	6 (38%)	0	100	100
15	C	204/232 (88%)	176 (86%)	28 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	G	148/178 (83%)	129 (87%)	19 (13%)	0	100	100
17	I	125/129 (97%)	107 (86%)	18 (14%)	0	100	100
18	J	96/103 (93%)	78 (81%)	18 (19%)	0	100	100
19	M	112/117 (96%)	98 (88%)	14 (12%)	0	100	100
20	N	92/100 (92%)	86 (94%)	6 (6%)	0	100	100
21	S	77/91 (85%)	64 (83%)	13 (17%)	0	100	100
All	All	2278/2561 (89%)	1935 (85%)	343 (15%)	0	100	100

There are no Ramachandran outliers to report.

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 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	D	172/172 (100%)	172 (100%)	0	100	100
3	E	113/125 (90%)	113 (100%)	0	100	100
4	F	87/116 (75%)	87 (100%)	0	100	100
5	H	104/104 (100%)	104 (100%)	0	100	100
6	K	90/98 (92%)	88 (98%)	2 (2%)	52	76
7	L	103/103 (100%)	102 (99%)	1 (1%)	76	89
8	O	76/77 (99%)	76 (100%)	0	100	100
9	P	65/65 (100%)	65 (100%)	0	100	100
10	Q	74/77 (96%)	74 (100%)	0	100	100
11	R	48/64 (75%)	47 (98%)	1 (2%)	53	77
12	T	65/65 (100%)	65 (100%)	0	100	100
13	B	180/198 (91%)	180 (100%)	0	100	100
14	U	15/61 (25%)	14 (93%)	1 (7%)	16	43
15	C	170/189 (90%)	169 (99%)	1 (1%)	86	93
16	G	123/146 (84%)	122 (99%)	1 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	I	105/106 (99%)	103 (98%)	2 (2%)	57	79
18	J	86/90 (96%)	83 (96%)	3 (4%)	36	66
19	M	92/95 (97%)	91 (99%)	1 (1%)	73	88
20	N	79/83 (95%)	77 (98%)	2 (2%)	47	74
21	S	70/78 (90%)	68 (97%)	2 (3%)	42	70
All	All	1917/2112 (91%)	1900 (99%)	17 (1%)	79	90

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	N	80	ARG
21	S	77	ARG
17	I	44	ARG
17	I	112	ARG
18	J	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
13	B	108	GLN
15	C	138	GLN
15	C	101	ASN
6	K	118	ASN
12	T	77	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1542 (99%)	468 (30%)	15 (0%)

5 of 468 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	A
1	A	9	G
1	A	18	C
1	A	20	U

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	923	A
1	A	1388	C
1	A	931	C
1	A	1390	U
1	A	1210	C

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.

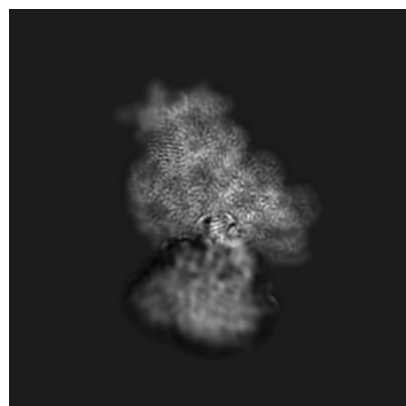
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12857. These allow visual inspection of the internal detail of the map and identification of artifacts.

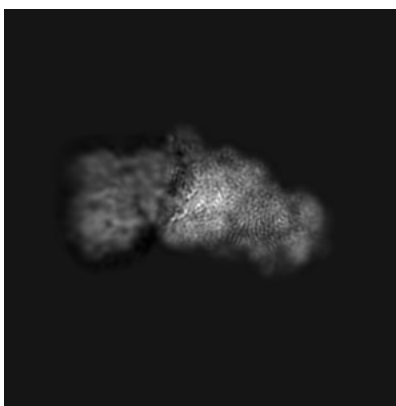
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

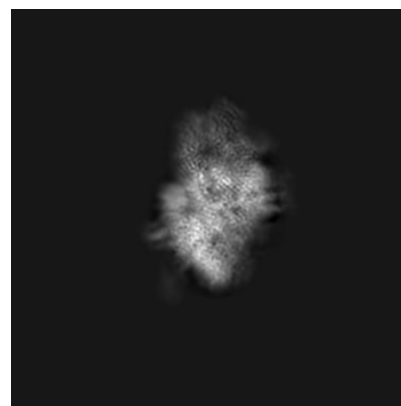
6.1.1 Primary map



X

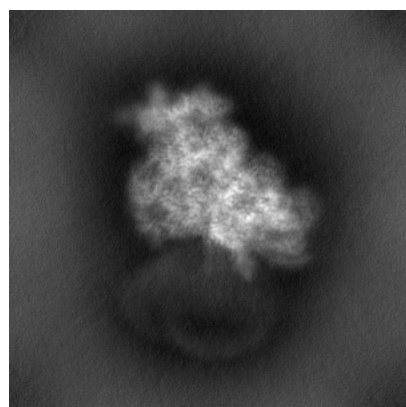


Y

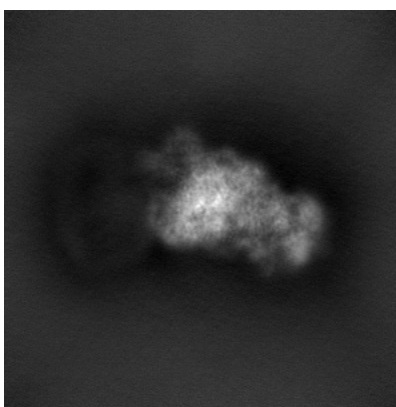


Z

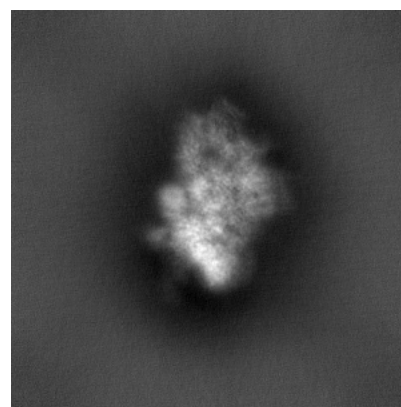
6.1.2 Raw map



X



Y

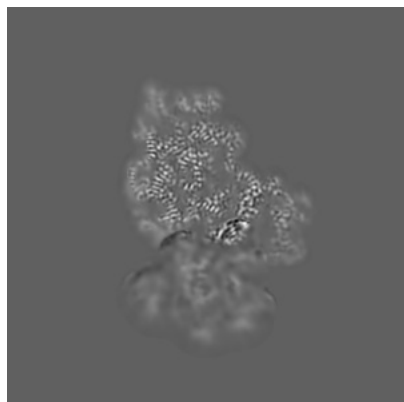


Z

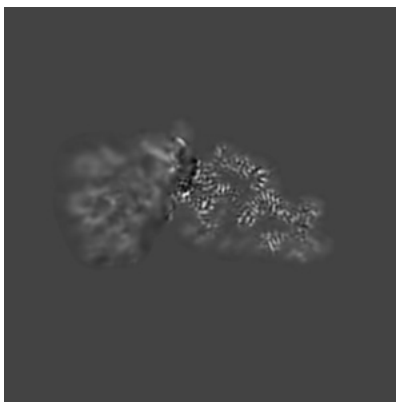
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

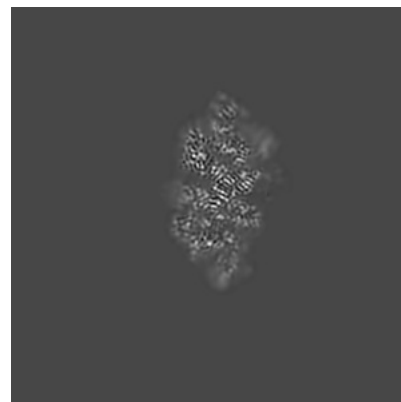
6.2.1 Primary map



X Index: 200

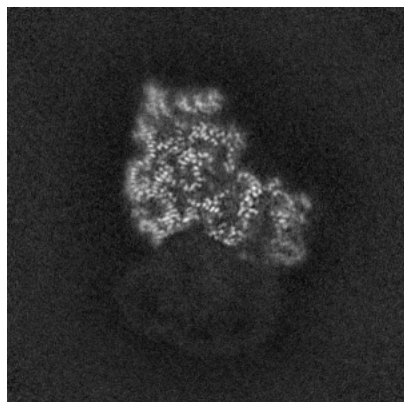


Y Index: 200

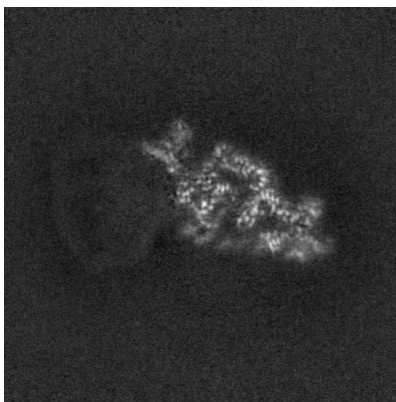


Z Index: 200

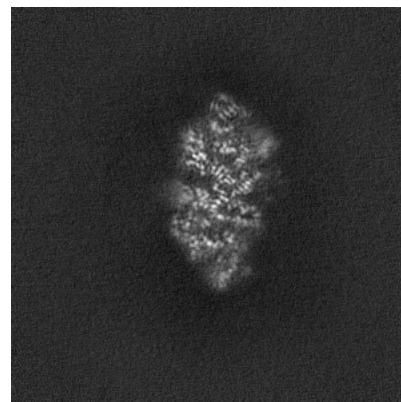
6.2.2 Raw map



X Index: 200



Y Index: 200

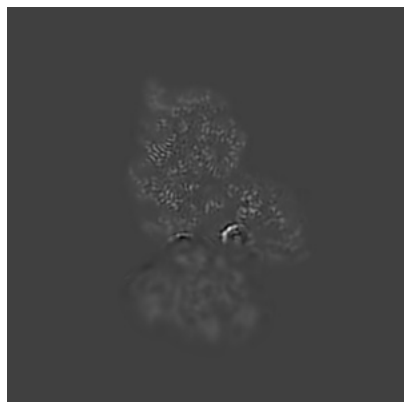


Z Index: 200

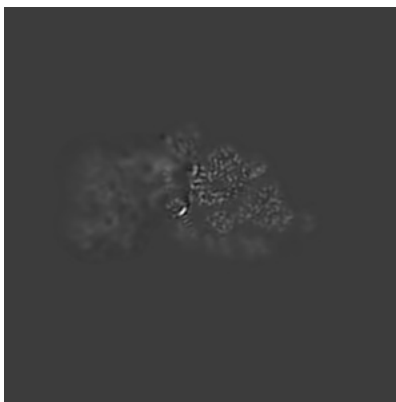
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

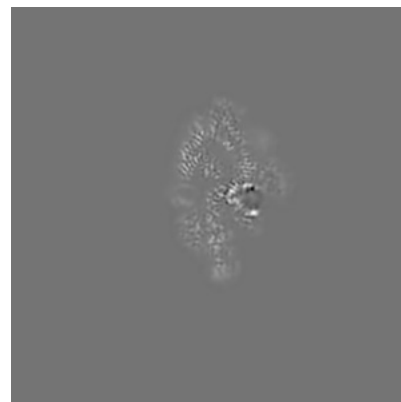
6.3.1 Primary map



X Index: 194

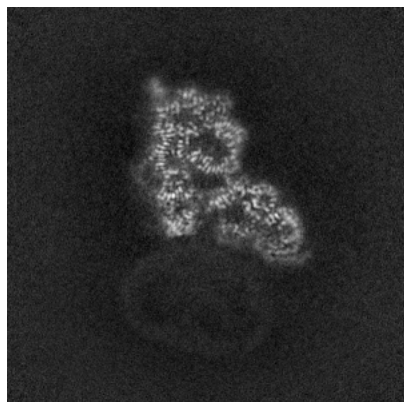


Y Index: 222

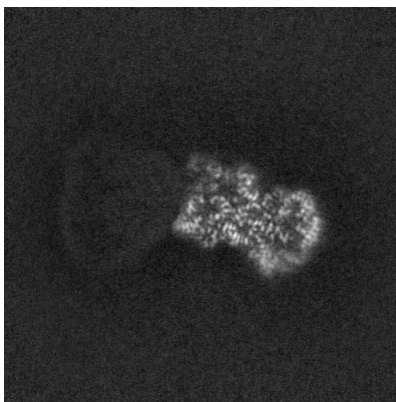


Z Index: 191

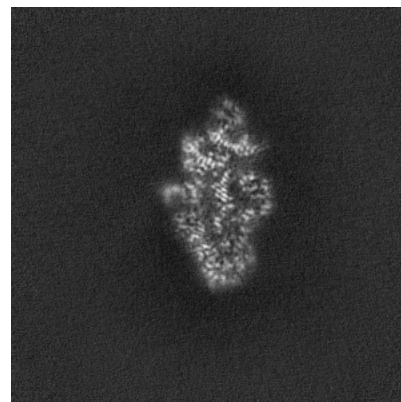
6.3.2 Raw map



X Index: 187



Y Index: 177

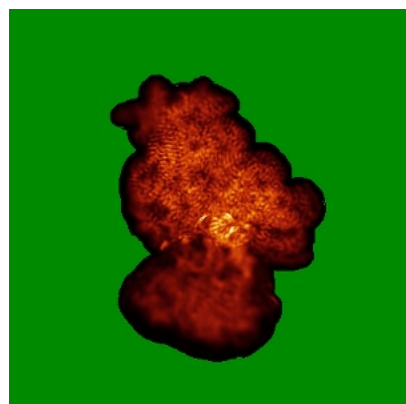


Z Index: 214

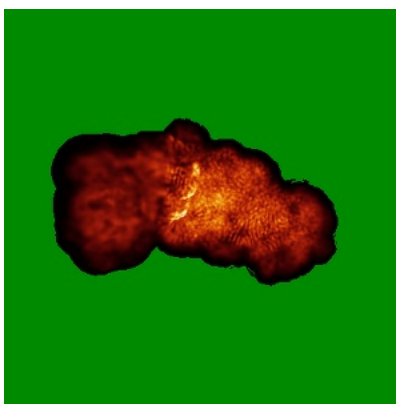
The images above show the largest variance slices of the map in three orthogonal directions.

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

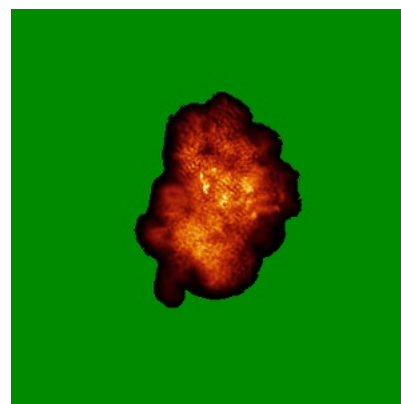
6.4.1 Primary map



X

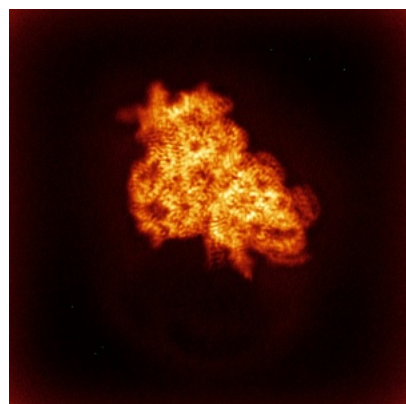


Y

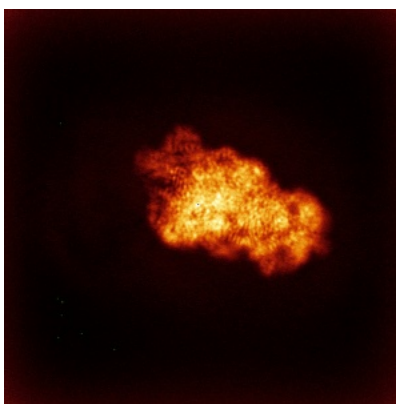


Z

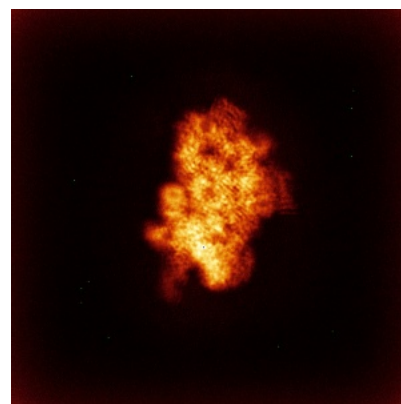
6.4.2 Raw map



X



Y

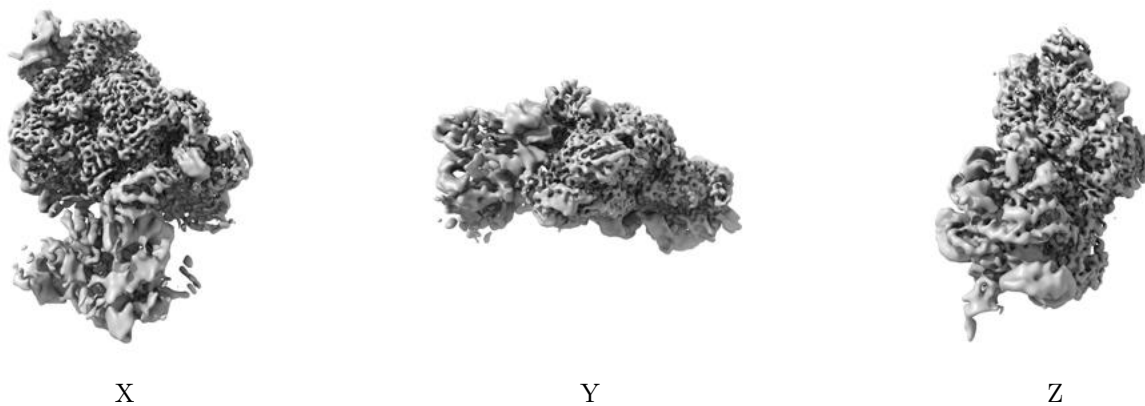


Z

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.

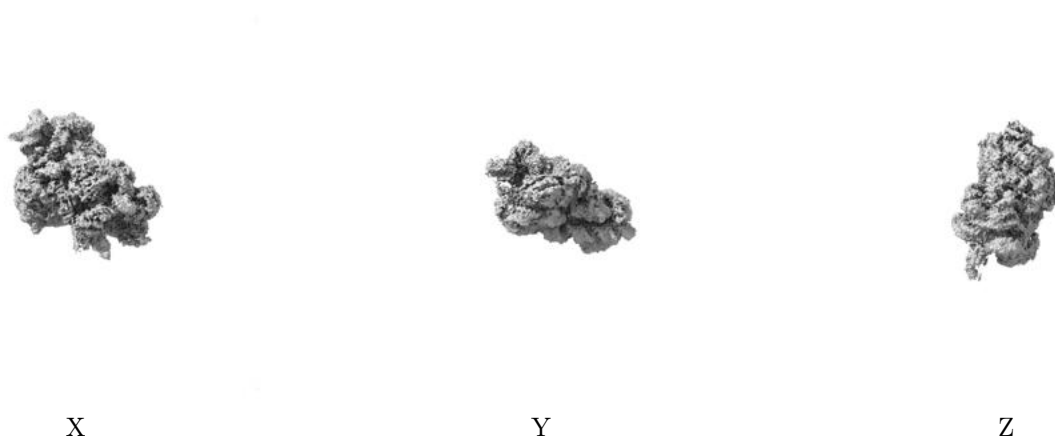
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.428. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

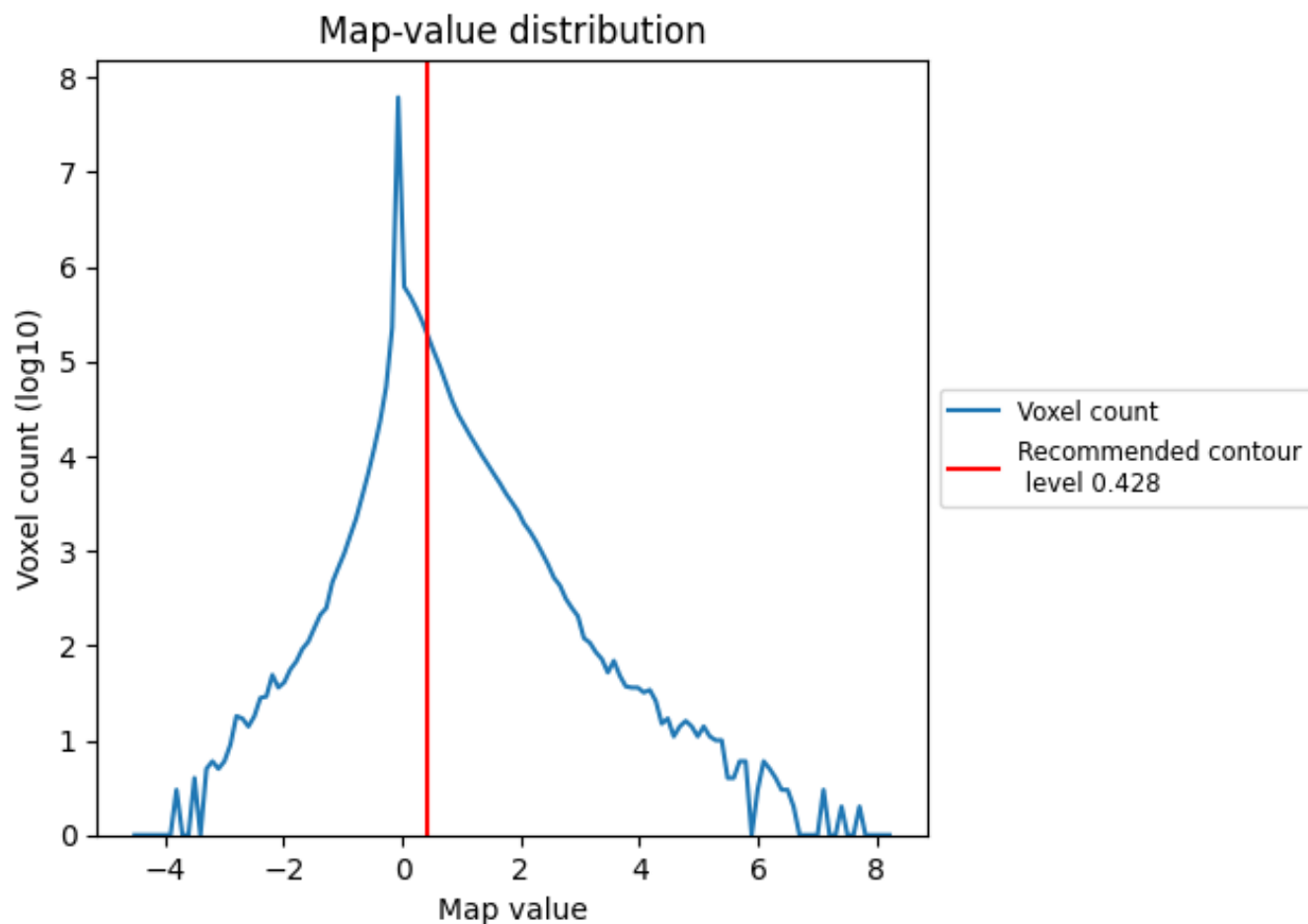
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

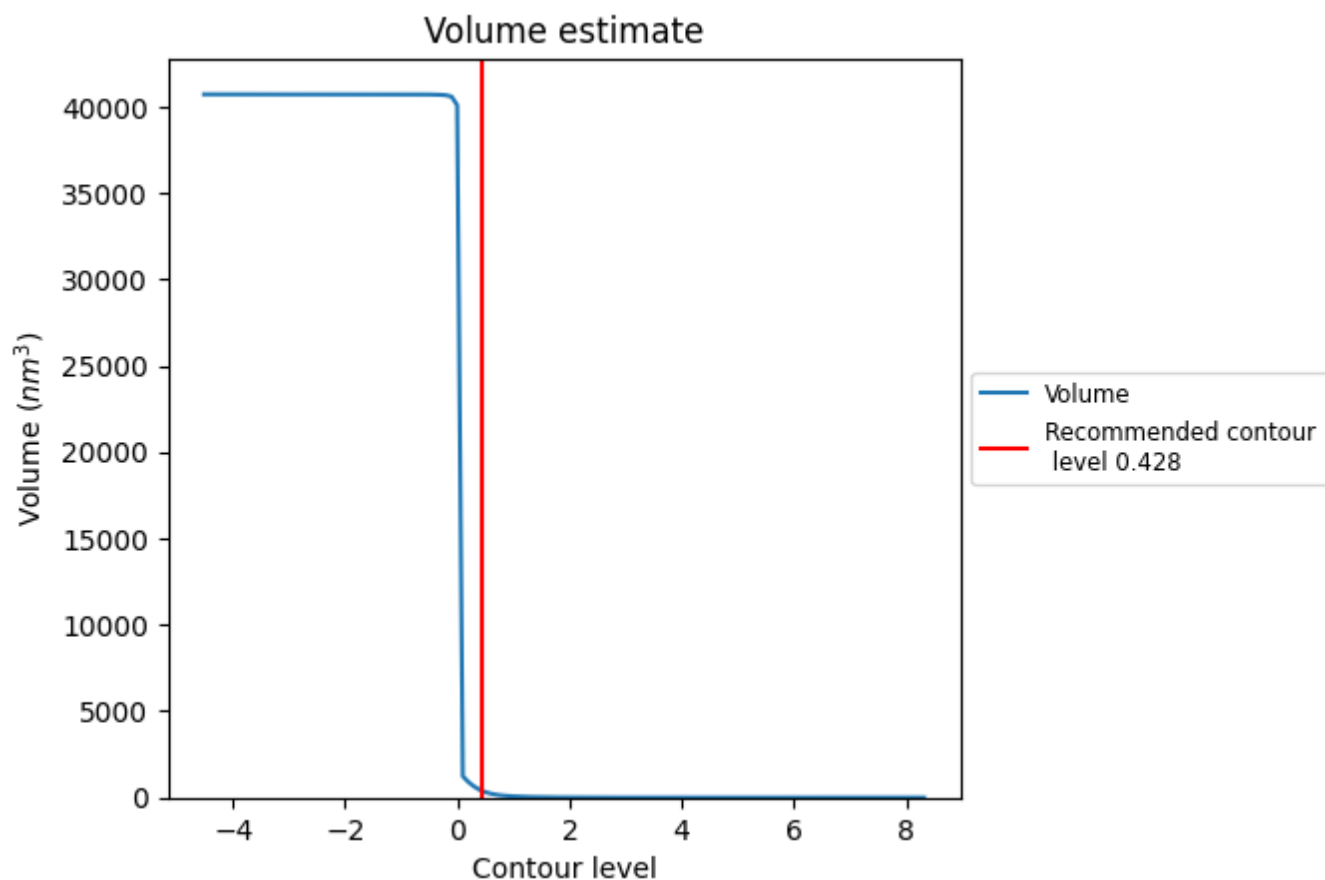
This section contains the results of statistical analysis of the map.

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.

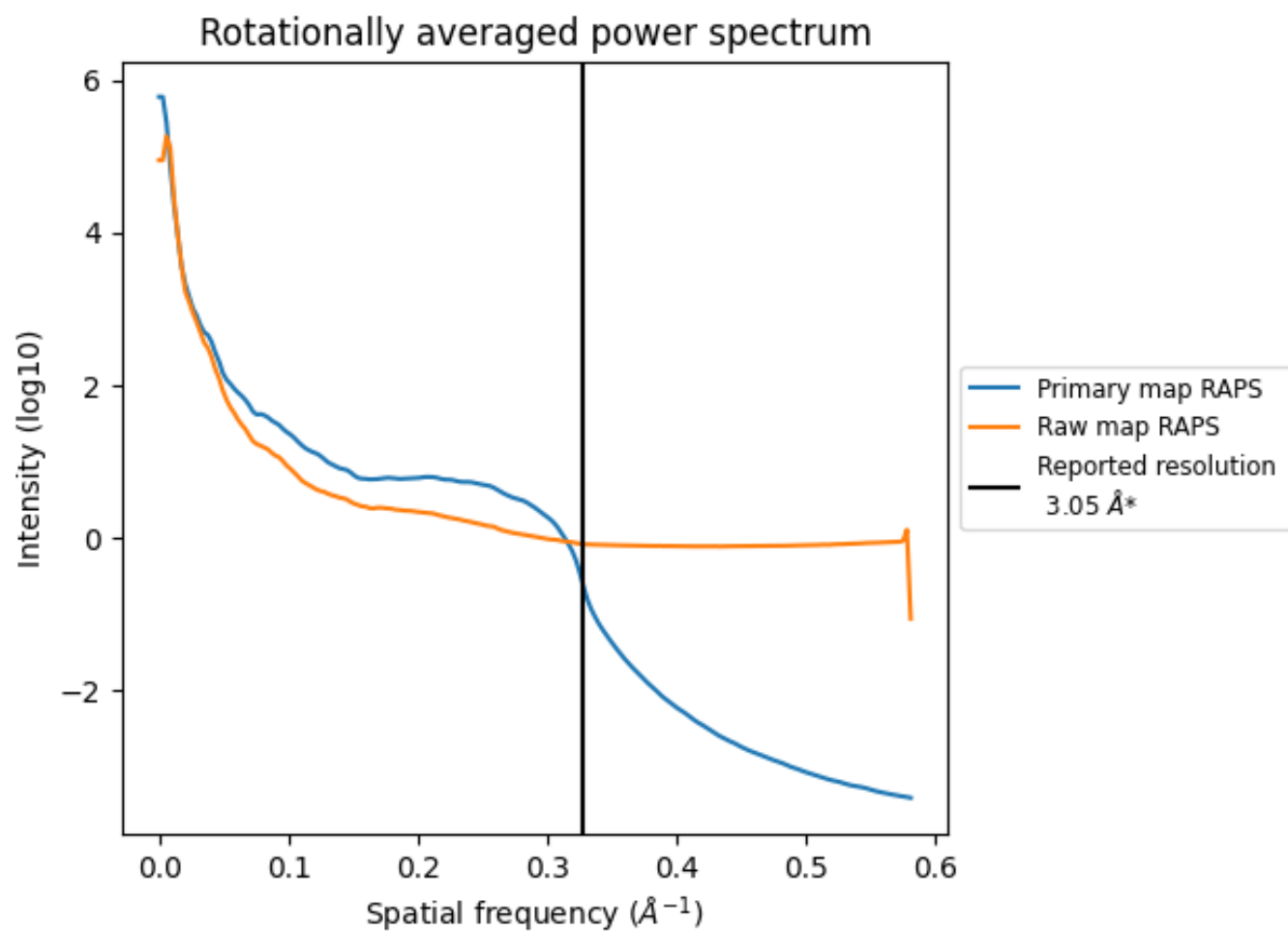
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 373 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 ⓘ

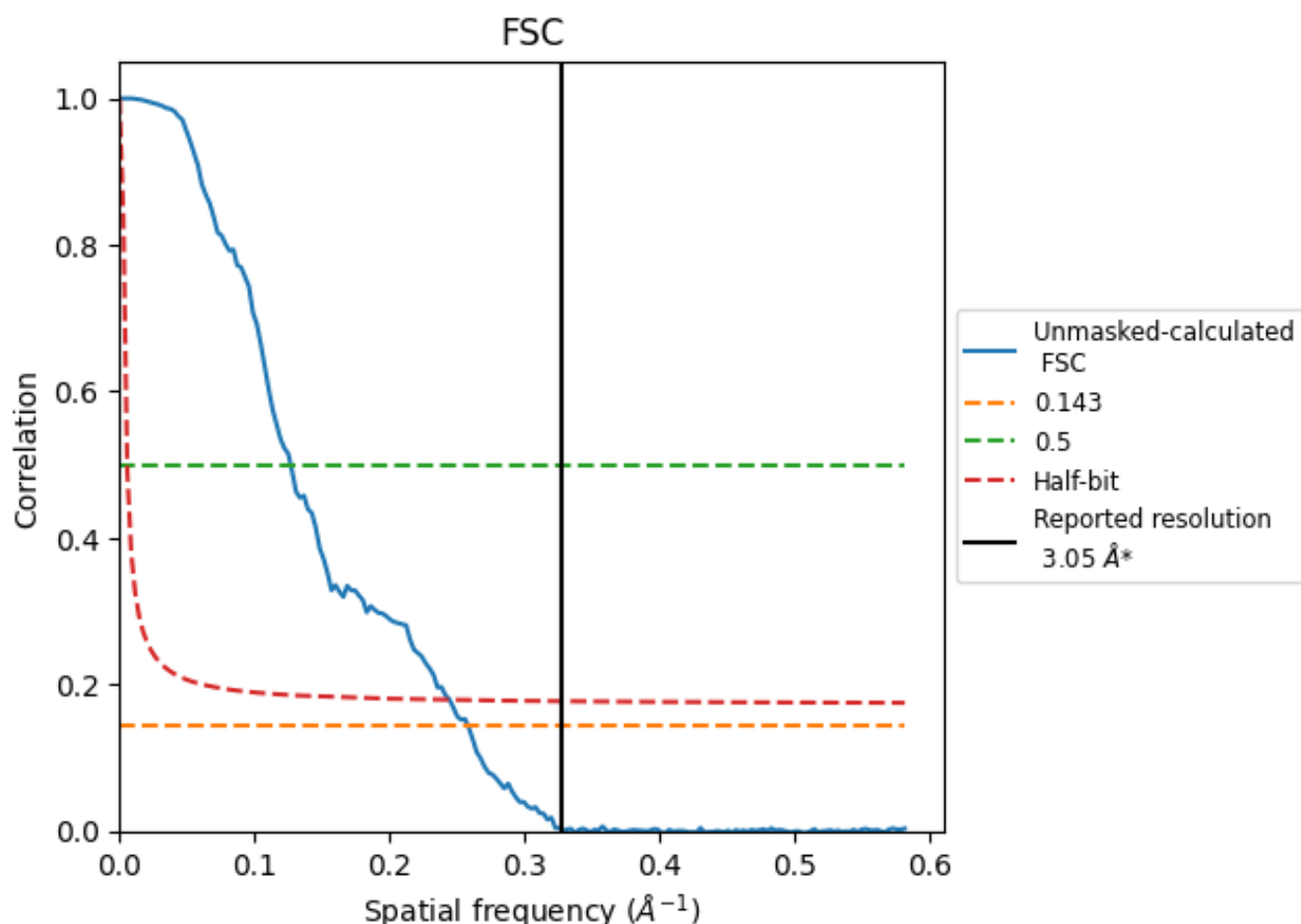


*Reported resolution corresponds to spatial frequency of 0.328 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

8.2 Resolution estimates [i](#)

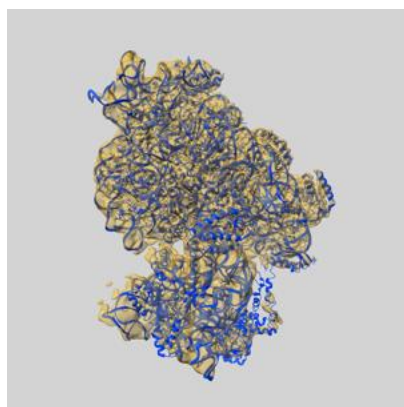
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.87	7.89	4.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.05 by more than 10 %

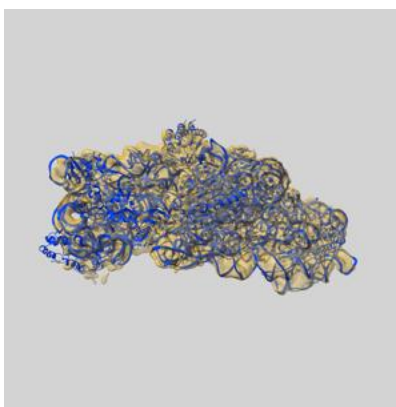
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12857 and PDB model 7OE1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

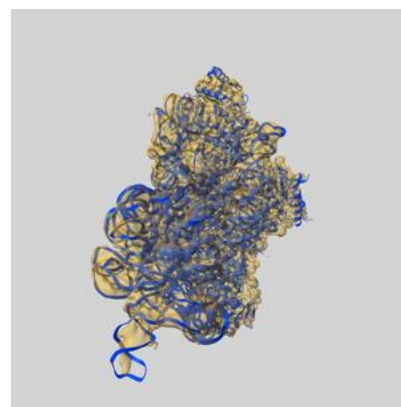
9.1 Map-model overlay [i](#)



X



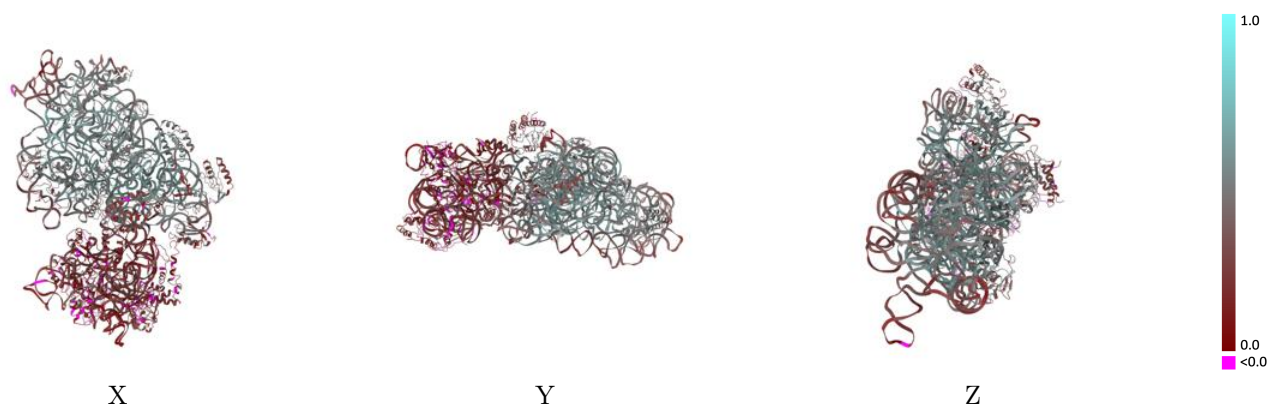
Y



Z

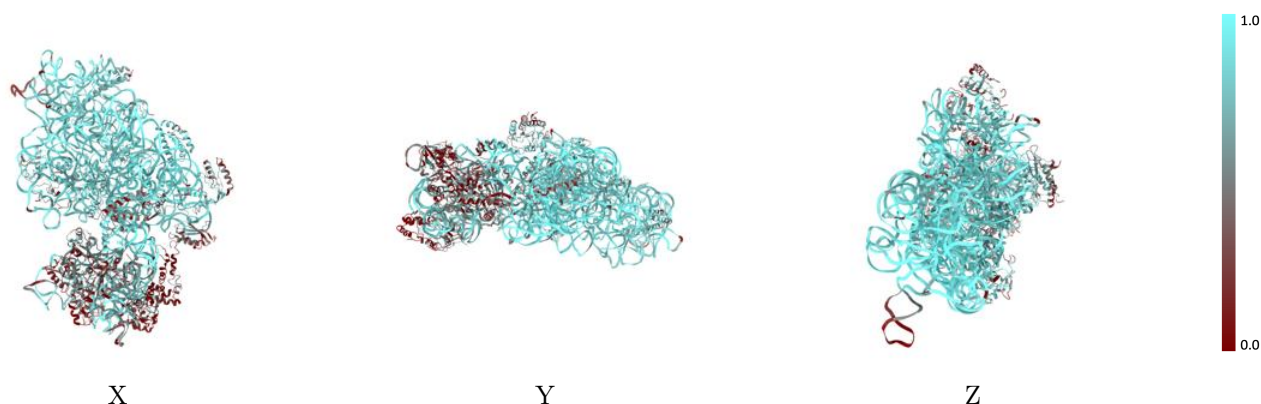
The images above show the 3D surface view of the map at the recommended contour level 0.428 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



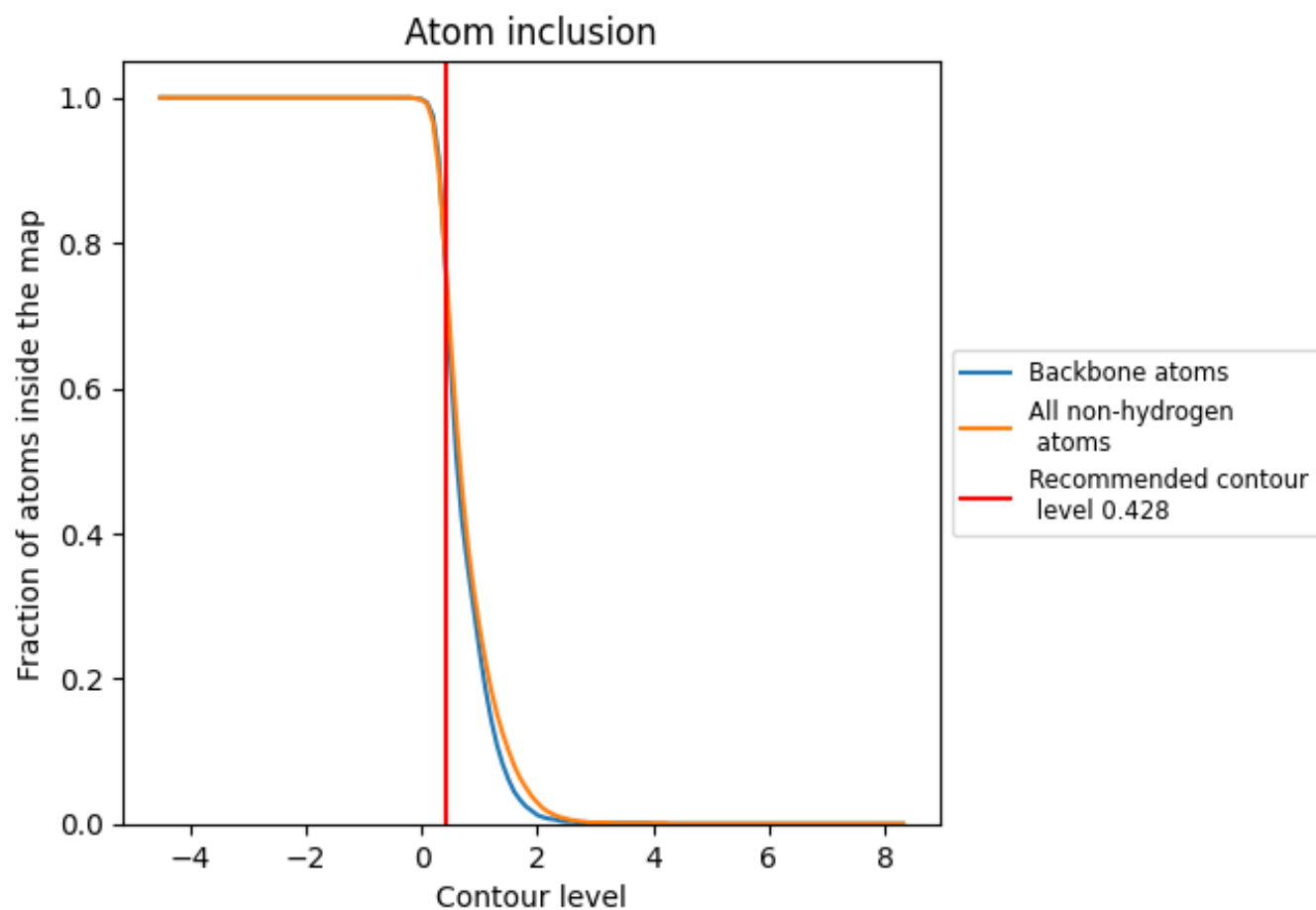
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.428).













































9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 76% 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 (0.428) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.3730
A	 0.8750	 0.4040
B	 0.6050	 0.2910
C	 0.3320	 0.1720
D	 0.6910	 0.4170
E	 0.8230	 0.4900
F	 0.5510	 0.3490
G	 0.1390	 0.1240
H	 0.8530	 0.5140
I	 0.2340	 0.1370
J	 0.1580	 0.1120
K	 0.4530	 0.3110
L	 0.8180	 0.4880
M	 0.1610	 0.1170
N	 0.3660	 0.1580
O	 0.7940	 0.4790
P	 0.8610	 0.5250
Q	 0.8100	 0.4950
R	 0.7500	 0.4740
S	 0.3240	 0.1270
T	 0.7940	 0.4650
U	 0.1820	 0.2380

