



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 04:06 AM UTC

PDB ID : 5LMU / pdb_00005lmu
EMDB ID : EMD-4080
Title : Structure of bacterial 30S-IF3-mRNA-tRNA translation pre-initiation complex, closed form (state-4)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 4.00 Å(reported)

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

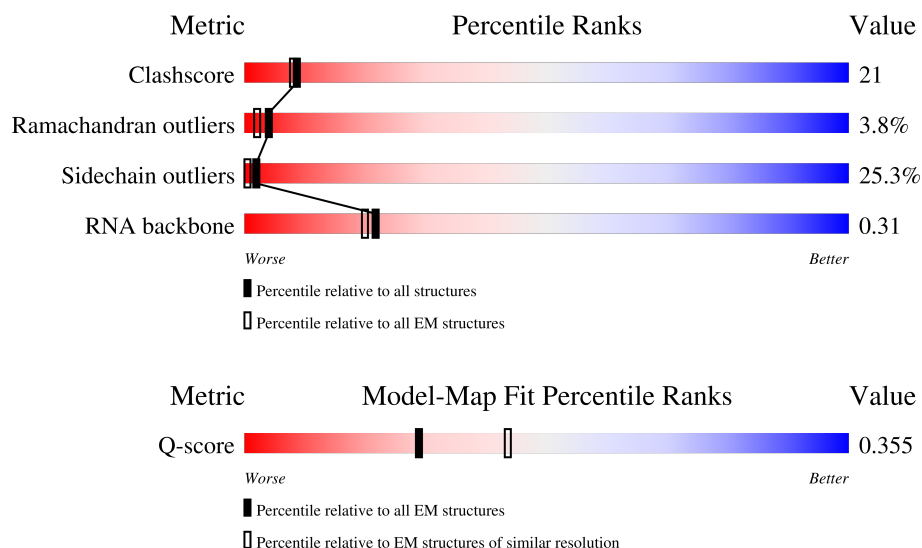
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	1522	
2	B	256	
3	C	239	

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	X	171	
23	Y	42	
24	Z	77	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 55195 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1515	Total	C	N	O	P	0	0
			32548	14490	6022	10523	1513		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	118	Total	C	N	O	S	0	0
			937	579	193	163	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			655	419	120	114	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	164	Total	C	N	O	S	0	0
			1336	841	245	241	9		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 24 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	77	Total	C	N	O	P	0	0
			1646	735	297	536	77		

- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
25	A	78	Total	Mg	0
			78	78	
25	L	1	Total	Mg	0
			1	1	
25	Z	1	Total	Mg	0
			1	1	

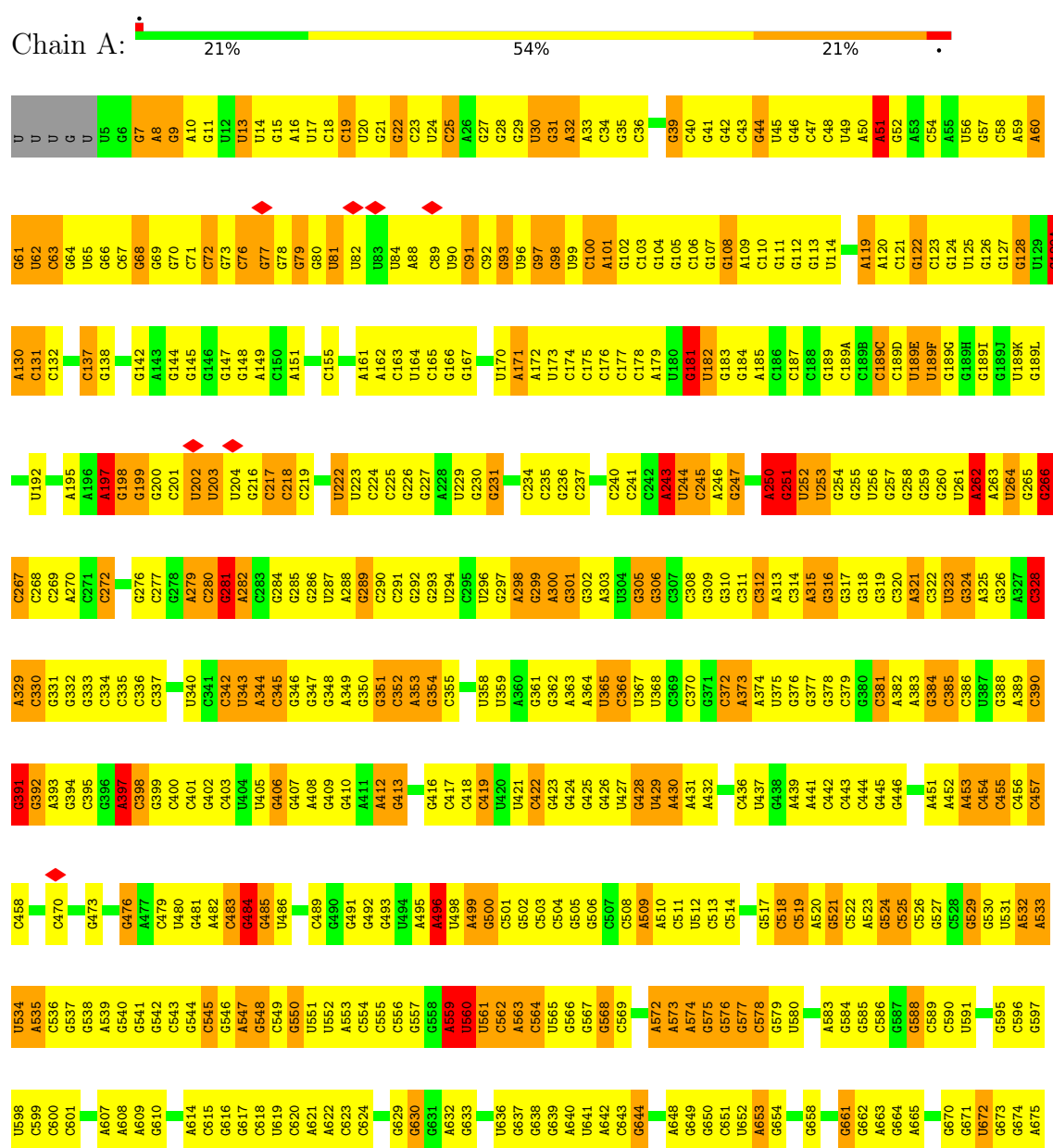
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	1	

3 Residue-property plots

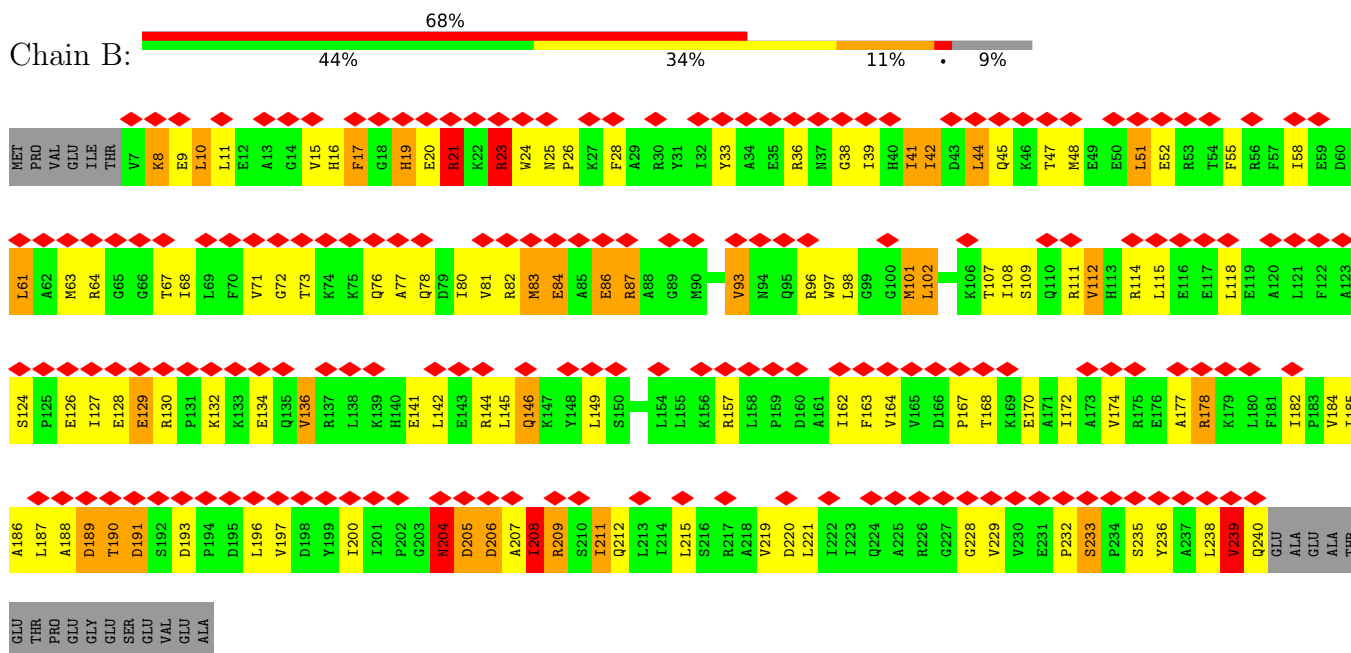
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

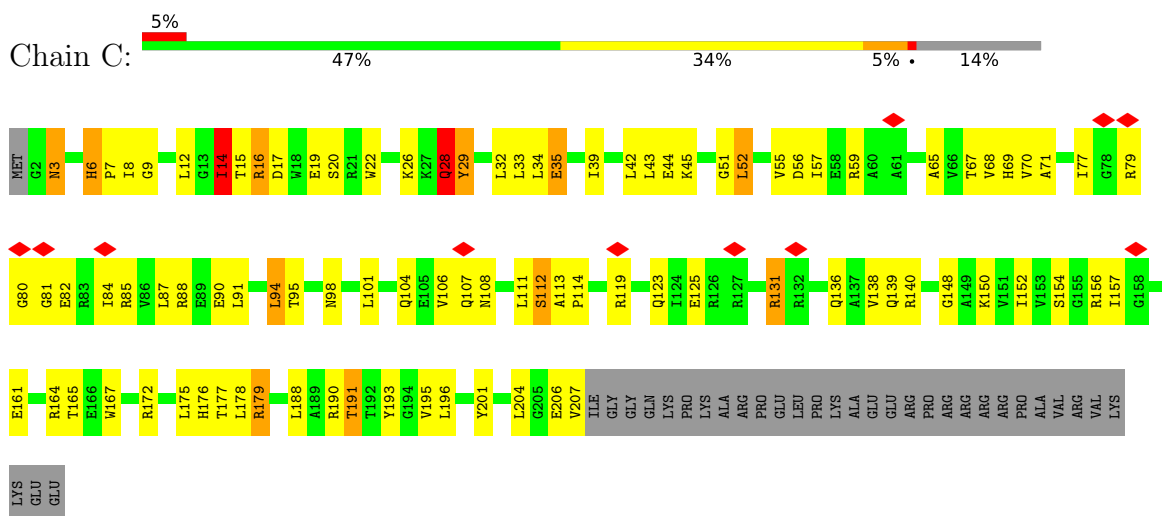


U1537	G1475	C1335	G1266	G1138	U1073	A1004	U943	C890	G809	U743	A676
C1538	U1407	C1336	G1207	G1139	G1074	A1005	G944	G881	C810	C744	U677
C1539	C1407	A1339	C1208	C1140	C1075	C1008	G945	C882	C811	C745	U678
U1540	A1408	A1339	C1209	C1141	C1076	G1009	A946	C883	C812	C746	C679
U1541	C1478	G1342	C1210	G1144	U1077	U1012	G947	U884	U813	C747	C680
U1542	A1409	G1343	U1211	C1145	U1078	U1013	A949	G885	A814	C748	C681
C	G1410	G1343	U1212	C1146	A1080	G1013	U950	G887	A815	C749	G682
U	C1411	G1344	A1213	A1147	A1081	A1013	U951	C888	A816	C750	G683
	C1412	U1345	G1214	C1147	G1082	A1015	U952	G889	U820	C751	A687
	A1413	G1346	G1215	U1148	U1083	A1016	G953	A890	G752	C752	G688
	U1414	G1347	G1216	C1149	G1084	A1017	G954	U891	A753	C753	G689
	G1415	U1217	C1217	U1150	U1085	G1017	U955	U892	G754	C754	G690
	U1348	U1281	C1218	A1151	U1086	C1018	U956	C893	G755	C755	G691
	A1349	U1282	U1219	A1152	U1087	G1022	U957	C894	C756	C756	U692
	A1350	C1283	G1220	C1153	G1087	G1023	U958	G895	G760	C760	U693
	U1351	C1284	G1221	G1154	U1088	G1024	A959	C896	G761	C761	A694
	C1352	A1285	G1222	G1155	U1089	U1025	U960	C897	C762	C762	A695
	G1353	A1286	C1223	G1156	U1090	G1026	U961	A900	G763	C763	A696
	G1354	A1287	G1224	U1159	G1094	G1027	G962	A901	C764	C764	C701
	G1355	A1287	A1225	G1160	U1095	C1028	G963	A902	G765	C765	A702
	G1356	A1288	C1226	C1161	C1096	C1029	A964	G903	A766	A766	G703
	A1357	G1293	A1227	C1162	C1097	C1030	A965	G904	A767	A767	A704
	U1358	C1294	C1228	C1163	U1098	G1030A	G966	U905	A768	A768	
	C1359	G1295	G1229	A1170	C1100	C1030B	C967	G906	G769	G769	
	A1360	G1295	C1230	C1171	A1101	C1030C	A968	A907	C770	C770	C707
	G1361	G1295	G1231	C1172	A1102	A1030D	A969	C910	G771	G771	G709
	C1362	C1298	G1232	G1173	C1103	G1031	G970	U911	G772	G772	G710
	C1363	A1299	U1233	C1174	G1104	G1031	G971	C912	G773	G773	G711
	A1363A	G1300	C1234	C1175	A1105	C1037	G972	A913	G774	G774	A712
	G1364	U1301	G1235	G1176	G1106	C1038	A973	A914	A777	A777	G713
	G1365	U1302	A1236	A1177	C1107	C1039	A974	A915	G778	G778	G714
	G1366	G1303	C1237	G1177	G1108	U1040	A975	U850	C779	C779	G715
	C1367	G1304	A1238	G1178	G1109	A1041	A976	G851	A780	A780	A716
	G1368	G1305	A1239	G1179	G1110	G1042	A977	G852	G717	G717	G718
	C1369	G1306	U1240	A1180	C1112	C1043	A978	A918	A781	A781	C719
	G1370	U1307	U1241	G1181	C1113	A1044	G979	U920	G782	G782	C720
	G1371	G1310	G1242	G1182	C1114	C1045	C980	U921	C783	C783	G721
	G1372	G1311	C1243	A1183	C1115	A1046	U981	G922	G784	G784	G722
	G1373	G1312	C1244	G1184	C1116	U1060	G982	A923	A785	A785	U723
	C1378	U1313	A1245	G1185	G1117	A1065	C985	G924	G786	G786	G724
	G1379	C1314	C1246	G1186	C1118	U1066	A986	G925	U787	U787	G725
	U1380	U1315	U1247	G1187	C1119	C1067	G987	G926	A788	A788	C726
	U1381	U1316	U1248	A1188	C1120	U1068	C988	G927	U789	U789	C727
	G1384	C1317	C1249	C1189	U1121	U1069	C989	G928	G791	G791	G728
	G1385	A1318	A1250	G1190	U1122	A1065	C990	G929	A792	A792	A729
	G1386	A1319	A1251	A1191	A1123	U1066	C991	C930	U793	U793	G730
	G1387	C1320	A1252	C1192	G1124	U1066	C992	C931	C795	C795	G731
	G1388	C1321	G1253	G1193	U1125	U1066	U991	C932	G796	G796	G734
	C1388	C1322	C1254	U1194	U1126	C1060	G992	G933	C797	C797	C735
	C1389	G1323	G1255	C1195	G1127	G1061	A994	C934	A872	A872	C736
	U1390	A1324	A1256	U1196	C1128	G1064	C995	A935	C737	C737	C738
	U1391	C1325	U1257	G1197	C1129	U1065	G998	A936	A873	A873	G739
	G1392	C1326	G1258	U1198	A1130	U1066	C999	C936	G798	G798	U740
	U1393	C1327	G1259	U1199	G1131	A1067	A1000	A937	C799	C799	G741
	A1394	C1328	C1260	G1200	C1132	U1067	A1001	A938	U804	U804	C808
	C1395	G1331	A1261	A1201	G1133	G1068	G939	G875	C805	C805	
	A1396	C1332	C1262	G1202	G1134	C1069	A1002	G876	C806	C806	
	C1397	A1332	C1263	C1203	U1135	U1070	G1001A	C877	U740	U740	
	A1398	A1333	C1264	A1204	U1136	G1071	G1002	G878	G741	G741	
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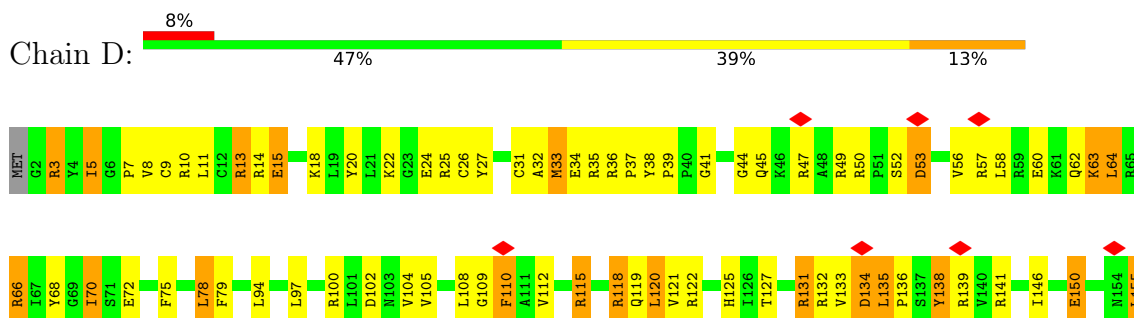
- Molecule 2: 30S ribosomal protein S2

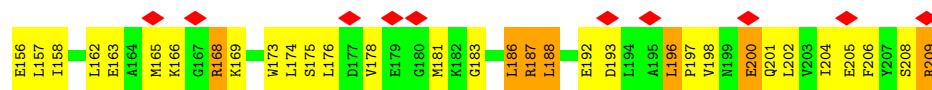


- Molecule 3: 30S ribosomal protein S3

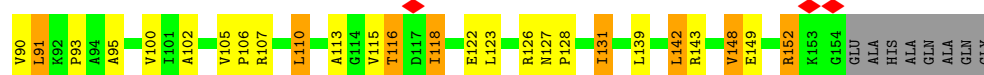
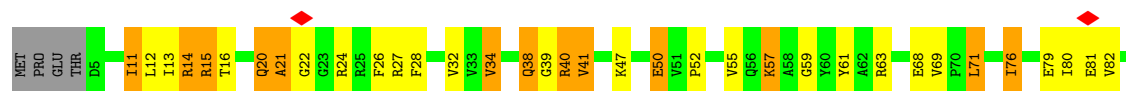


- Molecule 4: 30S ribosomal protein S4

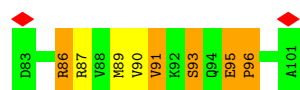
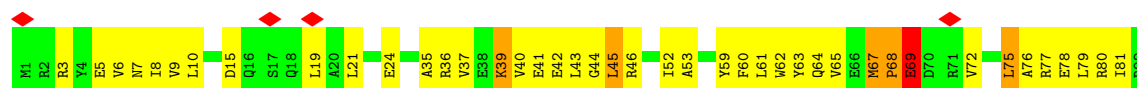




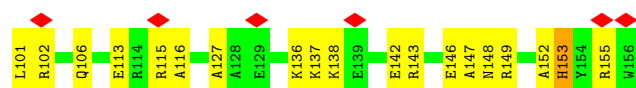
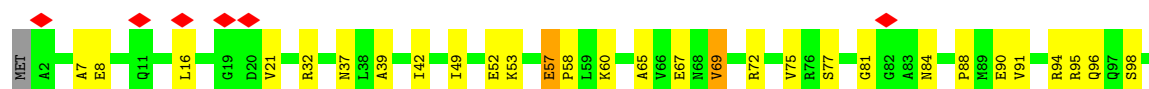
• Molecule 5: 30S ribosomal protein S5



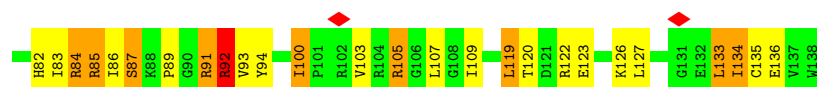
• Molecule 6: 30S ribosomal protein S6



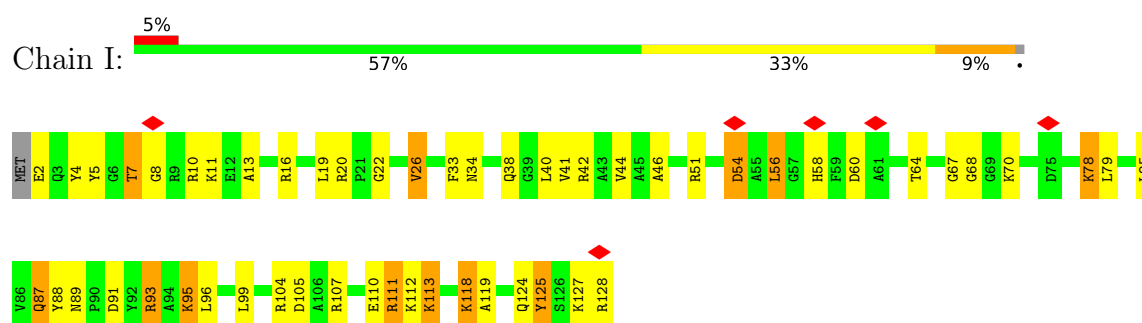
• Molecule 7: 30S ribosomal protein S7



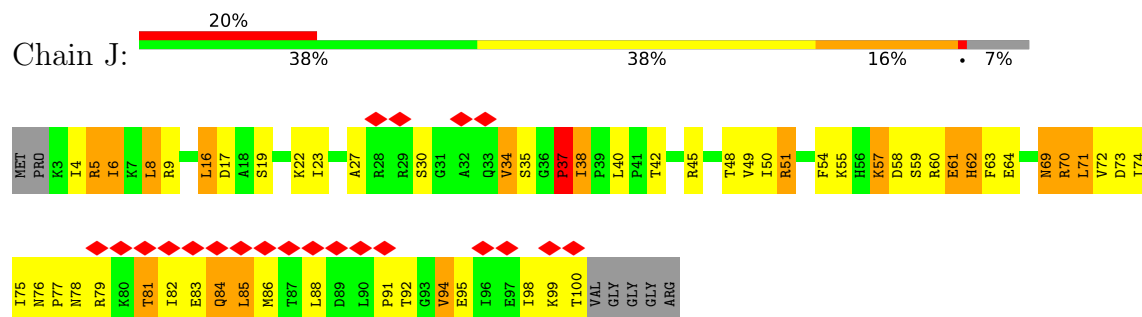
• Molecule 8: 30S ribosomal protein S8



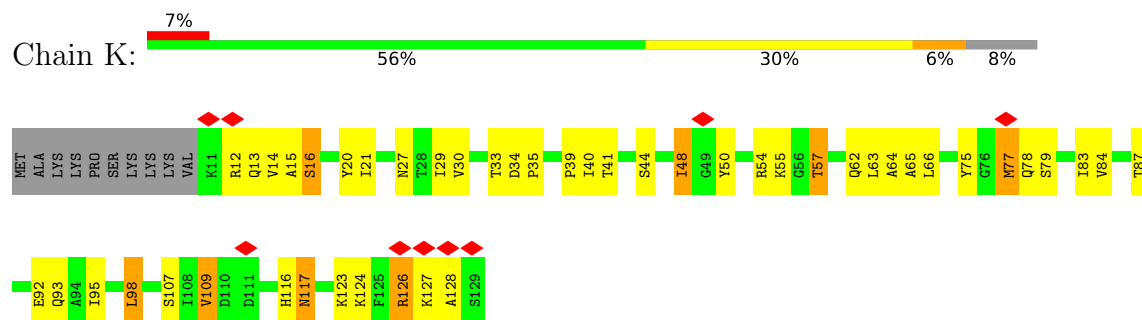
• Molecule 9: 30S ribosomal protein S9



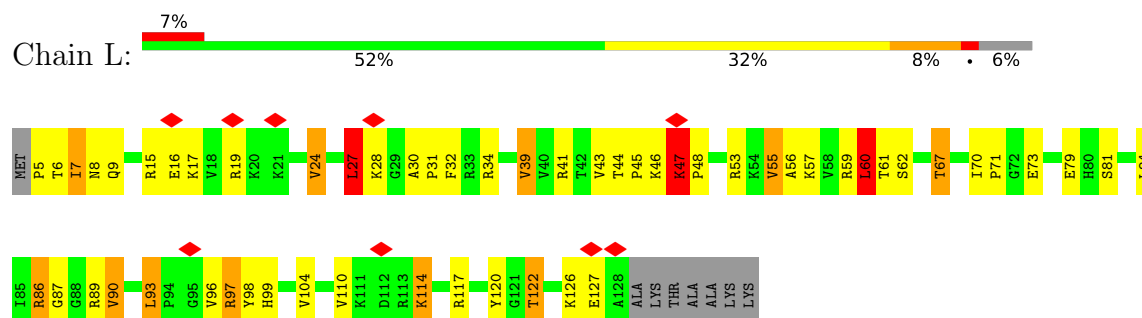
- Molecule 10: 30S ribosomal protein S10



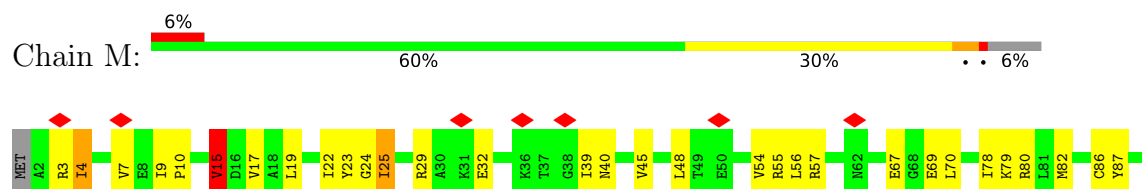
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

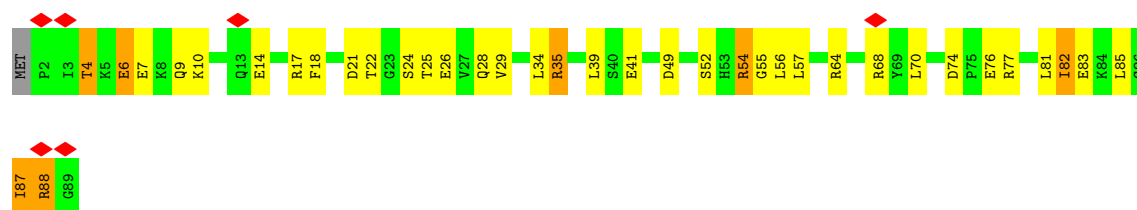




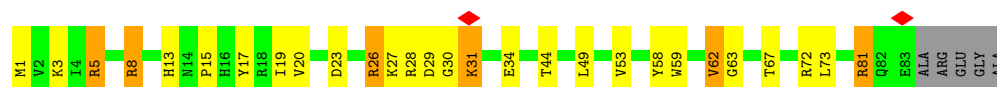
- Molecule 14: 30S ribosomal protein S14 type Z



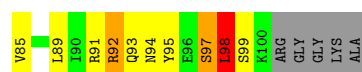
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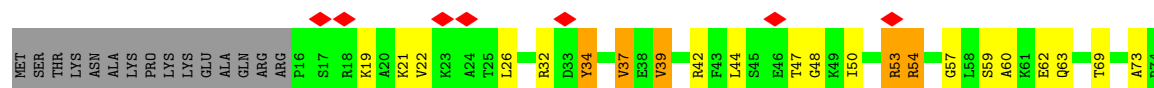
- Molecule 16: 30S ribosomal protein S16



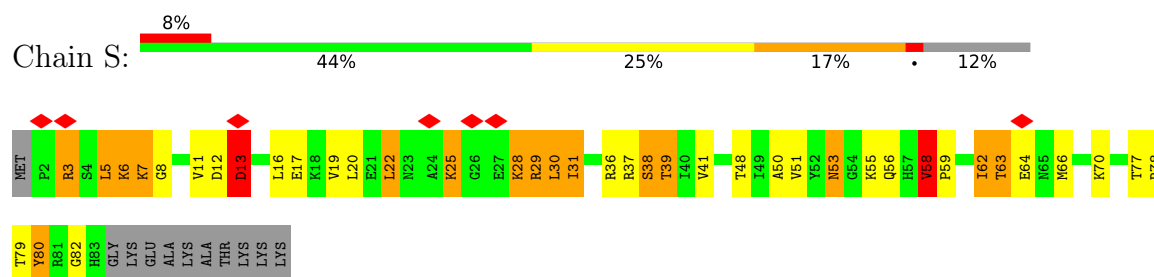
- Molecule 17: 30S ribosomal protein S17



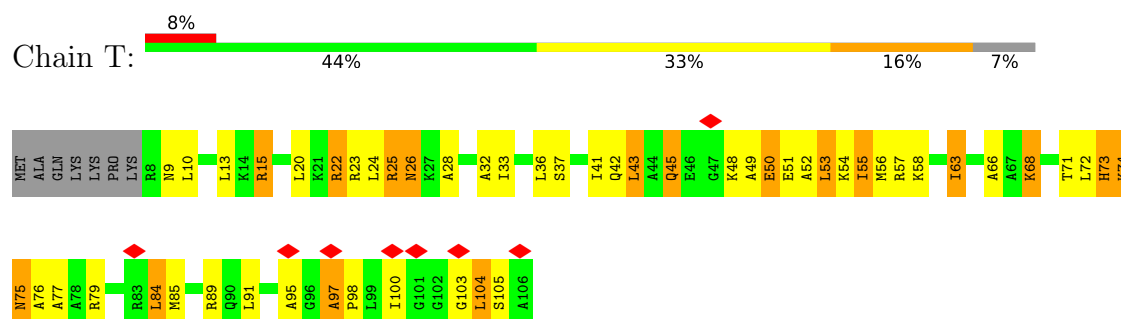
- Molecule 18: 30S ribosomal protein S18



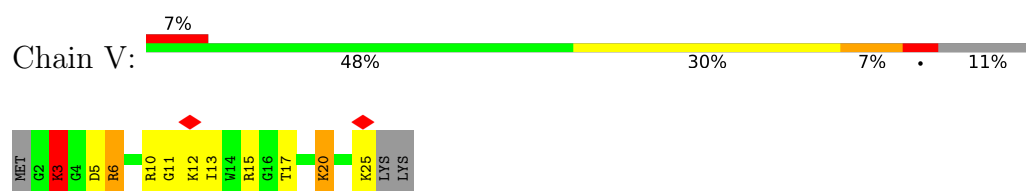
- Molecule 19: 30S ribosomal protein S19



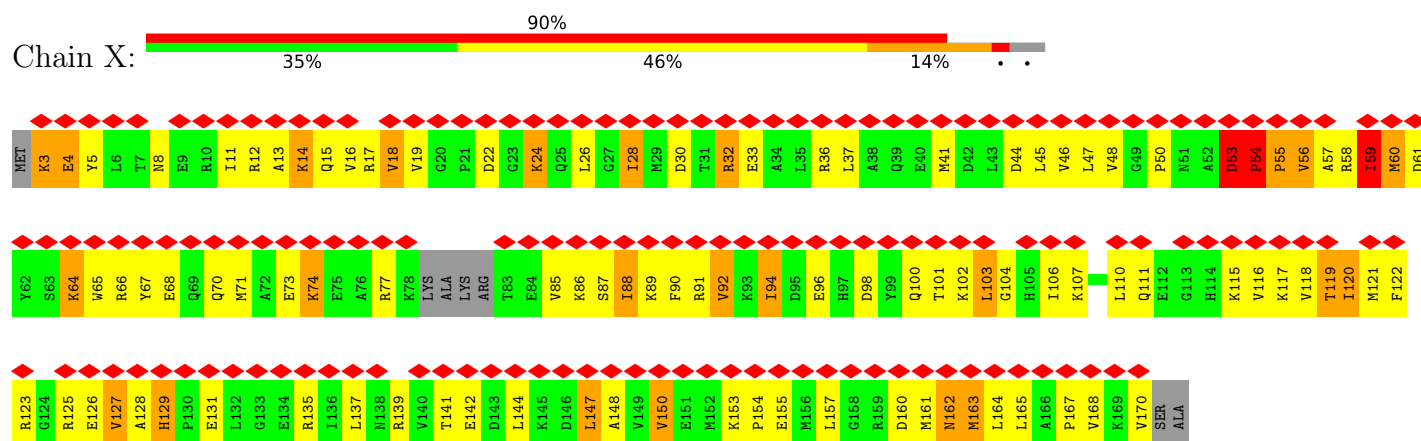
- Molecule 20: 30S ribosomal protein S20



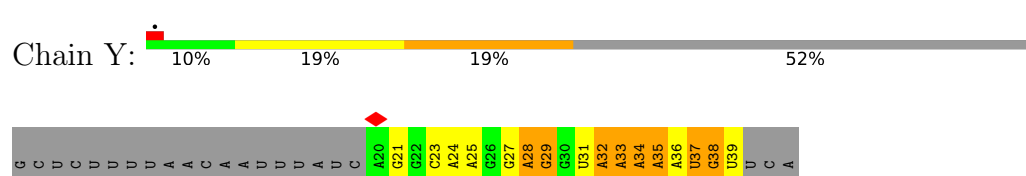
- Molecule 21: 30S ribosomal protein Thx



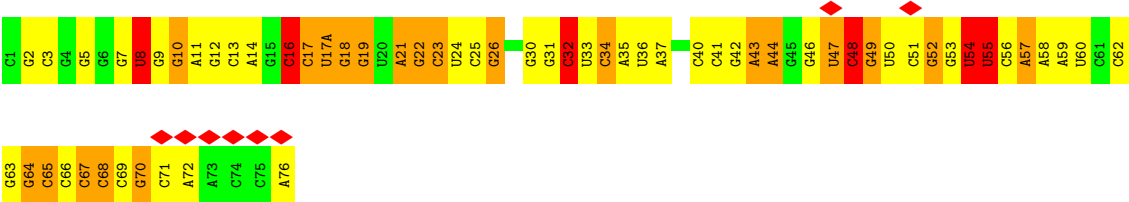
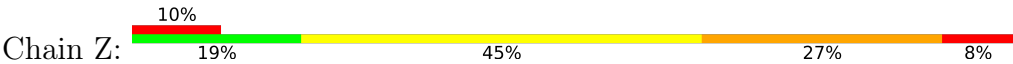
- Molecule 22: Translation initiation factor IF-3



- Molecule 23: mRNA



● Molecule 24: tRNAi



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.704	Depositor
Minimum map value	-0.271	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, G7M, ZN, MG, OMC, 4SU

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	0.42	0/36426	0.85	86/56837 (0.2%)
2	B	0.69	0/1935	1.26	3/2609 (0.1%)
3	C	0.57	0/1636	1.10	6/2205 (0.3%)
4	D	0.52	0/1733	1.20	8/2318 (0.3%)
5	E	0.55	0/1162	1.18	7/1564 (0.4%)
6	F	0.54	0/856	1.19	4/1154 (0.3%)
7	G	0.52	0/1276	1.17	0/1709
8	H	0.54	0/1136	1.07	3/1527 (0.2%)
9	I	0.54	0/1029	1.04	1/1379 (0.1%)
10	J	0.58	0/805	1.13	4/1082 (0.4%)
11	K	0.61	0/900	1.17	2/1213 (0.2%)
12	L	0.49	0/986	1.08	5/1320 (0.4%)
13	M	0.57	0/947	1.21	6/1270 (0.5%)
14	N	0.51	0/501	1.03	0/664
15	O	0.59	0/745	1.25	0/992
16	P	0.51	0/716	0.96	0/963
17	Q	0.48	0/836	1.03	1/1117 (0.1%)
18	R	0.55	0/604	1.12	0/801
19	S	0.57	0/670	1.14	1/903 (0.1%)
20	T	0.56	0/765	1.31	2/1007 (0.2%)
21	V	0.46	0/212	1.06	0/277
22	X	0.79	1/1354 (0.1%)	1.39	7/1813 (0.4%)
23	Y	0.46	0/493	0.90	0/766
24	Z	0.53	1/1721 (0.1%)	0.89	5/2682 (0.2%)
All	All	0.48	2/59444 (0.0%)	0.96	151/88172 (0.2%)

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	2
19	S	0	1
22	X	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	4	GLU	C-O	5.82	1.30	1.23
24	Z	8	4SU	O3'-P	5.79	1.62	1.56

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	X	4	GLU	N-CA-CB	-15.66	83.86	110.95
1	A	266	G	C2'-C3'-O3'	11.58	126.87	109.50
1	A	1145	C	C2'-C3'-O3'	10.72	125.58	109.50
1	A	1498	U	C2'-C3'-O3'	10.30	124.96	109.50
22	X	4	GLU	CB-CA-C	-10.18	96.78	111.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1445	C	Sidechain
1	A	218	C	Sidechain
19	S	3	ARG	Peptide
22	X	3	LYS	Peptide
22	X	53	ASP	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	32548	0	16440	1269	0
2	B	1900	0	1951	72	0
3	C	1612	0	1675	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1703	0	1767	93	0
5	E	1146	0	1207	46	0
6	F	843	0	857	27	0
7	G	1257	0	1296	15	0
8	H	1116	0	1177	20	0
9	I	1010	0	1037	32	0
10	J	792	0	834	99	0
11	K	885	0	904	17	0
12	L	970	0	1057	31	0
13	M	937	0	995	18	0
14	N	492	0	531	16	0
15	O	734	0	771	15	0
16	P	700	0	720	19	0
17	Q	823	0	891	24	0
18	R	598	0	670	17	0
19	S	655	0	672	26	0
20	T	763	0	861	46	0
21	V	208	0	221	9	0
22	X	1336	0	1388	87	0
23	Y	439	0	219	18	0
24	Z	1646	0	843	56	0
25	A	78	0	0	3	0
25	L	1	0	0	0	0
25	Z	1	0	0	0	0
26	D	1	0	0	1	0
26	N	1	0	0	1	0
All	All	55195	0	38984	1980	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 21.

The worst 5 of 1980 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)
10:J:38:ILE:HG23	10:J:71:LEU:CB	1.24	1.66
10:J:38:ILE:CG2	10:J:71:LEU:HB3	1.04	1.50
1:A:412:A:N3	4:D:35:ARG:NH1	1.66	1.44
1:A:1358:U:H3	1:A:1363(A):A:N6	1.13	1.43
1:A:1061:G:C5'	10:J:59:SER:OG	1.68	1.39

There are no symmetry-related clashes.

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 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	B	232/256 (91%)	184 (79%)	33 (14%)	15 (6%)	1	15
3	C	204/239 (85%)	174 (85%)	26 (13%)	4 (2%)	6	33
4	D	206/209 (99%)	176 (85%)	26 (13%)	4 (2%)	6	34
5	E	148/162 (91%)	125 (84%)	19 (13%)	4 (3%)	4	28
6	F	99/101 (98%)	87 (88%)	7 (7%)	5 (5%)	1	18
7	G	153/156 (98%)	132 (86%)	18 (12%)	3 (2%)	6	33
8	H	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	38
9	I	125/128 (98%)	104 (83%)	14 (11%)	7 (6%)	1	17
10	J	96/105 (91%)	79 (82%)	12 (12%)	5 (5%)	1	18
11	K	117/129 (91%)	94 (80%)	17 (14%)	6 (5%)	1	18
12	L	122/132 (92%)	95 (78%)	24 (20%)	3 (2%)	4	29
13	M	116/126 (92%)	100 (86%)	13 (11%)	3 (3%)	4	29
14	N	58/61 (95%)	44 (76%)	9 (16%)	5 (9%)	0	10
15	O	86/89 (97%)	77 (90%)	7 (8%)	2 (2%)	5	31
16	P	81/88 (92%)	71 (88%)	8 (10%)	2 (2%)	4	29
17	Q	97/105 (92%)	82 (84%)	10 (10%)	5 (5%)	1	18
18	R	71/88 (81%)	62 (87%)	8 (11%)	1 (1%)	9	39
19	S	80/93 (86%)	63 (79%)	12 (15%)	5 (6%)	1	15
20	T	97/106 (92%)	81 (84%)	11 (11%)	5 (5%)	1	18
21	V	22/27 (82%)	19 (86%)	1 (4%)	2 (9%)	0	10
22	X	160/171 (94%)	137 (86%)	17 (11%)	6 (4%)	2	22
All	All	2506/2709 (92%)	2111 (84%)	301 (12%)	94 (4%)	4	22

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
2	B	229	VAL
4	D	37	PRO
5	E	21	ALA

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	B	202/220 (92%)	150 (74%)	52 (26%)	0	4
3	C	160/188 (85%)	117 (73%)	43 (27%)	0	4
4	D	180/181 (99%)	130 (72%)	50 (28%)	0	3
5	E	115/123 (94%)	80 (70%)	35 (30%)	0	2
6	F	90/90 (100%)	73 (81%)	17 (19%)	1	11
7	G	126/127 (99%)	102 (81%)	24 (19%)	1	10
8	H	119/119 (100%)	79 (66%)	40 (34%)	0	2
9	I	98/99 (99%)	78 (80%)	20 (20%)	1	8
10	J	87/92 (95%)	69 (79%)	18 (21%)	1	7
11	K	90/99 (91%)	68 (76%)	22 (24%)	1	5
12	L	104/109 (95%)	76 (73%)	28 (27%)	0	4
13	M	94/101 (93%)	78 (83%)	16 (17%)	2	13
14	N	49/50 (98%)	37 (76%)	12 (24%)	1	5
15	O	79/80 (99%)	53 (67%)	26 (33%)	0	2
16	P	72/74 (97%)	58 (81%)	14 (19%)	1	10
17	Q	94/97 (97%)	75 (80%)	19 (20%)	1	9
18	R	64/77 (83%)	46 (72%)	18 (28%)	0	3
19	S	71/80 (89%)	48 (68%)	23 (32%)	0	2
20	T	76/82 (93%)	52 (68%)	24 (32%)	0	2
21	V	19/22 (86%)	15 (79%)	4 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	X	145/150 (97%)	110 (76%)	35 (24%)	1	5
All	All	2134/2260 (94%)	1594 (75%)	540 (25%)	2	4

5 of 540 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
19	S	79	THR
19	S	29	ARG
22	X	77	ARG
6	F	79	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	78	ASN
12	L	99	HIS
22	X	129	HIS
10	J	84	GLN
12	L	8	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1522 (99%)	460 (30%)	109 (7%)
23	Y	19/42 (45%)	10 (52%)	1 (5%)
24	Z	76/77 (98%)	37 (48%)	5 (6%)
All	All	1604/1641 (97%)	507 (31%)	115 (7%)

5 of 507 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	19	C
1	A	22	G

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	932	C
24	Z	3	C
1	A	1145	C
23	Y	32	A
1	A	1442(B)	A

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

5 non-standard protein/DNA/RNA residues 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$
24	4SU	Z	8	24	18,21,22	1.77	5 (27%)	25,30,33	2.43	8 (32%)
24	G7M	Z	46	24	23,26,27	2.43	5 (21%)	34,39,42	3.01	13 (38%)
24	5MU	Z	54	24	19,22,23	1.57	4 (21%)	27,32,35	1.85	6 (22%)
24	PSU	Z	55	24	18,21,22	1.47	3 (16%)	21,30,33	2.46	6 (28%)
24	OMC	Z	32	24	19,22,23	0.93	1 (5%)	25,31,34	1.27	3 (12%)

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
24	4SU	Z	8	24	-	0/7/25/26	0/2/2/2
24	G7M	Z	46	24	-	0/7/25/26	0/3/3/3
24	5MU	Z	54	24	-	3/7/25/26	0/2/2/2
24	PSU	Z	55	24	-	5/7/25/26	0/2/2/2
24	OMC	Z	32	24	-	3/9/27/28	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	46	G7M	C8-N7	7.98	1.46	1.33
24	Z	55	PSU	C6-C5	4.61	1.40	1.35
24	Z	46	G7M	C8-N9	4.58	1.48	1.35
24	Z	8	4SU	C4-S4	-4.54	1.60	1.68
24	Z	46	G7M	C5-C4	4.19	1.48	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	46	G7M	CN7-N7-C8	-8.30	112.22	124.79
24	Z	46	G7M	N9-C8-N7	-6.58	96.51	112.48
24	Z	46	G7M	C8-N7-C5	6.10	115.41	107.78
24	Z	55	PSU	C6-C5-C4	-5.83	114.24	118.17
24	Z	55	PSU	N1-C2-N3	5.76	121.24	115.17

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	Z	32	OMC	O4'-C4'-C5'-O5'
24	Z	54	5MU	O4'-C4'-C5'-O5'
24	Z	55	PSU	C2'-C1'-C5-C4
24	Z	55	PSU	C2'-C1'-C5-C6
24	Z	55	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Z	8	4SU	1	0
24	Z	54	5MU	1	0
24	Z	55	PSU	2	0
24	Z	32	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 82 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
23	Y	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1442(A):G	O3'	1442(B):A	P	5.11
1	A	84:U	O3'	88:A	P	5.07
1	A	93:G	O3'	96:U	P	4.99
1	A	204:U	O3'	216:G	P	4.97
1	A	841:U	O3'	848:C	P	4.05

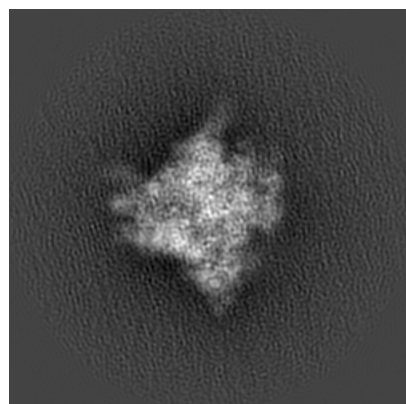
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4080. These allow visual inspection of the internal detail of the map and identification of artifacts.

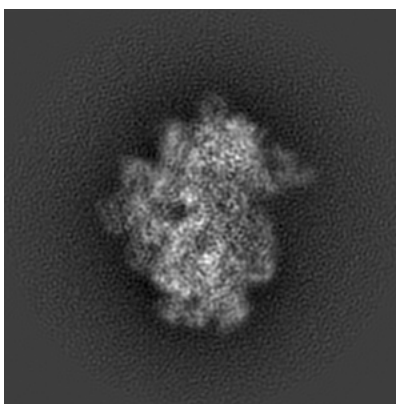
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

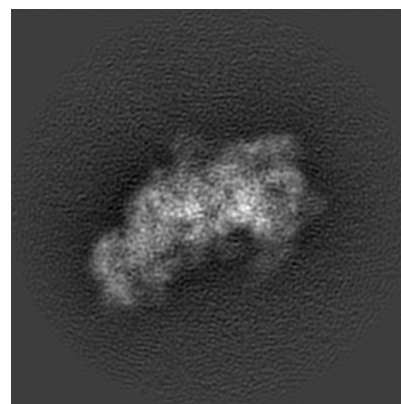
6.1.1 Primary map



X

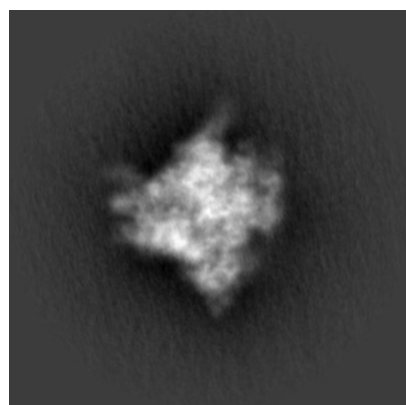


Y

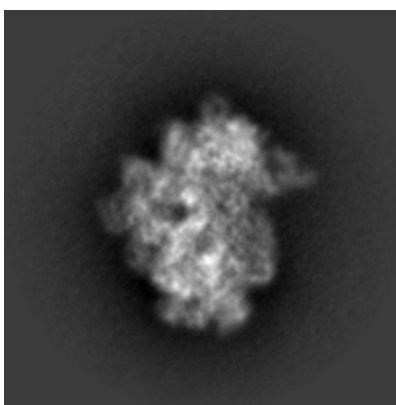


Z

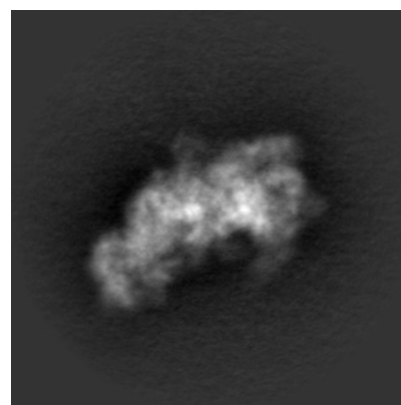
6.1.2 Raw map



X



Y

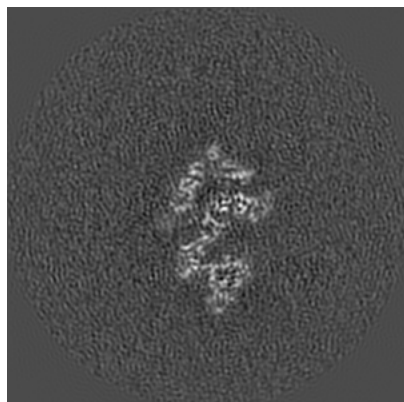


Z

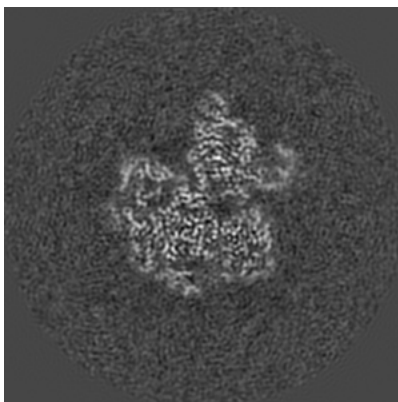
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

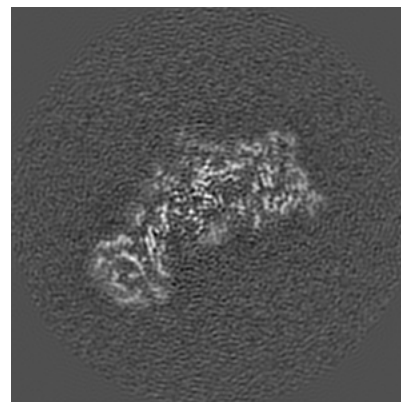
6.2.1 Primary map



X Index: 130

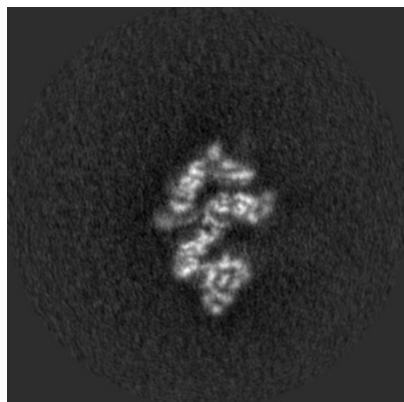


Y Index: 130

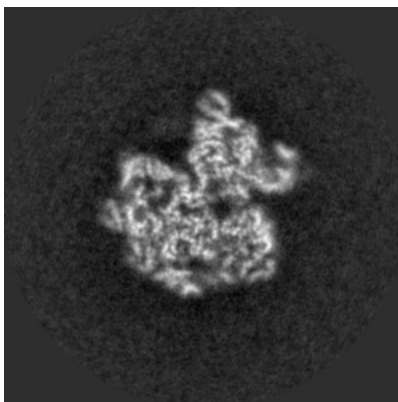


Z Index: 130

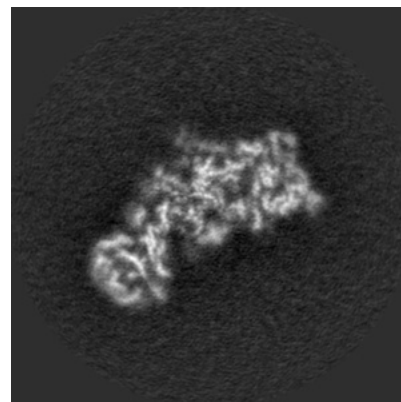
6.2.2 Raw map



X Index: 130



Y Index: 130

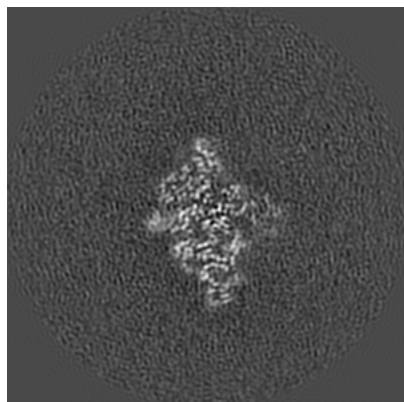


Z Index: 130

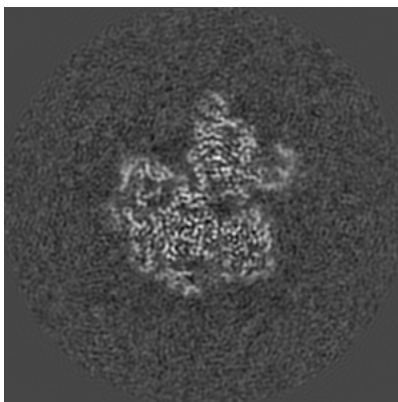
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

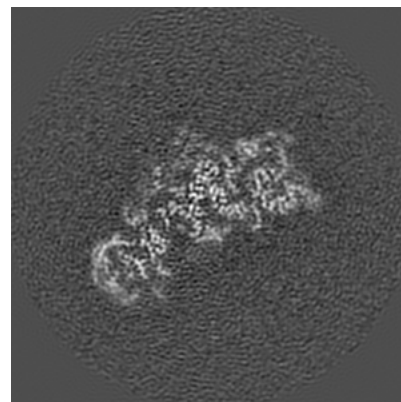
6.3.1 Primary map



X Index: 119

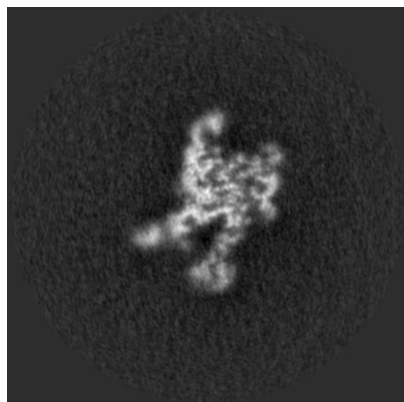


Y Index: 130

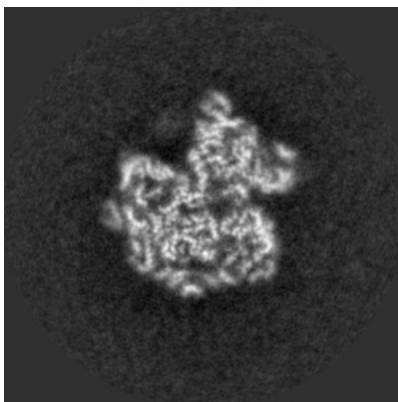


Z Index: 128

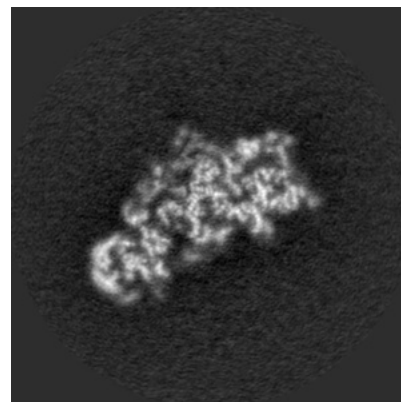
6.3.2 Raw map



X Index: 161



Y Index: 129

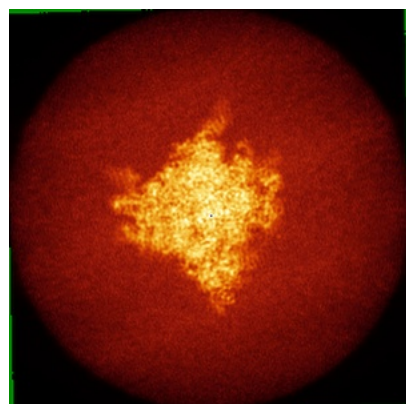


Z Index: 127

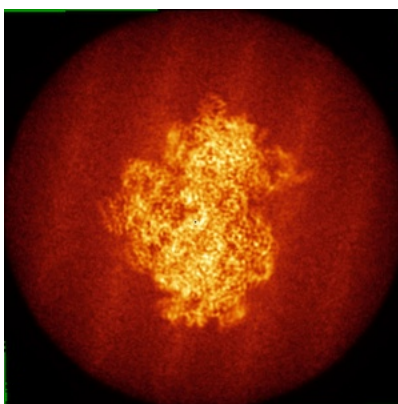
The images above show the largest variance slices of the map in three orthogonal directions.

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

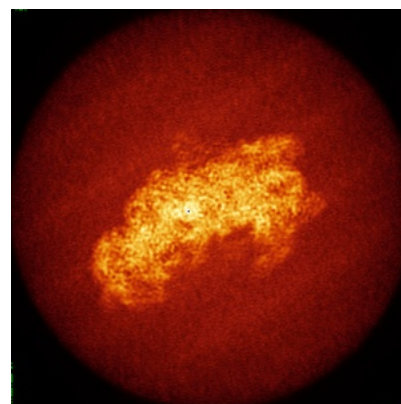
6.4.1 Primary map



X

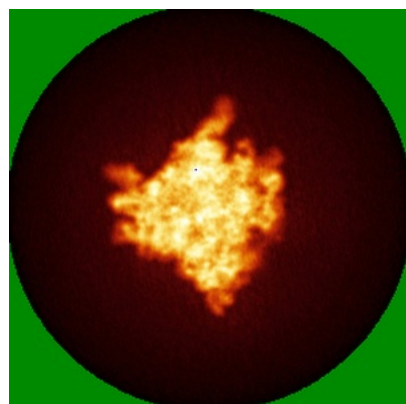


Y

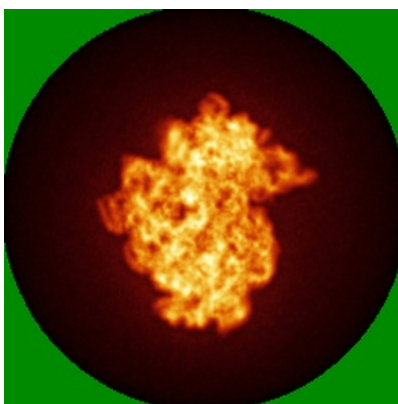


Z

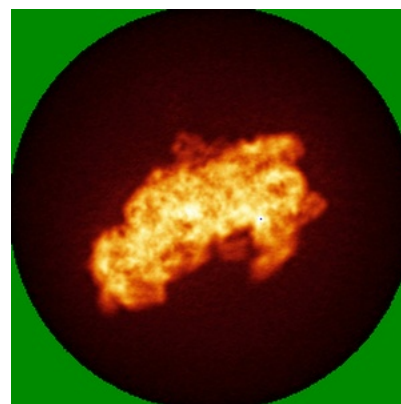
6.4.2 Raw map



X



Y

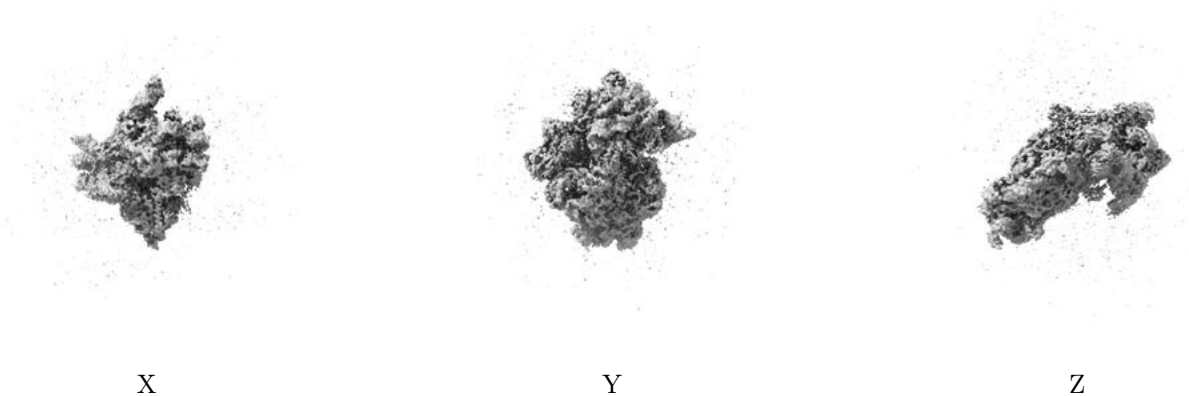


Z

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.

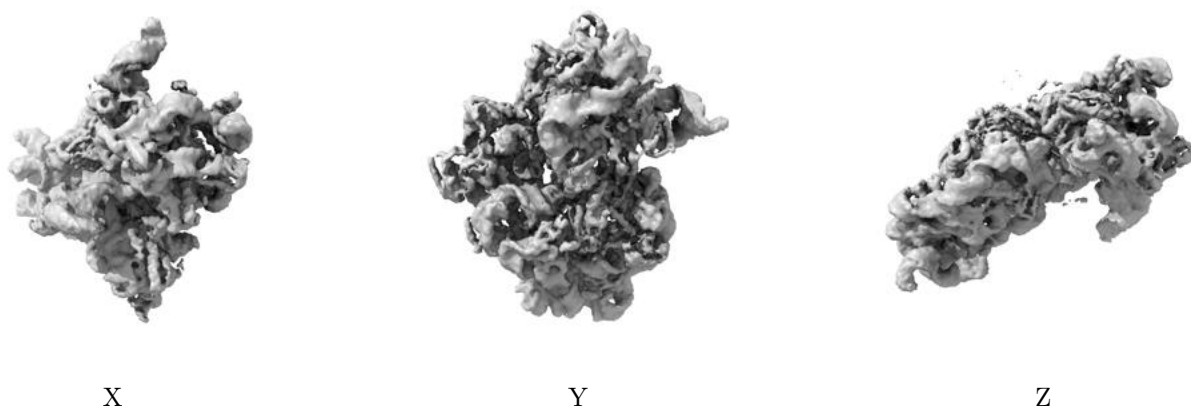
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

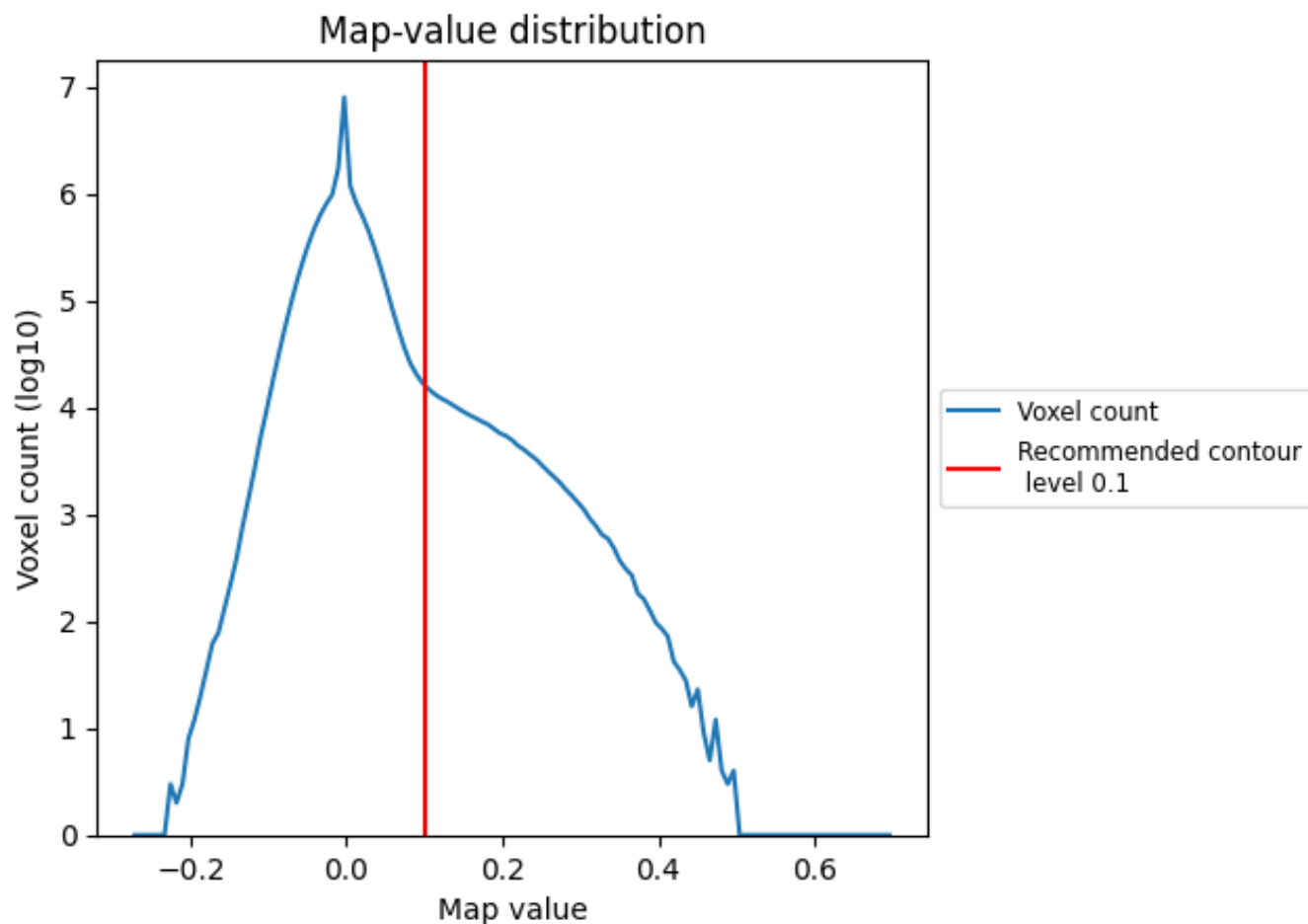
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

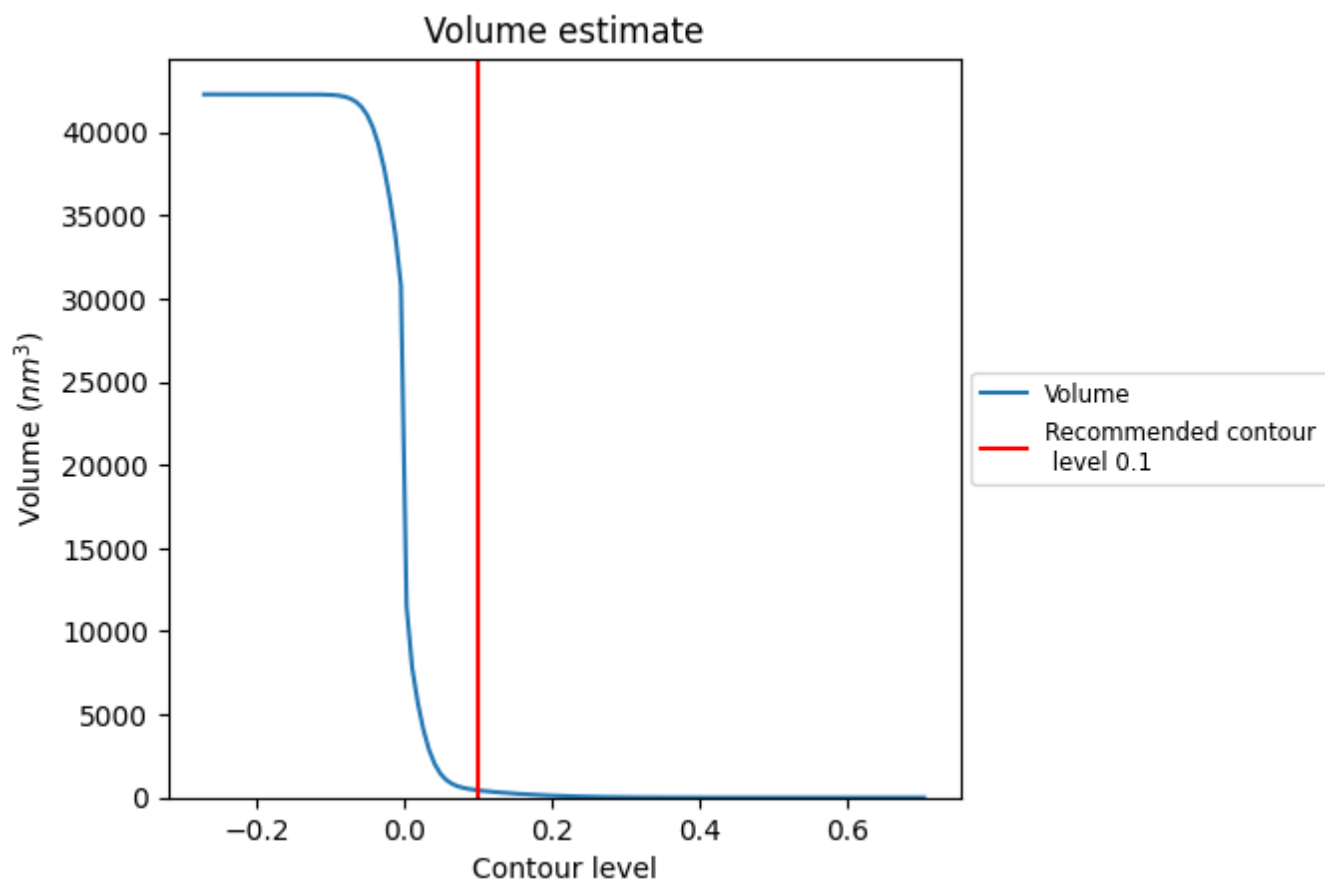
This section contains the results of statistical analysis of the map.

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.

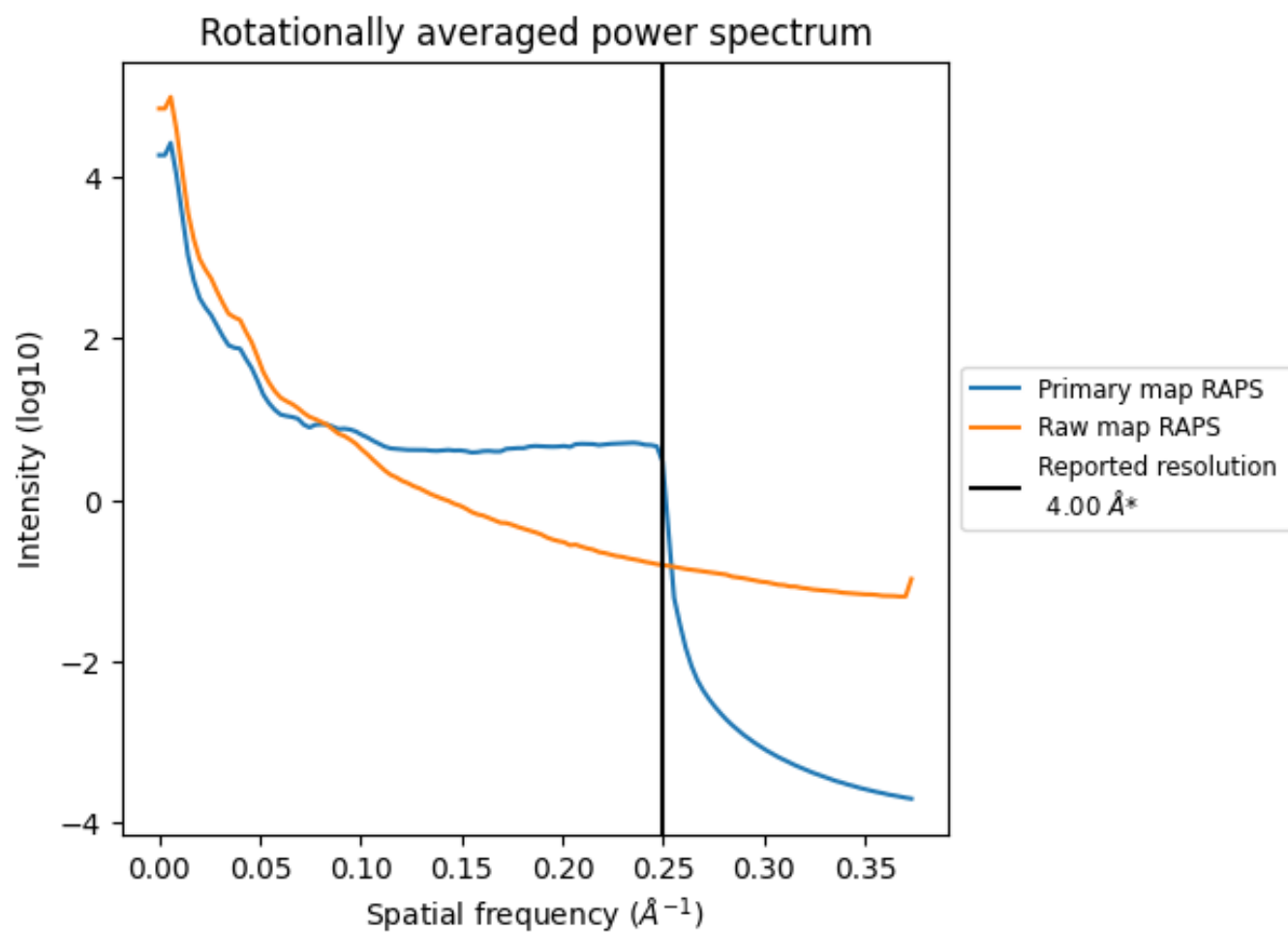
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 435 nm³; this corresponds to an approximate mass of 393 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 ⓘ

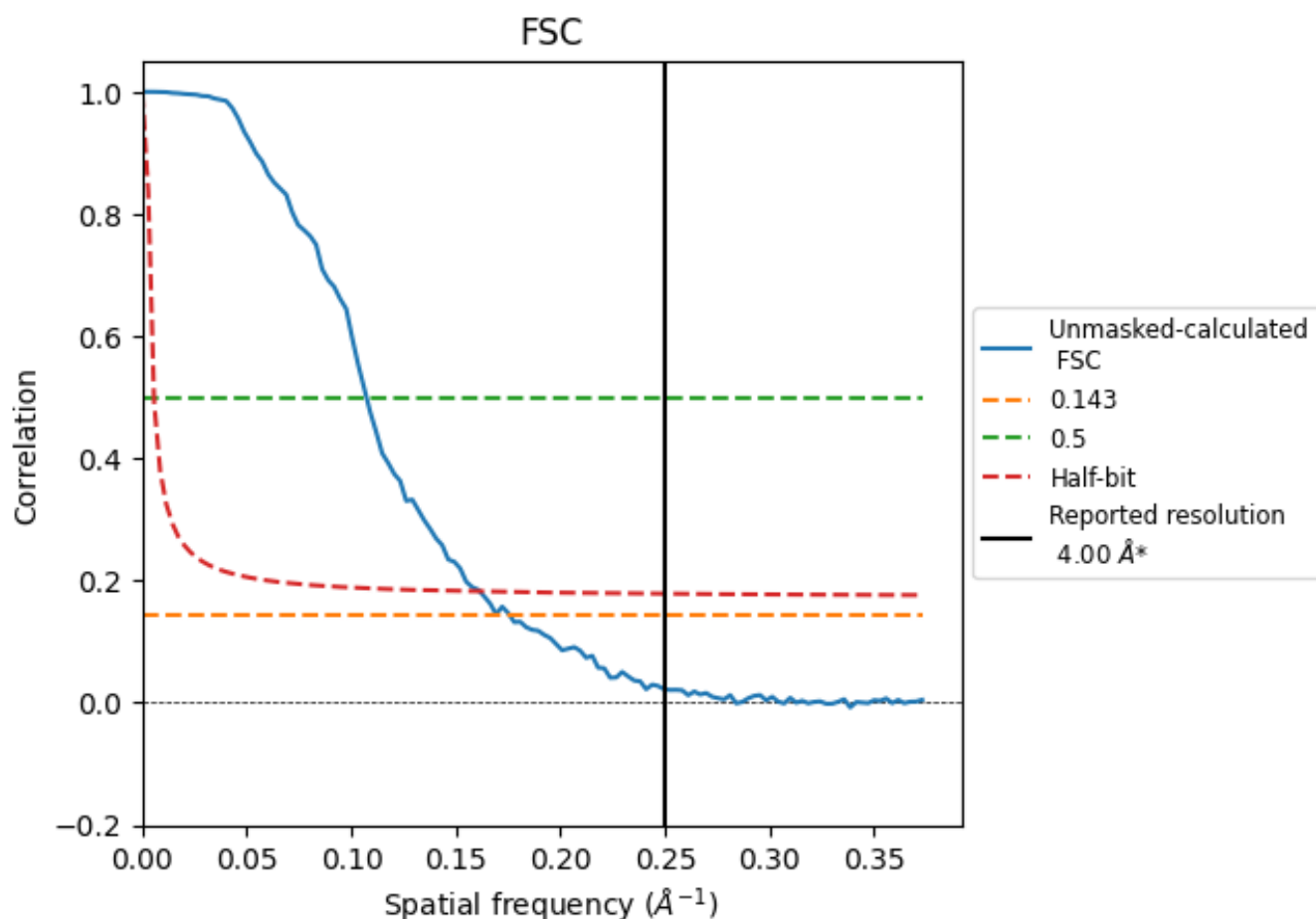


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

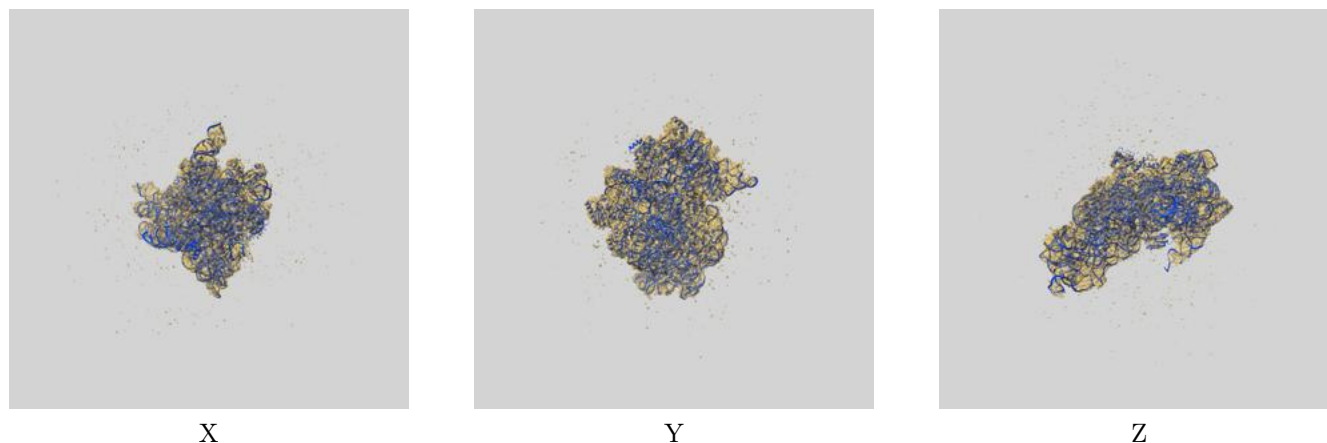
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.69	9.32	6.19

*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 5.69 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

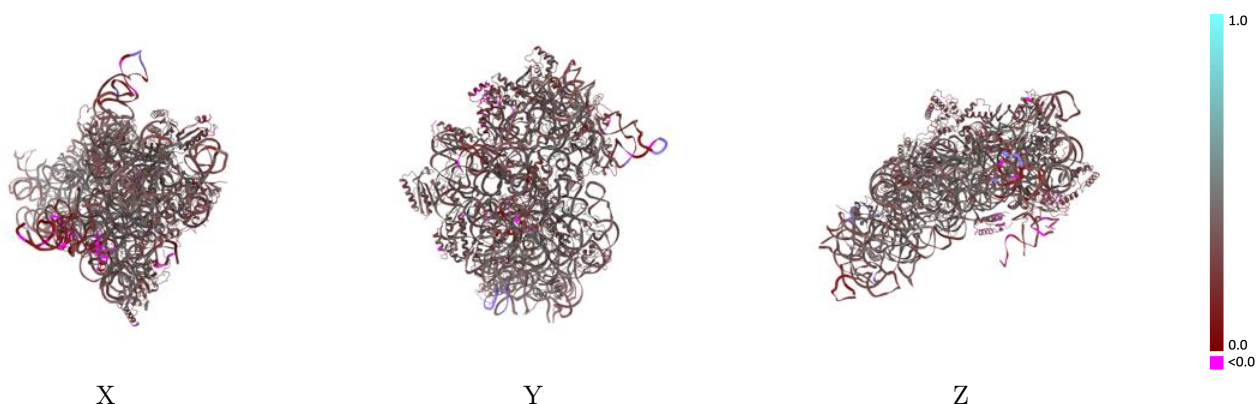
This section contains information regarding the fit between EMDB map EMD-4080 and PDB model 5LMU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



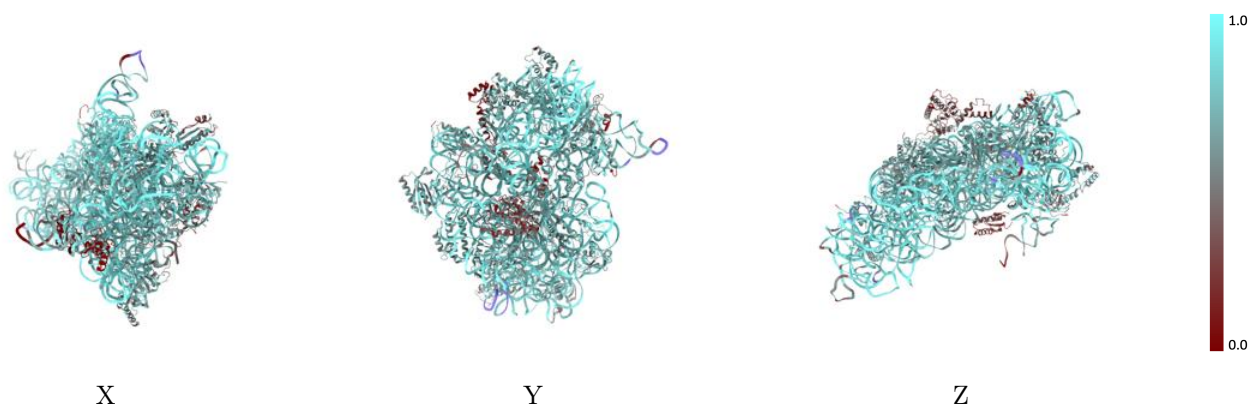
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



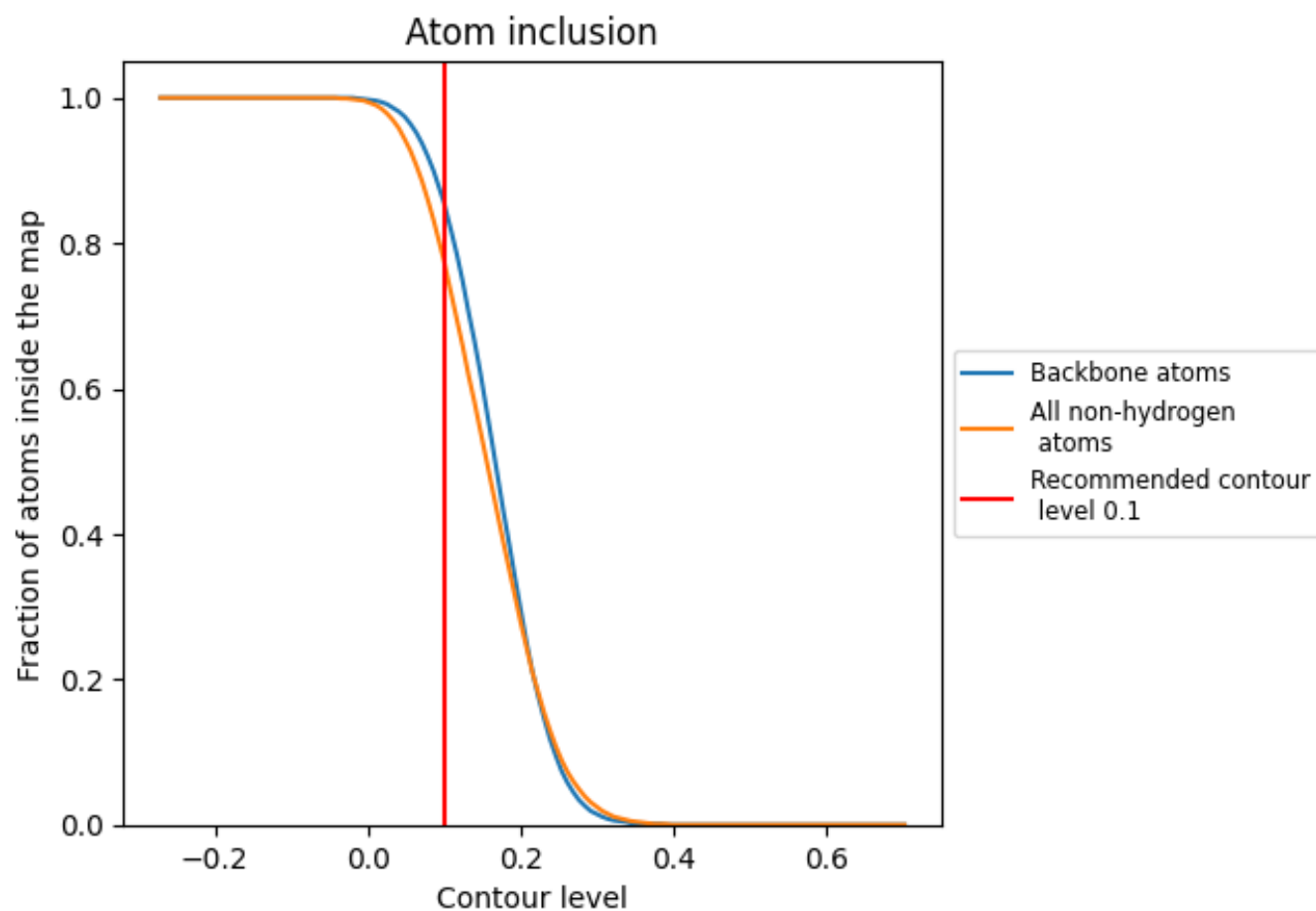
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.3550
A	 0.8820	 0.3710
B	 0.2920	 0.2820
C	 0.6890	 0.3870
D	 0.6780	 0.3620
E	 0.6920	 0.3980
F	 0.6460	 0.3530
G	 0.6610	 0.3550
H	 0.6850	 0.3790
I	 0.6910	 0.3680
J	 0.5780	 0.3320
K	 0.6640	 0.3540
L	 0.6920	 0.4180
M	 0.6860	 0.3420
N	 0.7350	 0.4010
O	 0.6650	 0.3500
P	 0.7420	 0.3990
Q	 0.6980	 0.4060
R	 0.6420	 0.3500
S	 0.6750	 0.3360
T	 0.6620	 0.3310
V	 0.7490	 0.3640
X	 0.1150	 0.1040
Y	 0.7450	 0.2960
Z	 0.7240	 0.1910

