



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 12:40 PM JST

PDB ID : 3J2E
EMDB ID : EMD-5507
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 : 15.30 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

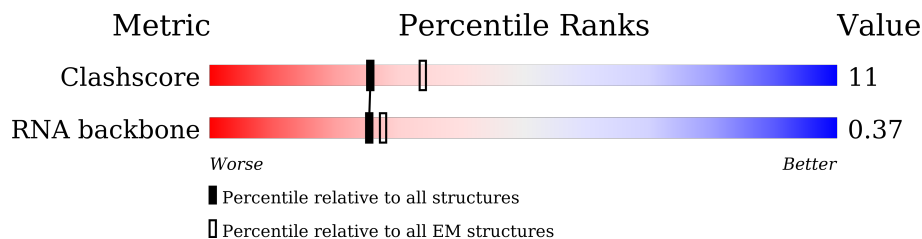
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 15.30 Å.

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



Metric	Whole archive (#Entries)	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.

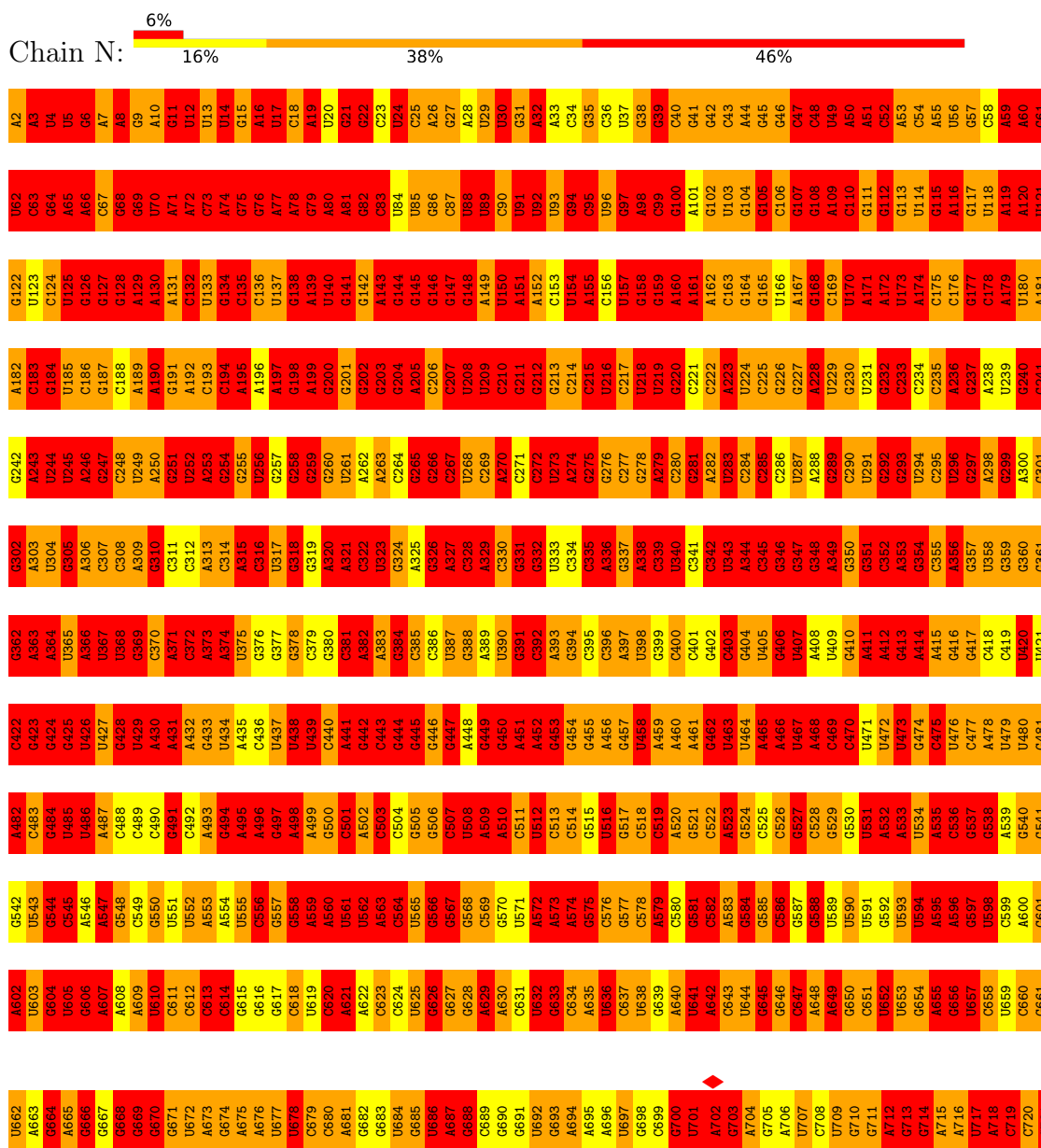
- Molecule 1 is a RNA chain called 16S rRNA.

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

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



A1502	G1442	C1382	U1302	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	C1203	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	A1324	A1204	G1144	G1084	G1024	G964	U904	G844	A784	G724
G1505	G1385	U1284	U1205	A1145	U1085	U1025	U965	U905	A845	G785	G725
U1506	U1445	G1386	G1206	C1146	G1086	G1026	G966	A906	G846	G786	G726
A1507	A1446	G1387	G1207	C1147	G1087	G1027	C967	A907	G847	A787	A727
A1508	A1447	C1388	C1208	U1148	G1088	C1028	A968	A908	C848	U788	A728
C1509	C1448	C1389	C1209	C1149	G1089	C1029	A969	A909	C849	U789	A729
C1510	C1449	A1289	G1210	A1150	U1090	C1028	A969	C910	U850	A790	A730
G1511	G1331	G1270	U1211	A1151	U1091	U1029	A969	U911	G851	G791	G731
G1512	A1332	A1271	U1212	A1152	A1092	U1030	G971	C912	G852	A792	C732
A1513	A1333	G1272	A1213	G1153	A1093	U1030	C972	A913	C853	U793	G733
A1514	G1334	C1273	G1214	A1154	G1094	C1031	G973	A914	U854	A794	G734
G1515	U1335	A1274	G1215	A1155	U1095	G1032	A974	A915	U855	C795	C735
G1516	C1336	A1275	G1216	G1156	C1096	G1033	A975	U916	C856	C796	C736
G1517	G1337	A1276	A1217	A1157	C1097	G1034	G976	G917	C857	C797	C737
A1518	G1338	C1277	C1218	U1158	C1098	A1035	A977	A918	G858	U798	C738
A1519	A1339	G1278	G1219	U1159	G1099	A1035	A978	A919	G859	C799	C739
C1520	A1340	G1279	G1220	G1160	C1100	A1036	C979	U920	A860	G800	U740
C1521	U1341	A1280	G1221	C1161	A1101	C1037	C980	U921	C861	U801	G741
G1522	G1342	C1281	G1222	C1162	A1102	C1038	U981	G922	C862	A802	G742
G1523	G1343	U1282	C1223	A1163	C1103	G1039	U982	A923	U863	G803	A743
G1524	C1344	U1283	C1224	G1164	C1104	U1040	A983	C924	A864	U804	C744
G1525	U1345	U1284	U1225	U1165	A1105	G1041	C984	G925	A865	C805	G745
G1526	A1346	C1285	A1226	G1166	G1106	A1042	C985	G926	G866	C806	A746
U1527	G1347	U1286	C1227	A1167	C1107	A1043	U986	G927	C867	A807	A747
U1528	U1348	A1287	A1228	U1168	G1108	G1043	G987	G928	C868	C808	G748
U1529	A1349	A1288	A1229	A1169	C1109	A1044	G988	G929	C869	G809	A749
G1530	A1350	A1289	C1230	A1170	A1110	C1045	U989	C930	U870	C810	C750
A1531	U1351	G1290	G1231	A1171	A1111	A1046	C990	C931	U871	C811	U751
U1532	C1352	U1291	U1232	C1172	C1112	G1047	U991	C932	A872	G812	G752
C1533	G1353	G1292	G1233	U1173	C1113	G1048	U992	C933	A873	U813	A753
C1534	U1354	C1293	C1234	G1174	C1114	U1049	G993	C934	G874	A814	G754
U1470	A1413	G1294	U1235	G1175	U1115	G1050	A994	A935	U875	A815	G755
U1471	G1414	U1295	A1236	A1176	C1116	C1051	C995	C936	C876	A816	C756
U1472	G1415	U1296	C1237	G1177	A1117	U1052	A996	A937	G877	C817	U757
G1473	G1416	G1297	A1238	U1178	U1118	G1053	U997	A938	A878	G818	C758
U1474	G1417	U1298	U1239	A1179	C1119	A1055	C998	C939	C879	A819	A759
U1475	A1418	A1299	A1240	A1180	C1120	U1056	C999	C940	C880	U820	G760
U1476	G1419	G1300	G1241	G1181	U1121	G1057	A1000	G941	G881	G821	G761
U1477	U1420	U1301	G1242	U1182	U1122	C1058	C1001	G942	C882	U822	U762
U1478	G1421	C1302	G1243	U1183	U1123	C1059	G1002	U943	C883	C823	G763
U1479	G1422	C1303	G1244	G1184	G1124	U1060	G1003	G944	U884	G824	C764
U1480	G1423	G1304	C1245	G1185	U1125	U1061	A1004	G945	G885	A825	G765
U1481	U1424	G1305	A1246	G1186	U1126	U1062	A1005	A946	G886	C826	A766
U1482	C1425	A1306	U1247	G1187	G1127	G1063	G1006	G947	C887	U827	A767
G1426	G1426	U1307	U1248	A1188	C1128	G1064	G1007	C948	G888	U828	A768
G1427	G1371	U1308	C1249	U1189	C1129	G1065	U1007	A949	A889	G829	G769
G1428	U1372	G1311	A1251	U1190	A1130	U1066	U1008	U950	G890	G830	C770
A1428	G1373	G1312	A1252	A1191	G1131	C1067	U1009	G951	U891	A831	G771
A1429	A1374	U1313	G1253	G1192	C1132	A1068	U1010	U952	G892	G832	U772
A1430	A1375	C1314	G1254	U1193	G1133	G1069	U1011	G953	C893	G833	G773
A1431	U1376	U1315	G1255	C1194	U1134	U1070	C1011	G954	G894	U834	G774
G1432	G1377	G1316	A1256	U1195	U1135	U1071	A1012	U955	G895	U835	G775
G1433	C1378	G1317	U1257	A1197	C1136	G1072	G1013	U956	C896	G836	G776
G1434	U1379	A1318	G1258	G1198	G1137	U1073	A1014	U957	U837	U837	A777
G1435	U1380	A1319	G1259	U1199	G1138	G1074	G1015	A958	G838	G838	G778
U1436	C1320	A1319	G1260	C1200	C1139	U1075	A1016	A959	C899	C899	C779
U1437	C1321	U1321	A1261	A1201	C1141	U1076	G1017	U960	A900	A900	A780
G1438	U1321	U1321	A1261	A1201	C1141	U1078	G1019	U961	A901	C841	A781

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29012	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	3.830	Depositor
Minimum map value	-6.331	Depositor
Average map value	-4.159	Depositor
Map value standard deviation	0.542	Depositor
Recommended contour level	-2.5	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, 3, 3	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	3.49	5336/36831 (14.5%)	3.98	9479/57458 (16.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1016

The worst 5 of 5336 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	119	A	N7-C5	-20.91	1.26	1.39
1	N	1181	G	N7-C5	-19.67	1.27	1.39
1	N	1155	A	N7-C5	-19.13	1.27	1.39
1	N	262	A	N7-C5	-18.91	1.27	1.39
1	N	663	A	N7-C5	-18.43	1.28	1.39

The worst 5 of 9479 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1362	A	P-O3'-C3'	28.51	153.91	119.70
1	N	1309	G	N1-C6-O6	27.84	136.60	119.90
1	N	780	A	N1-C6-N6	27.41	135.04	118.60
1	N	790	A	N1-C6-N6	26.54	134.52	118.60
1	N	309	A	N1-C6-N6	25.21	133.72	118.60

There are no chirality outliers.

5 of 1016 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	2	A	Sidechain
1	N	3	A	Sidechain
1	N	4	U	Sidechain
1	N	6	G	Sidechain
1	N	8	A	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	16522	562	0
All	All	32892	16554	16522	562	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 11.

The worst 5 of 562 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:594:U:C4	1:N:595:A:C6	2.75	0.74
1:N:120:A:C2	1:N:122:G:C6	2.78	0.72
1:N:67:C:H2'	1:N:68:G:C8	2.25	0.71
1:N:1343:G:C5	1:N:1344:C:C4	2.79	0.70
1:N:411:A:H61	1:N:428:G:H1'	1.56	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%)	456 (29%)	155 (10%)

5 of 456 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	3	A
1	N	4	U
1	N	5	U
1	N	6	G
1	N	8	A

5 of 155 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1167	A
1	N	1364	U
1	N	1191	A
1	N	1299	A
1	N	1498	U

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.

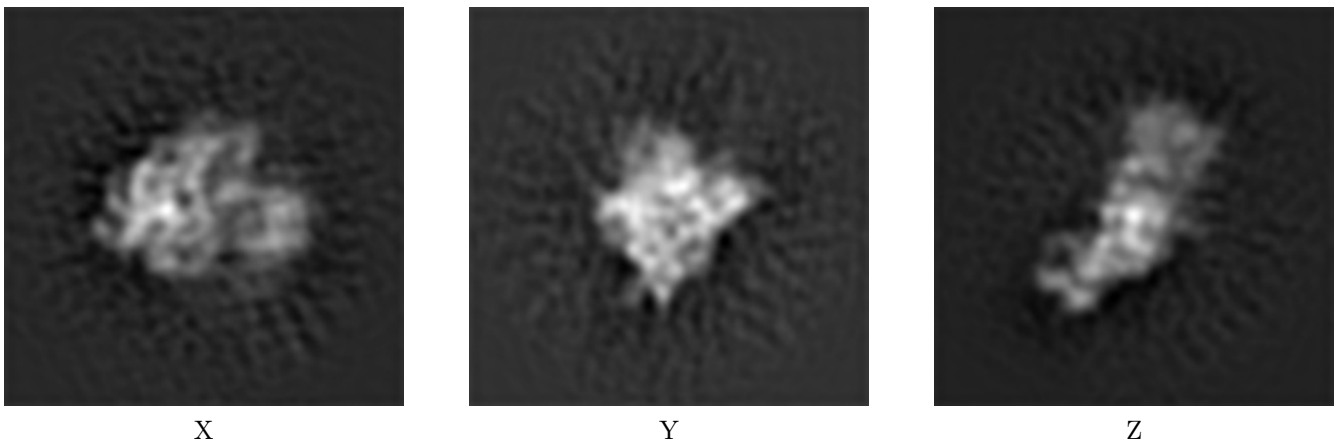
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5507. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

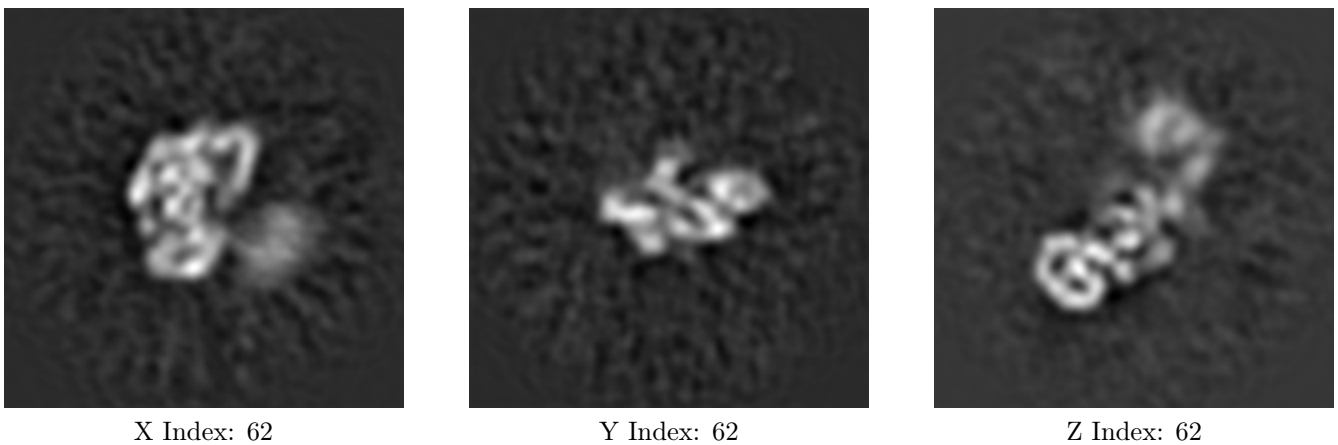
6.1.1 Primary map



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

6.2 Central slices [i](#)

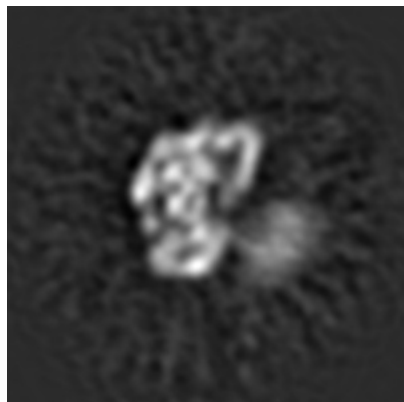
6.2.1 Primary map



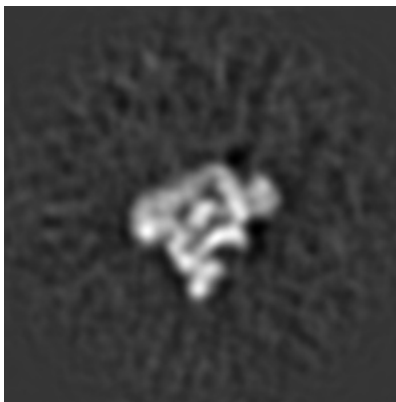
The images above show central slices of the map in three orthogonal directions.

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

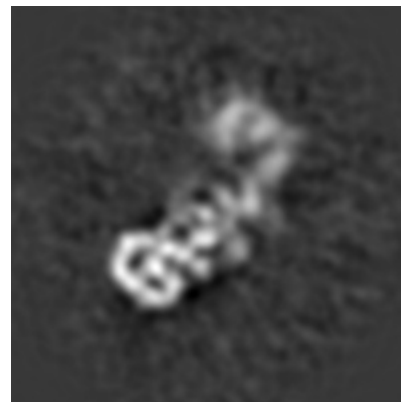
6.3.1 Primary map



X Index: 62



Y Index: 51

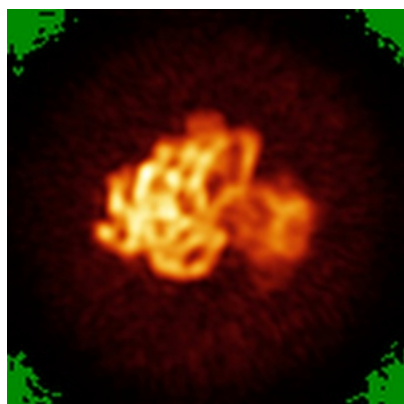


Z Index: 61

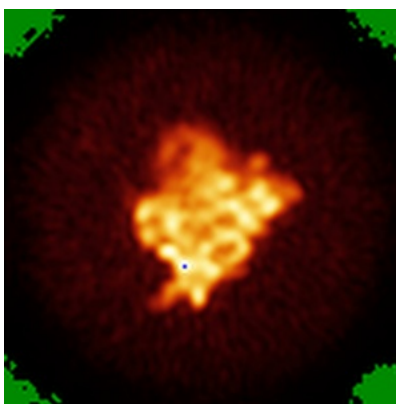
The images above show the largest variance slices of the map in three orthogonal directions.

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

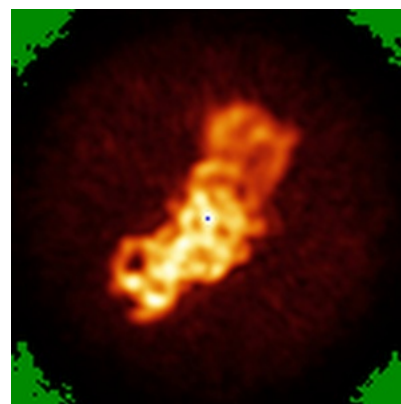
6.4.1 Primary map



X



Y

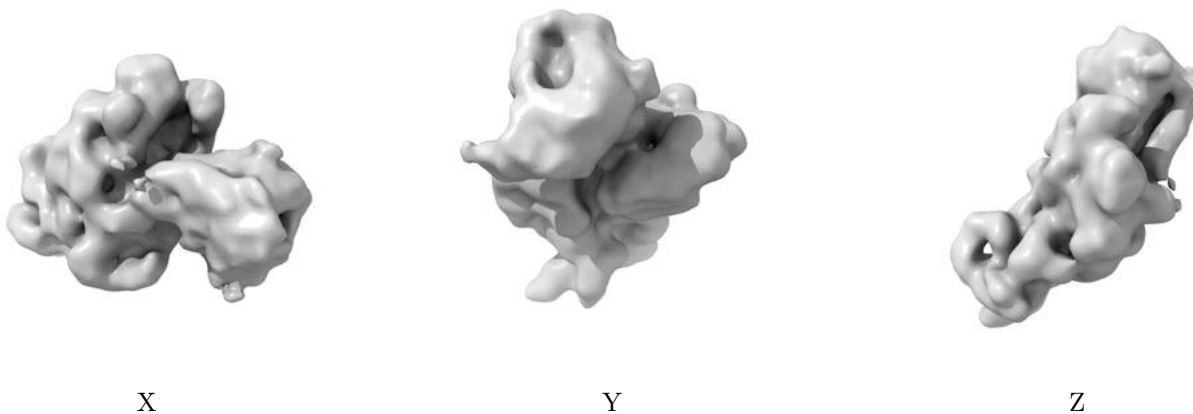


Z

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

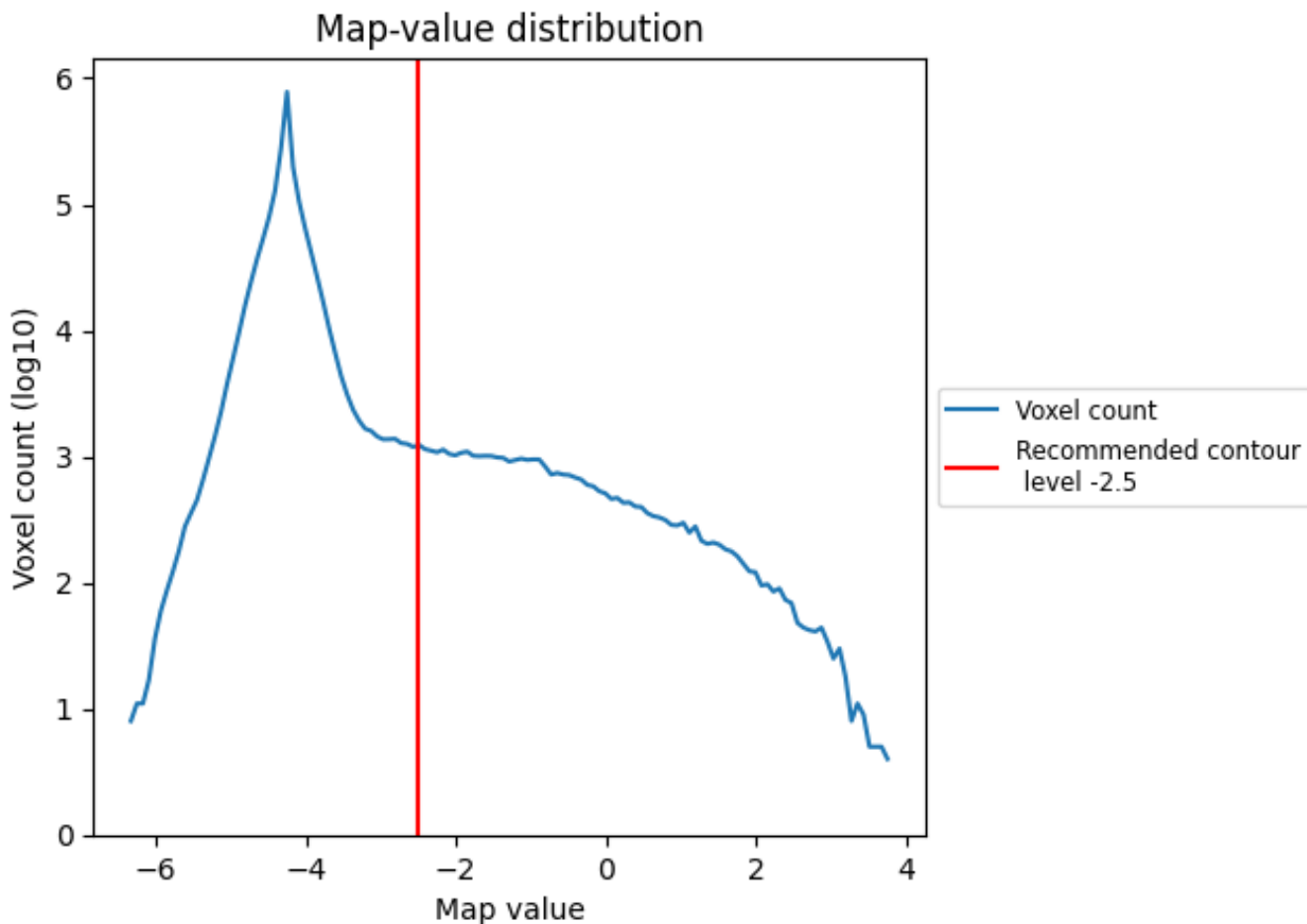
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

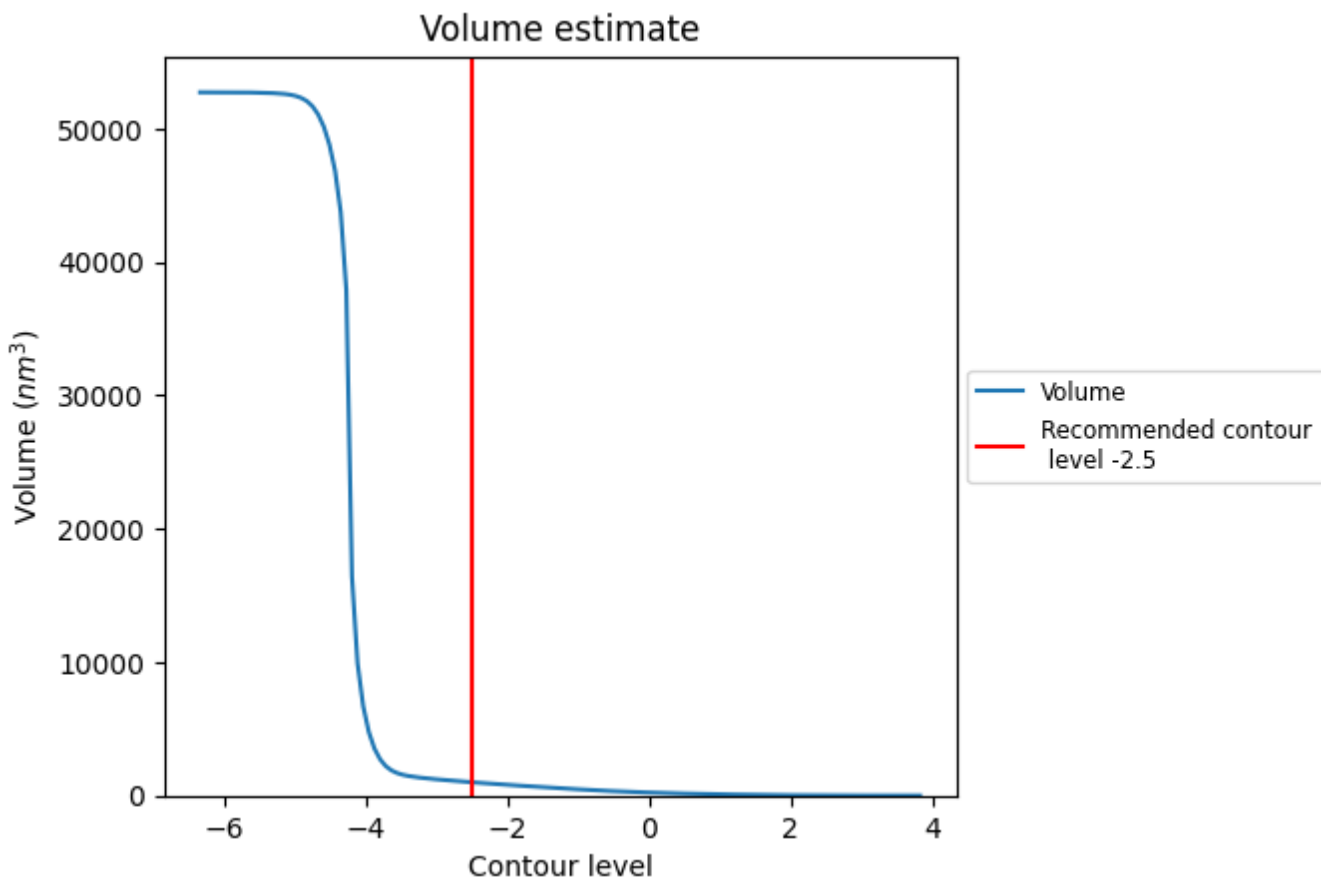
This section contains the results of statistical analysis of the map.

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.

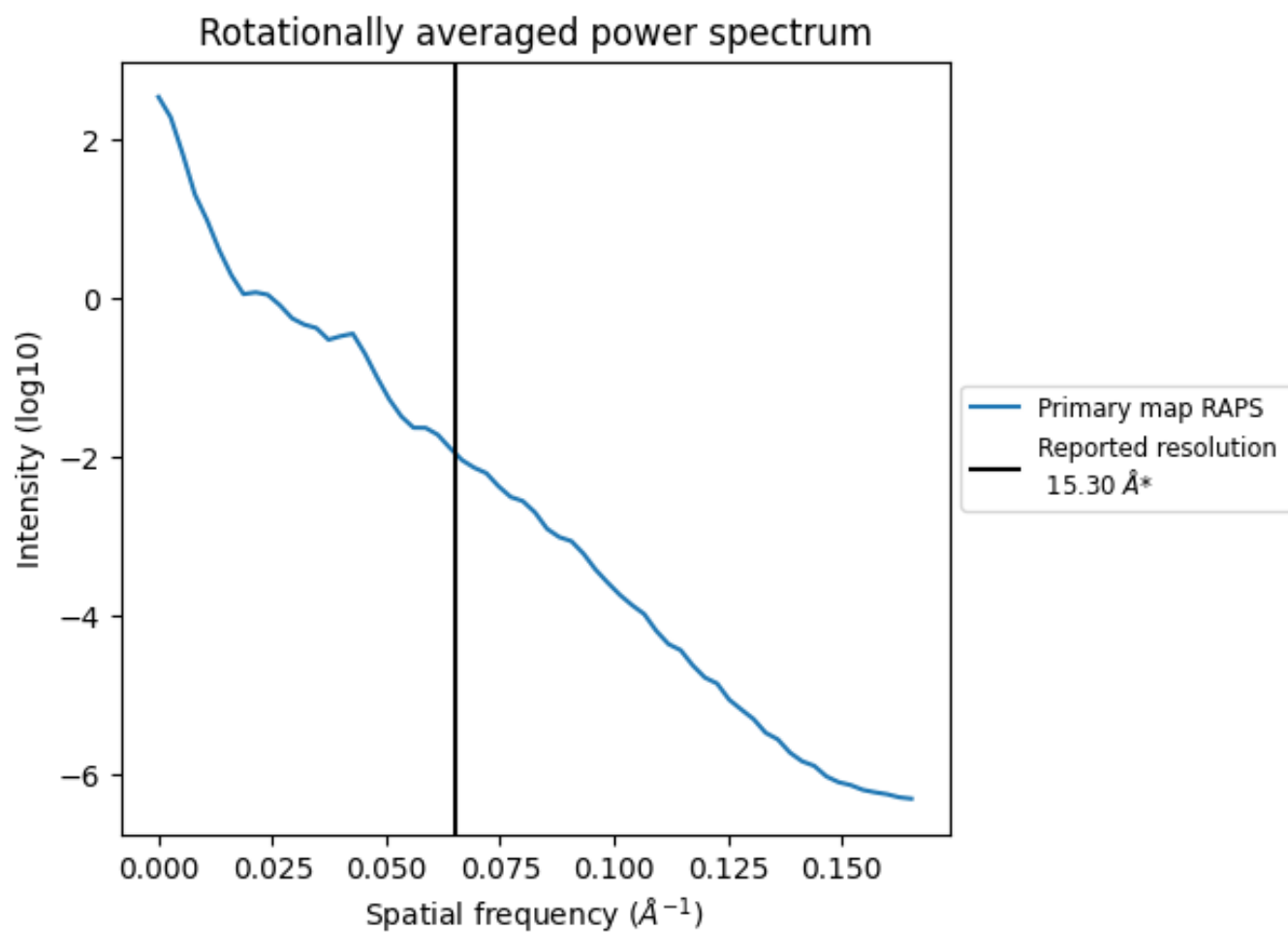
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 998 nm³; this corresponds to an approximate mass of 901 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 0.065 Å⁻¹

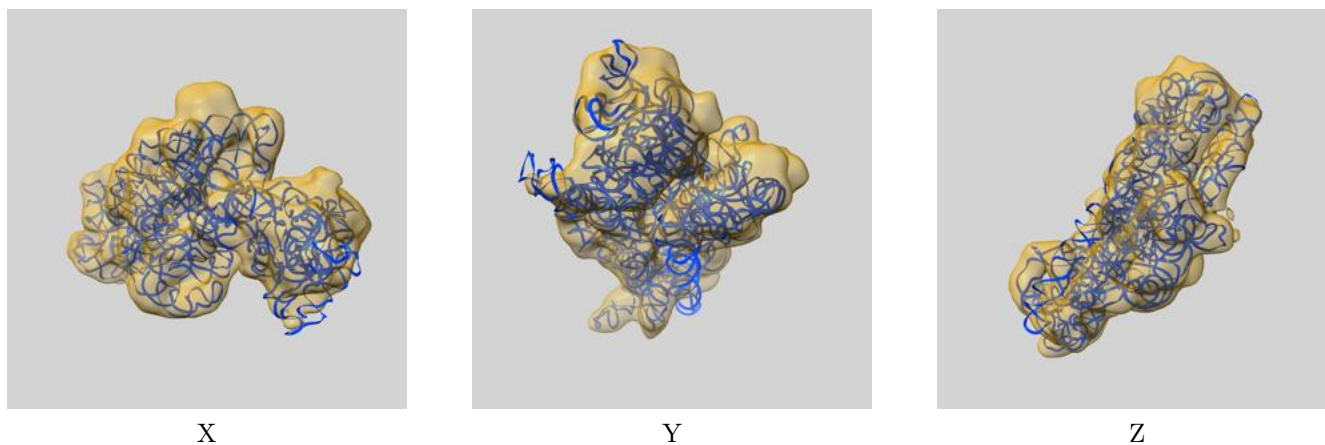
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

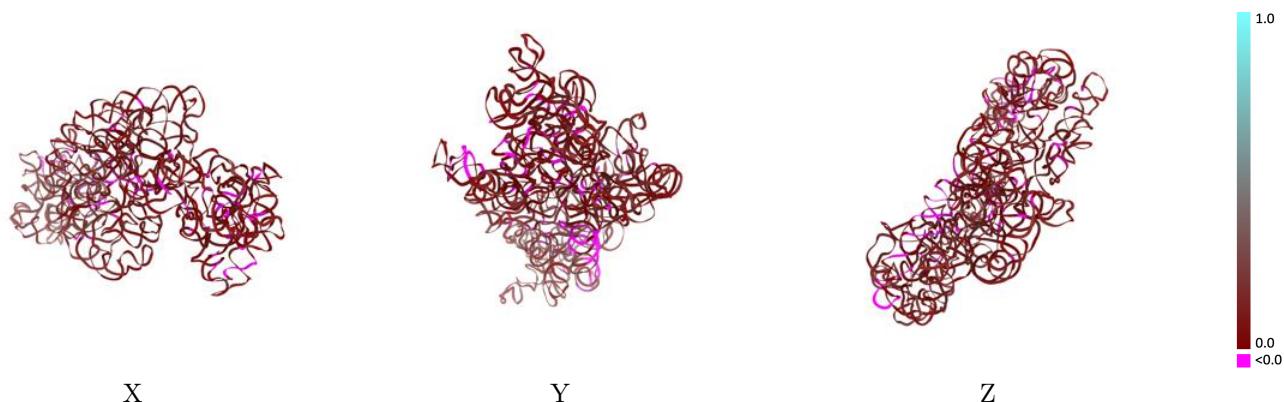
This section contains information regarding the fit between EMDB map EMD-5507 and PDB model 3J2E. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



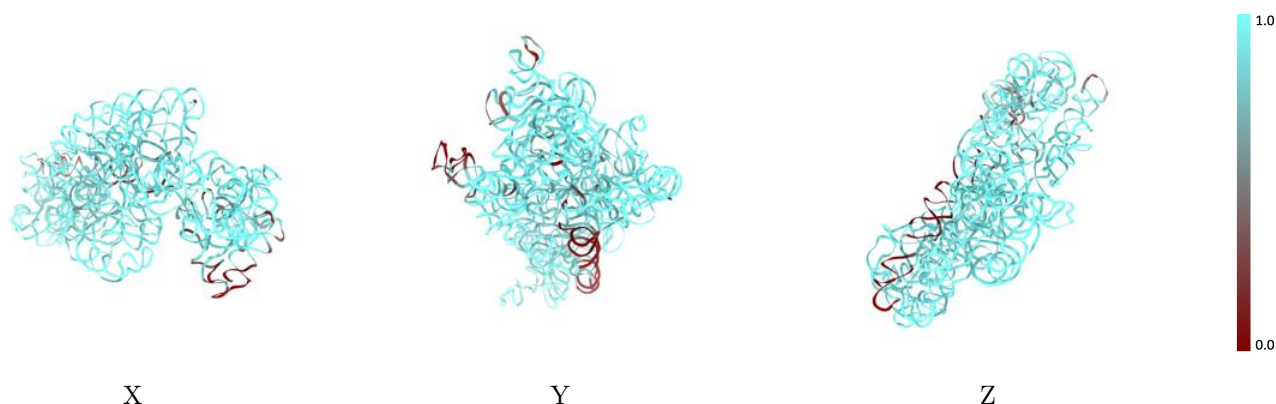
The images above show the 3D surface view of the map at the recommended contour level -2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



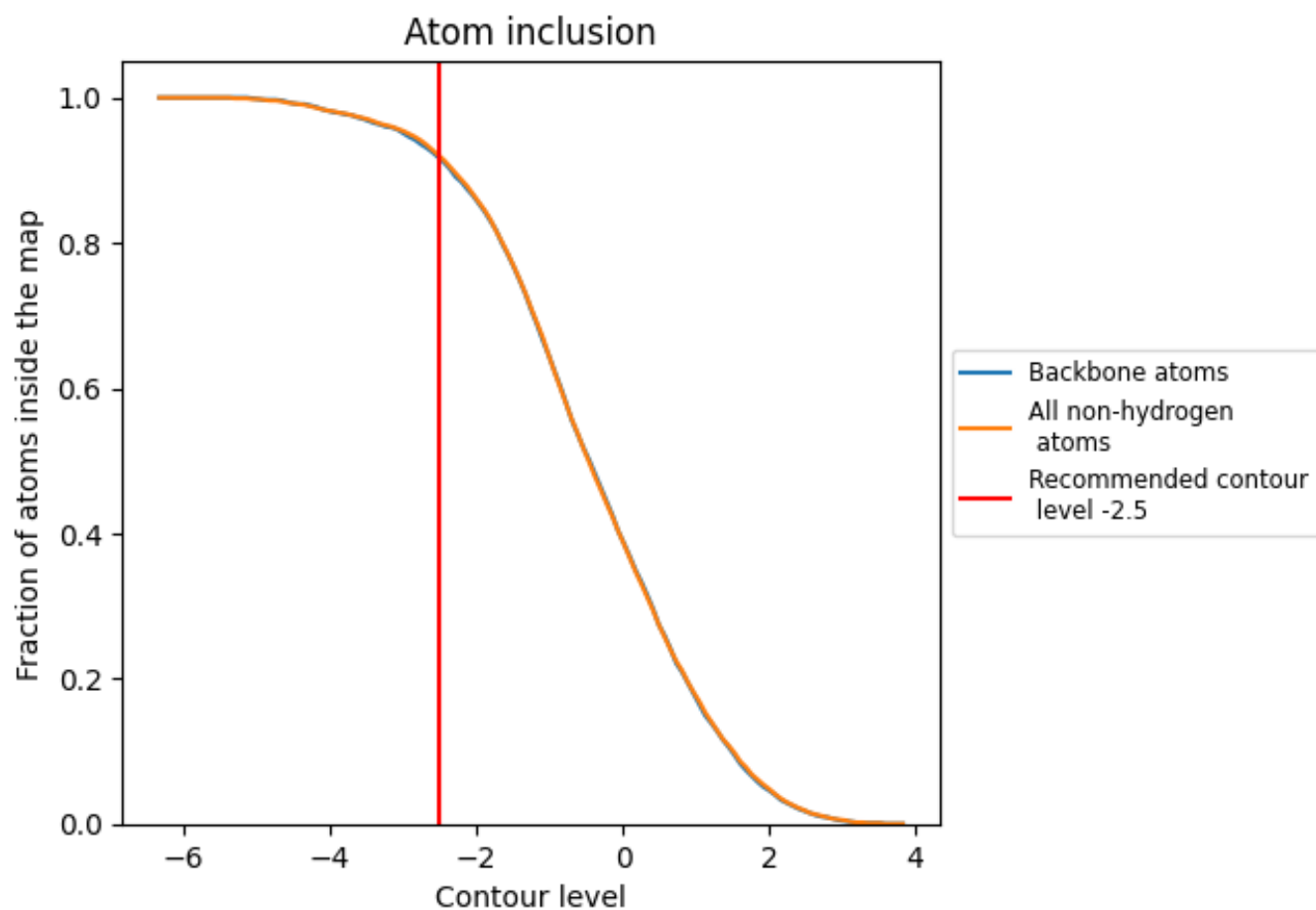
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (-2.5).





9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (-2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.0900
N	 0.9190	 0.0900

