



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 12:42 PM JST

PDB ID : 3J2F
EMDB ID : EMD-5508
Title : Dissecting the in vivo assembly of the 30S ribosomal subunit reveals the role of RimM
Authors : Guo, Q.; Goto, S.; Chen, Y.; Muto, A.; Himeno, H.; Deng, H.; Lei, J.; Gao, N.
Deposited on : 2012-09-28
Resolution : 17.60 Å (reported)
Based on initial model : 3OFA

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.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

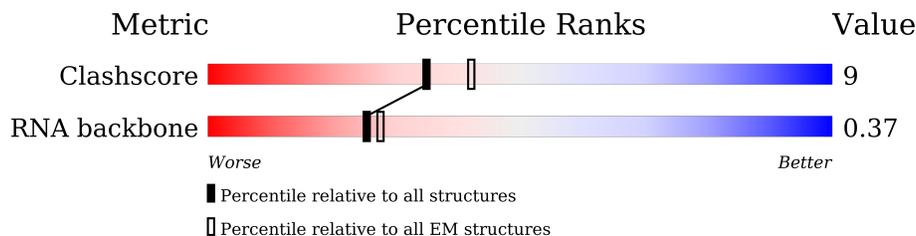
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.60 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
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	N	1533	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49446 atoms, of which 16554 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.

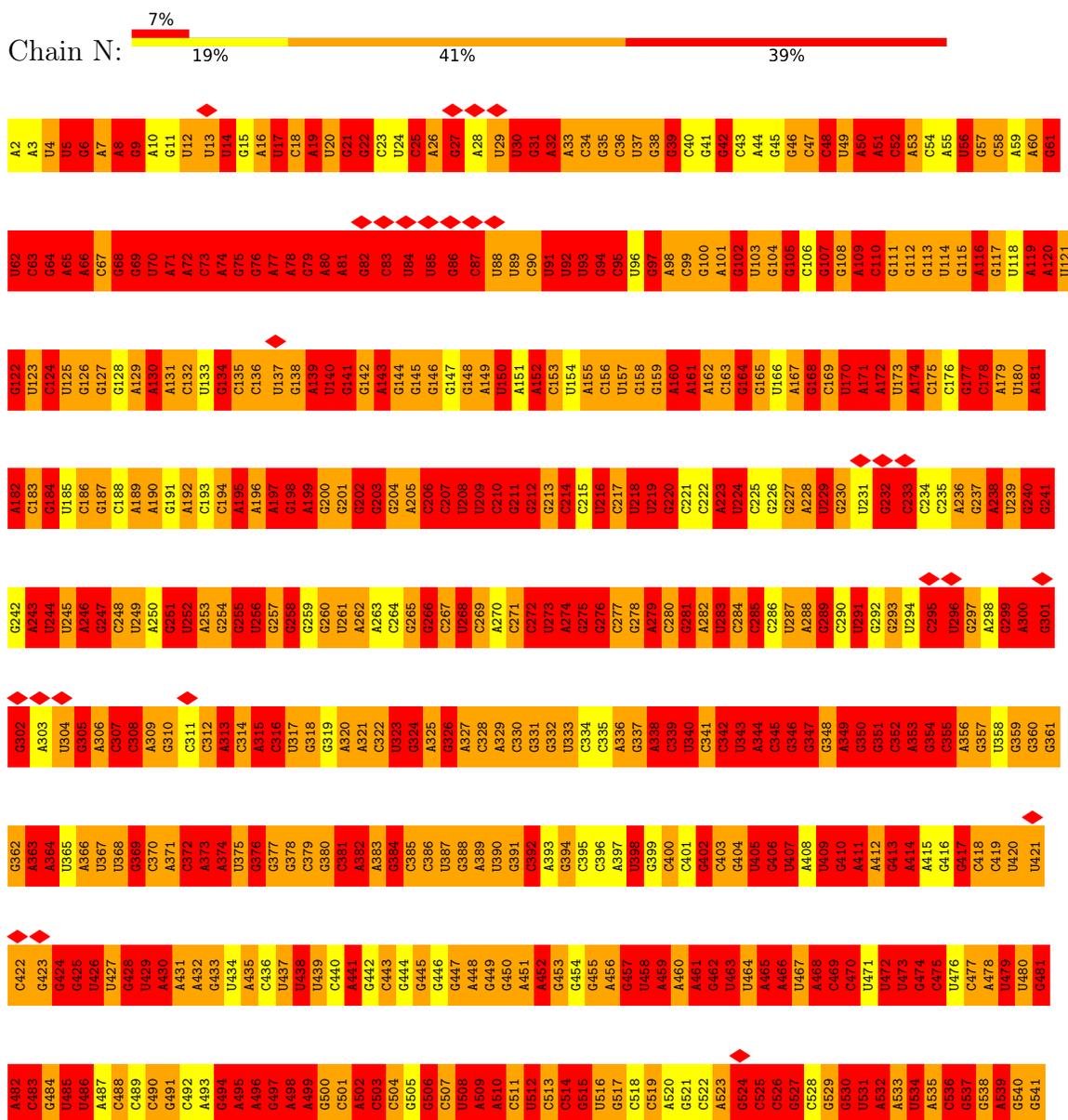
- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
1	N	1533	49446	14671	16554	6036	10653	1532	0	0

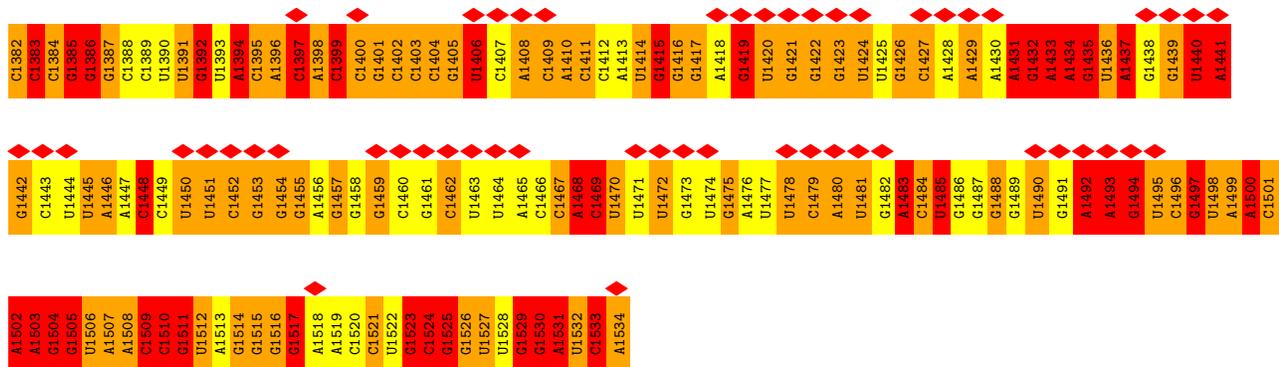
3 Residue-property plots i

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: 16S rRNA



C1322	C1323	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	A1346	G1347	A1348	A1349	A1350	U1351	U1352	C1353	G1354	G1355	G1356	A1357	C1358	A1360	G1361	A1362	A1363	U1364	G1365	C1366	C1367	A1368	C1369	G1370	G1371	U1372	A1373	A1374	A1375	U1376	A1377	C1378	G1379	U1380	U1381				
C1262	C1263	C1264	C1265	C1266	C1268	A1269	C1270	A1271	C1272	C1273	A1274	A1275	C1276	C1277	C1278	G1279	A1280	C1281	C1282	C1283	C1284	C1285	U1286	A1287	A1288	A1289	A1290	U1291	U1292	C1293	C1294	U1295	C1296	G1297	U1298	A1299	G1300	C1301	C1302	C1303	U1304	G1305	A1306	U1307	U1308	G1309	G1310	A1311	G1312	U1313	G1253	A1254	U1315	G1316	C1317	A1318	A1319	C1320	U1321		
G1142	G1143	A1144	U1145	A1146	C1147	U1148	C1149	A1150	A1151	A1152	G1153	G1154	A1155	G1156	A1157	U1158	U1159	G1160	C1161	C1162	A1163	G1164	U1165	G1166	A1167	U1168	A1169	A1170	A1171	C1172	U1173	G1174	G1175	A1176	G1177	G1178	A1179	A1180	G1181	U1182	U1183	G1184	G1185	U1186	G1187	A1188	U1189	G1190	A1191	C1192	G1193	U1194	C1195	A1196	U1197	G1198	U1199	C1200	A1201		
U1202	C1203	A1204	U1205	G1206	C1207	U1208	C1209	C1210	U1211	U1212	A1213	C1214	G1215	A1216	C1217	G1218	A1219	C1220	G1221	G1222	C1223	U1224	A1225	C1226	A1227	C1228	A1229	U1230	G1231	U1232	C1233	C1234	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1242	C1243	G1244	C1245	A1246	U1247	A1248	C1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1258	C1259	G1260	A1261		
G1082	U1083	G1084	U1085	U1086	G1087	U1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	C1096	G1097	C1098	G1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	G1114	U1115	U1116	A1117	U1118	C1119	C1120	U1121	U1122	U1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	G1133	G1134	U1135	U1136	C1137	U1138	G1139	C1140	C1141		
A1022	U1023	G1024	U1025	U1026	G1027	C1028	U1029	U1030	C1031	C1032	G1033	A1034	A1035	A1036	C1037	C1038	G1039	A1040	G1041	A1042	G1043	A1044	C1045	G1046	G1047	U1048	U1049	C1050	C1051	U1052	G1053	A1054	A1055	U1056	G1057	G1058	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	U1073	G1074	U1075	U1076	G1077	U1078	G1079	A1080	A1081		
C982	G983	U984	U985	U986	A987	A988	A989	A990	C991	G992	C993	A994	A995	A996	C997	A998	C999	A1000	C1001	G1002	C1003	U1004	G1005	A1006	G1006	U1007	C1008	U1009	U1010	G1011	U1012	G1013	A1014	G1015	U1016	U1017	A1018	G1019	U1020	A1021																					
U842	U843	G844	U845	G846	G847	C848	G849	U850	G851	C852	U853	U854	U855	C856	G857	G858	U859	A860	C861	G862	A863	U864	A865	C866	C867	C868	G869	C870	U871	U872	U873	A874	C875	U876	G877	U878	C879	U880	C881	U882	C883	U884	G885	G886	U887	G888	G889	U890	A891	C892	U893	C894	U895	U896	U897	A898	G899	A900	A901		
G922	G923	U924	U925	G926	G927	C928	U929	C930	C931	C932	G933	C934	A935	C936	U937	A938	C939	C940	G941	G942	C943	G944	G945	A946	U947	C948	A949	U950	U951	U952	G953	U954	G955	U956	U957	A958	G959	U960	U961																						
A782	C783	G784	U785	G786	C787	U788	U789	A790	G791	C792	U793	A794	U795	C796	C797	U798	G799	A800	U801	G802	C803	U804	C805	C806	A807	C808	G809	C810	U811	U812	U813	A814	A815	U816	C817	G818	A819	U820	C821	U822	C823	U824	C825	C826	U827	U828	G829	U830	C831	C832	G833	A834	C835	U836	U837	C838	U839	C840	C841		
G722	U723	G724	U725	G726	C727	U728	A729	G730	C731	U732	G733	A734	C735	C736	C737	U738	C739	G740	G741	A822	G823	U824	C825	A826	C827	G828	C829	G830	C831	U832	U833	A834	A835	U836	C837	U838	C839	G700	U701	A641	C642	U643	G644	A704	G705	A706	U707	C708	U709	G710	U711	A712	U713	G714	A715	U716	C717	A718	C719	U720	G721
U662	A663	G664	U665	G666	C667	U668	A669	G670	U671	C672	U673	A674	C675	A676	U677	C678	C679	A680	C681	A682	G683	U684	C685	U686	A687	G688	C689	G690	C691	U692	G693	A694	A695	U696	C697	U698	C699	G700	U701	A641	C642	U643	G644	A704	G705	A706	U707	C708	U709	G710	U711	A712	U713	G714	A715	U716	C717	A718	C719	U720	G721
U542	U543	G544	U545	C546	A547	G548	C549	U550	U551	U552	A553	A554	U555	C556	G557	U558	A559	U560	U561	U562	A563	C564	U565	G566	C567	U568	C569	G570	U571	A572	A573	U574	G575	C576	U577	C578	U579	A580	C581	C582	A583	G584	U585	C586	G587	U588	U589	U590	U591	U592	U593	U594	A595	U596	A597	U598	C599	A600	G601		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9609	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	6.063	Depositor
Minimum map value	-8.451	Depositor
Average map value	-4.957	Depositor
Map value standard deviation	0.711	Depositor
Recommended contour level	-2.8	Depositor
Map size (\AA)	375.0, 375.0, 375.0	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	3.0, 3.0, 3.0	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	N	3.47	5279/36831 (14.3%)	3.93	9337/57458 (16.3%)

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	N	0	941

The worst 5 of 5279 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1299	A	N9-C4	19.01	1.49	1.37
1	N	250	A	N7-C5	-17.90	1.28	1.39
1	N	942	G	N7-C5	-17.43	1.28	1.39
1	N	1093	A	C6-N6	17.36	1.47	1.33
1	N	710	G	N7-C5	-17.22	1.28	1.39

The worst 5 of 9337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1399	C	P-O3'-C3'	28.06	153.38	119.70
1	N	913	A	P-O3'-C3'	27.42	152.60	119.70
1	N	168	G	N1-C6-O6	27.05	136.13	119.90
1	N	1157	A	N1-C6-N6	26.02	134.21	118.60
1	N	168	G	C5-C6-O6	-25.86	113.09	128.60

There are no chirality outliers.

5 of 941 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	5	U	Sidechain
1	N	6	G	Sidechain
1	N	7	A	Sidechain
1	N	8	A	Sidechain
1	N	9	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	32892	16554	16526	428	0
All	All	32892	16554	16526	428	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 9.

The worst 5 of 428 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:N:203:G:H22	1:N:206:C:H41	1.34	0.73
1:N:594:U:C4	1:N:595:A:C6	2.77	0.73
1:N:67:C:H2'	1:N:68:G:C8	2.25	0.72
1:N:664:G:H22	1:N:741:G:H1	1.39	0.70
1:N:780:A:C2	1:N:801:U:C5	2.80	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	1532/1533 (99%)	452 (29%)	147 (9%)

5 of 452 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	4	U
1	N	5	U
1	N	6	G
1	N	8	A
1	N	9	G

5 of 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1214	C
1	N	1502	A
1	N	1251	A
1	N	1345	U
1	N	372	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

There are no chain breaks in this entry.

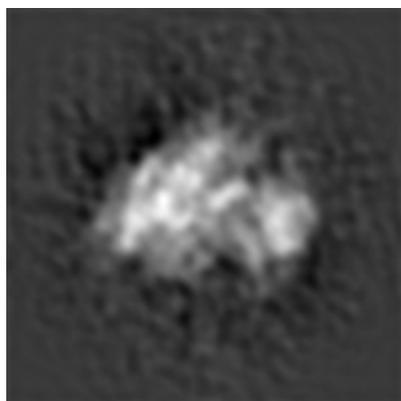
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5508. These allow visual inspection of the internal detail of the map and identification of artifacts.

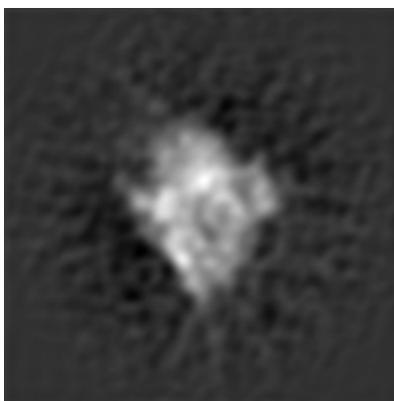
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

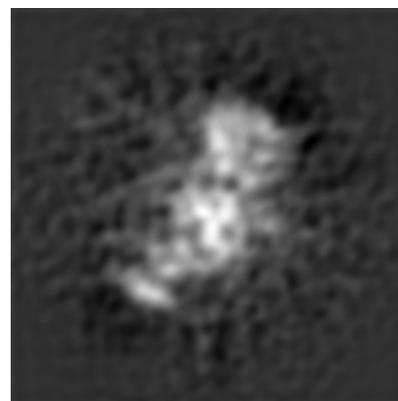
6.1.1 Primary map



X



Y

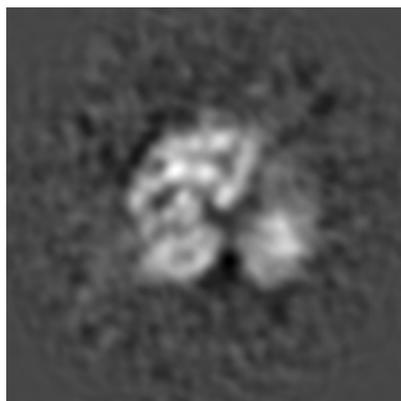


Z

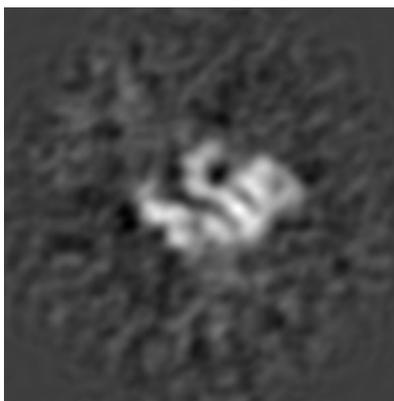
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

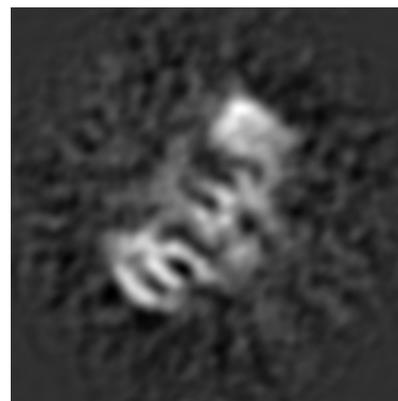
6.2.1 Primary map



X Index: 62



Y Index: 62

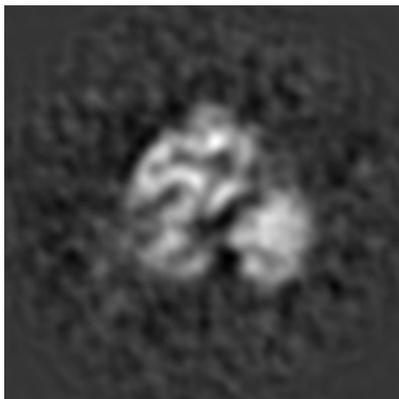


Z Index: 62

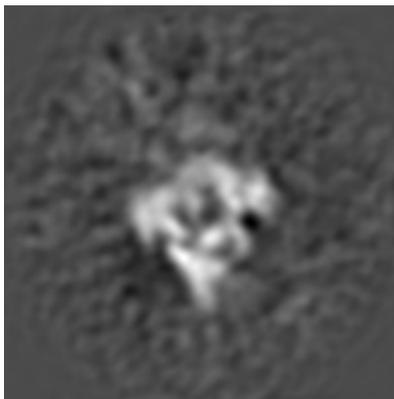
The images above show central slices of the map in three orthogonal directions.

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

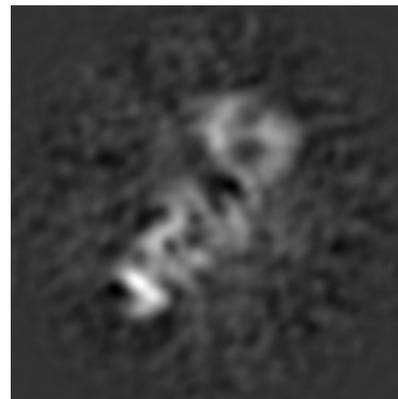
6.3.1 Primary map



X Index: 65



Y Index: 50

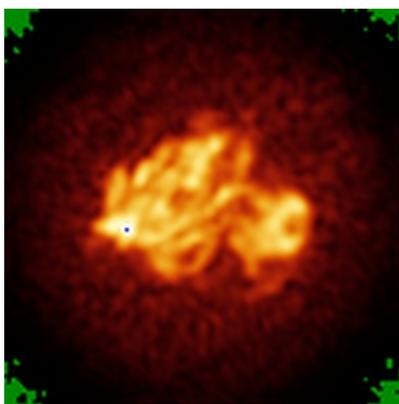


Z Index: 57

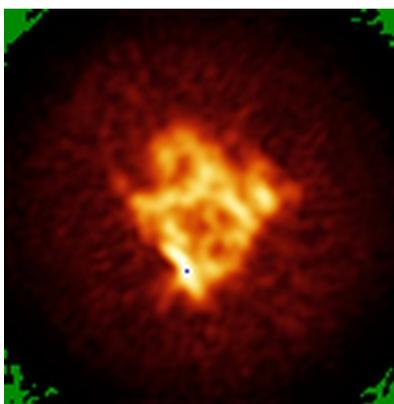
The images above show the largest variance slices of the map in three orthogonal directions.

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

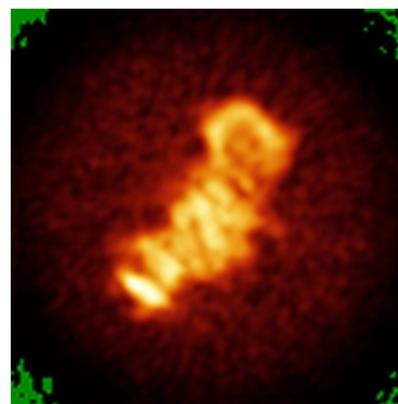
6.4.1 Primary map



X



Y

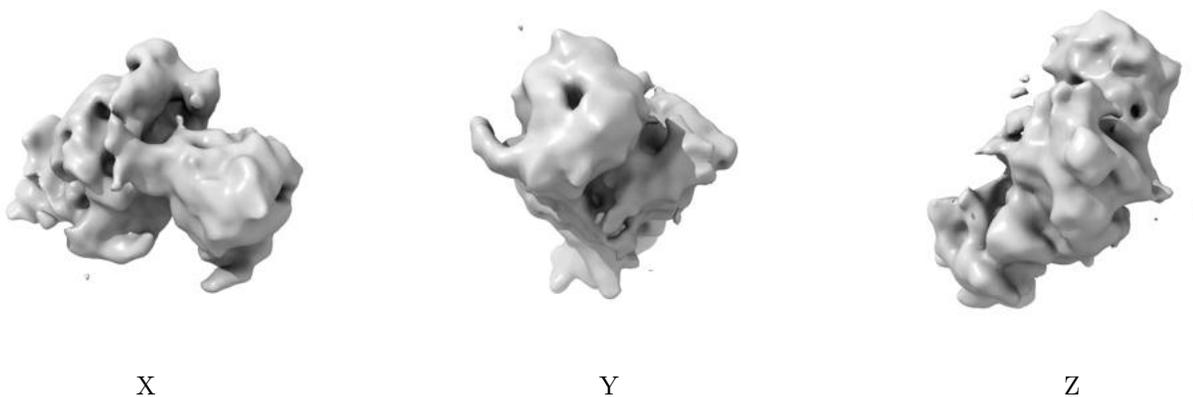


Z

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 - 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

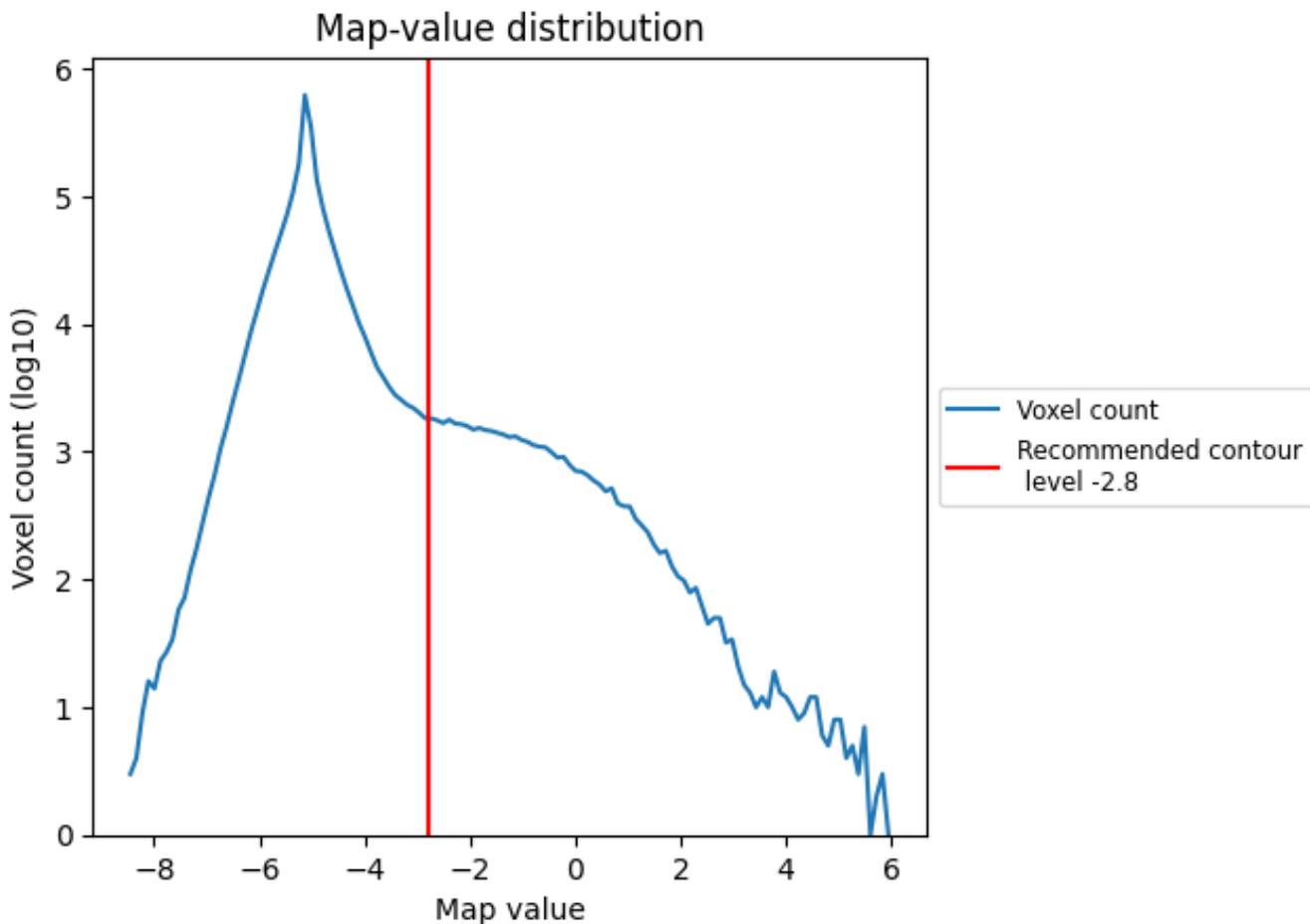
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

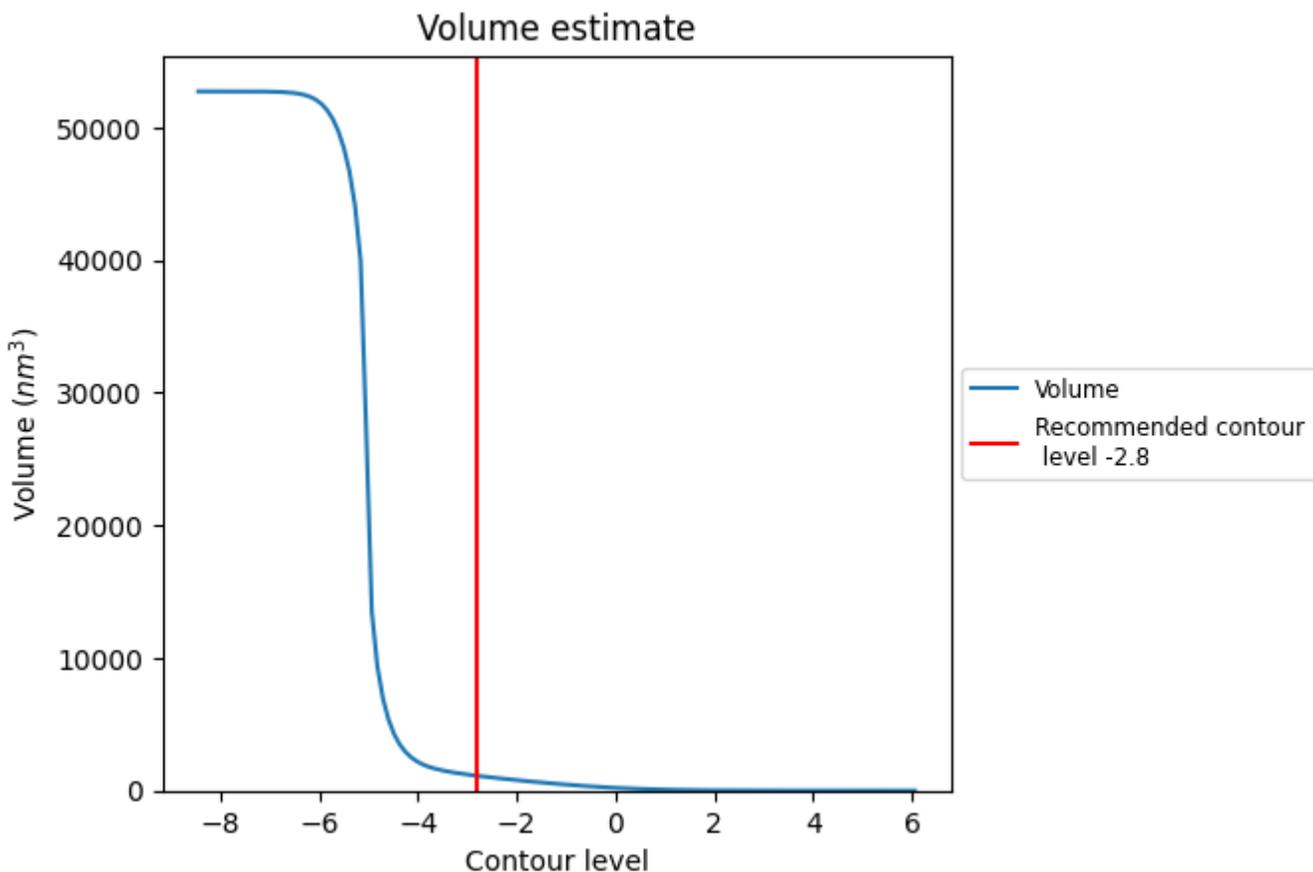
This section contains the results of statistical analysis of the map.

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.

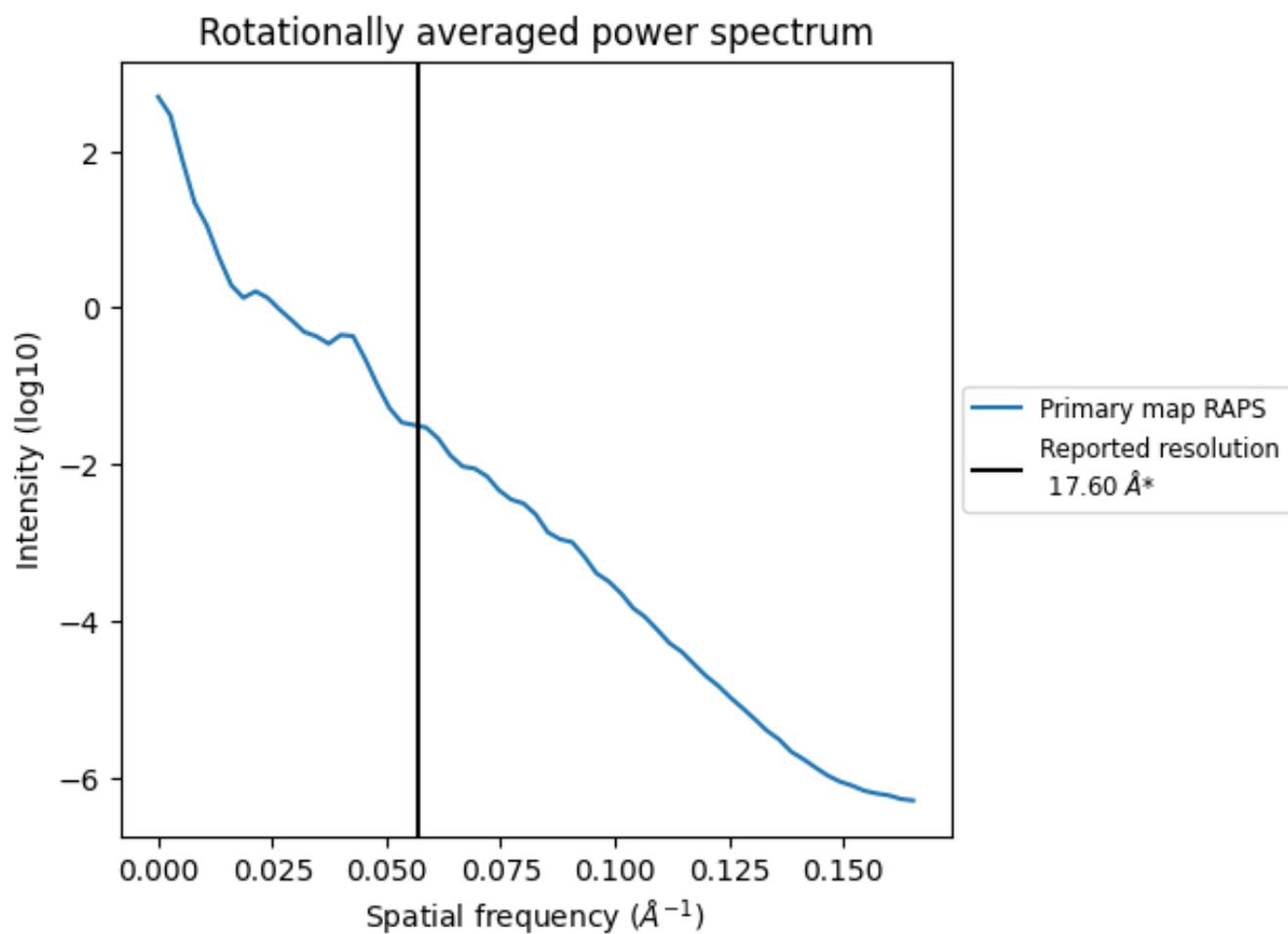
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1116 nm³; this corresponds to an approximate mass of 1009 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 0.057 Å⁻¹

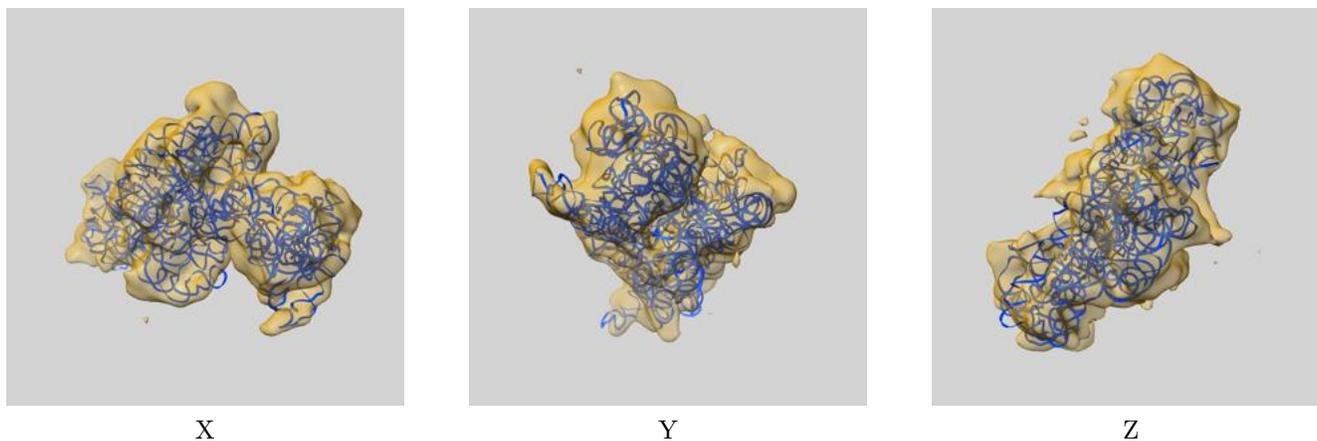
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

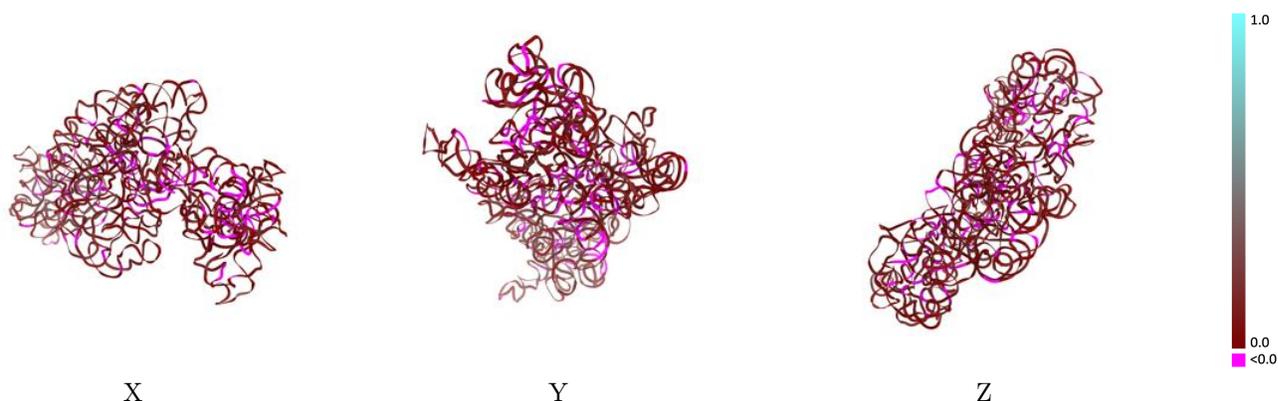
This section contains information regarding the fit between EMDB map EMD-5508 and PDB model 3J2F. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



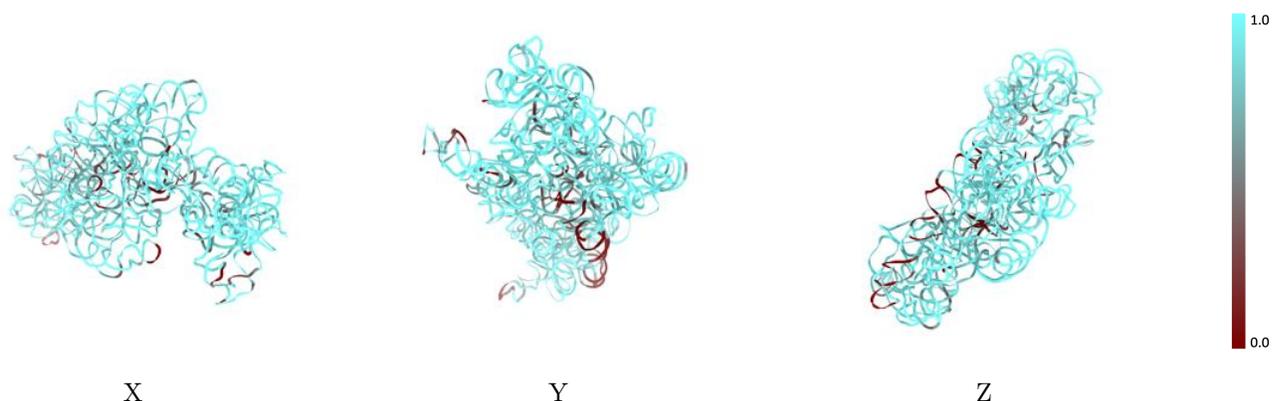
The images above show the 3D surface view of the map at the recommended contour level -2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



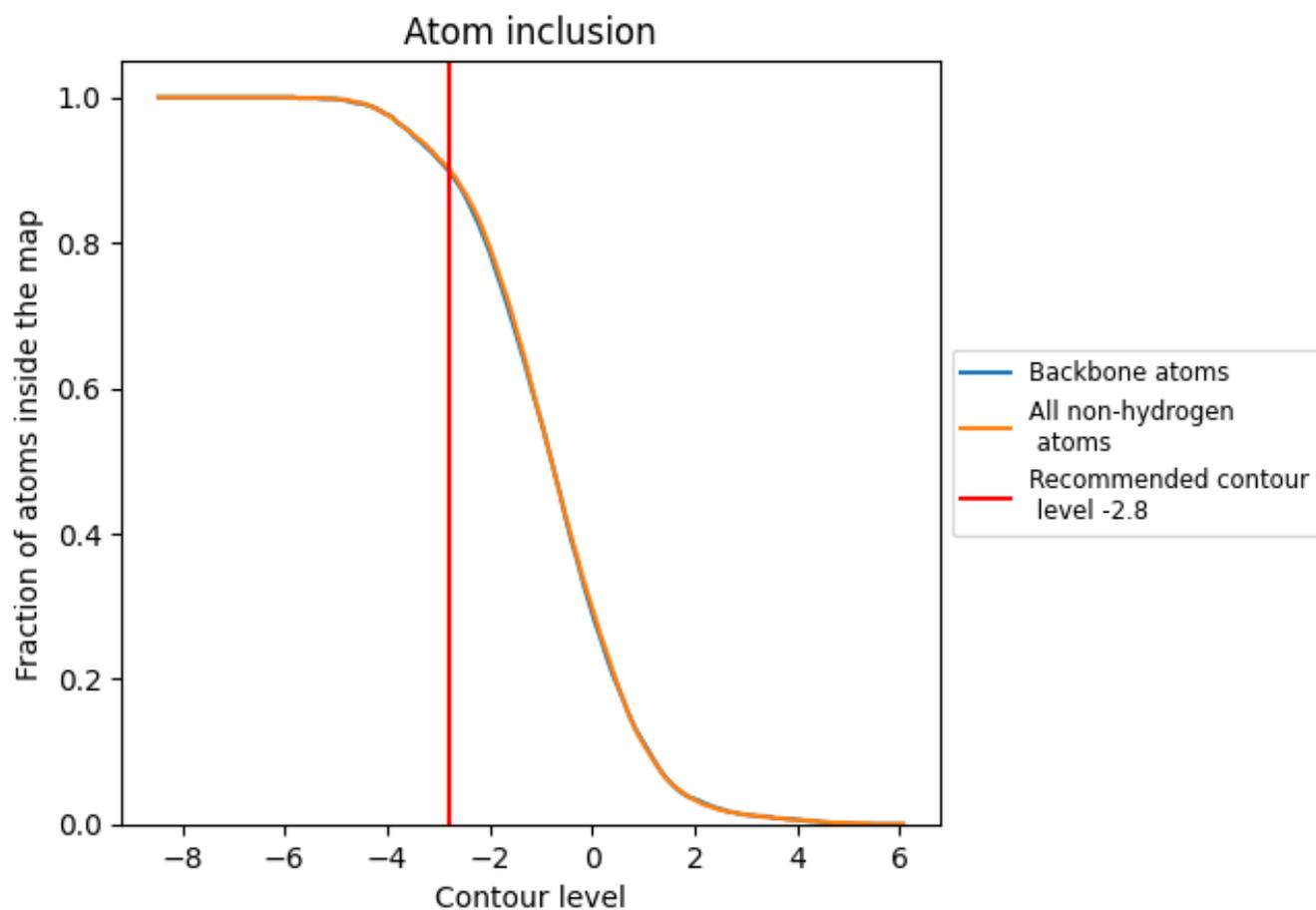
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (-2.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (-2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9020	 0.0710
N	 0.9020	 0.0710

