



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 01:21 PM EST

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

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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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

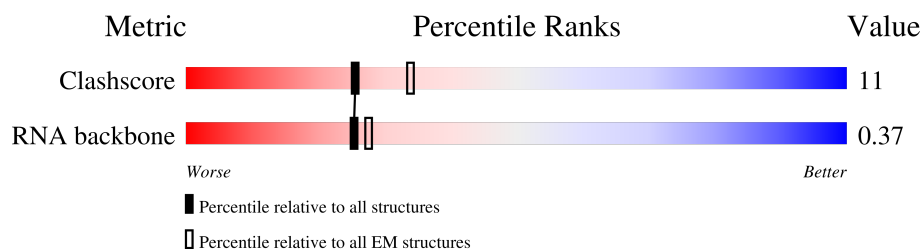
1 Overall quality at a glance

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 [i](#)

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.

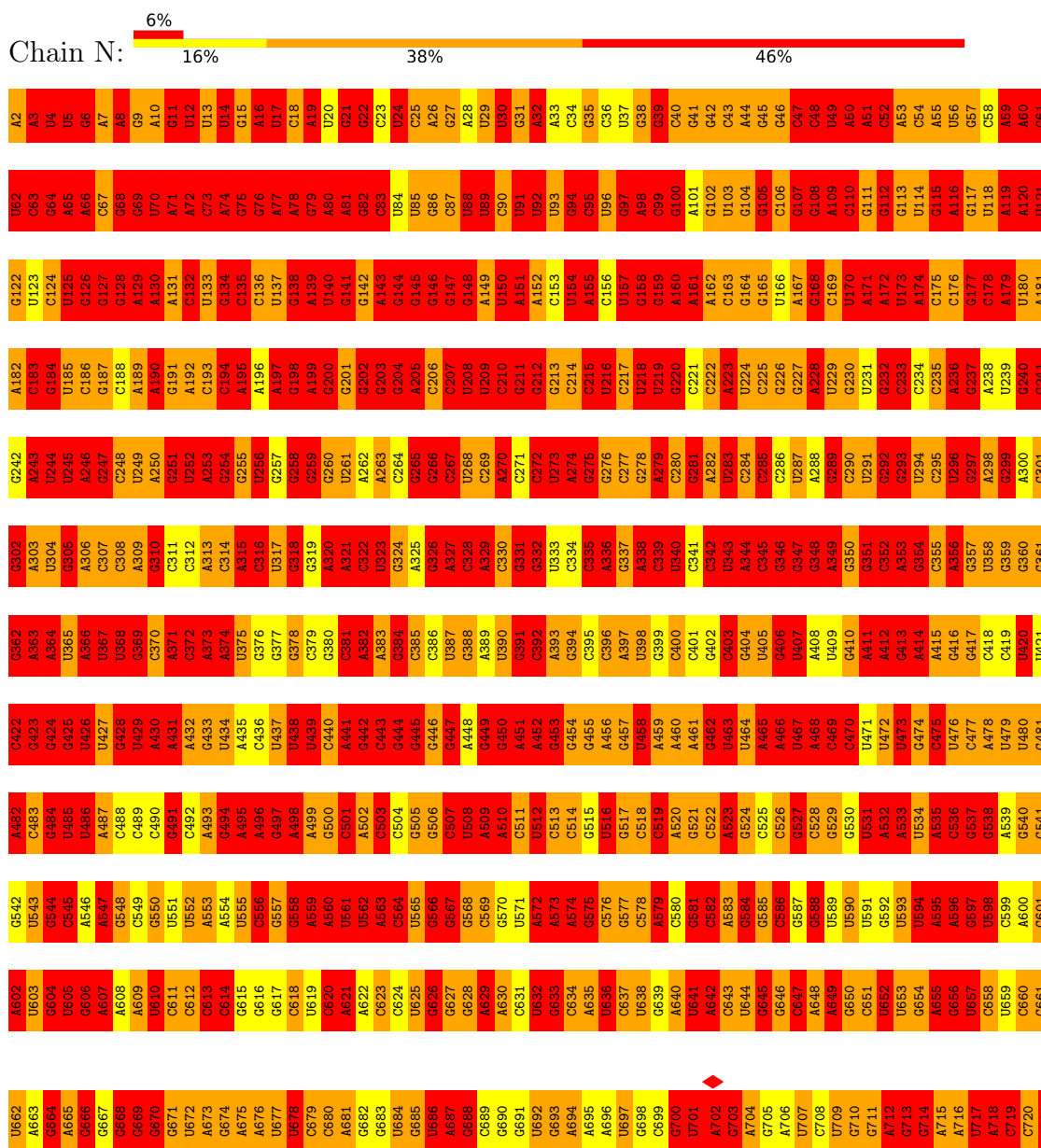
- Molecule 1 is a RNA chain called 16S rRNA.

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

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	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	C1384	G1144	G1084	G1024	A964	U904	G844	C784	U724
G1505	U1445	C1385	A1145	U1085	G1025	U965	U905	A845	G785	G725
U1506	U1446	U1386	A1146	U1086	U1026	G966	A906	G846	G786	G726
A1508	A1447	G1387	C1147	U1087	G1027	C967	A907	G847	G787	G727
A1509	C1448	C1388	U1148	G1088	C1027	A968	A908	C848	U788	A728
C1510	C1449	A1389	C1149	U1089	C1028	A969	A909	G849	U789	A729
G1511	G1531	G1390	A1150	G1090	U1028	A969	C910	U850	A790	G730
U1512	U1450	U1391	A1151	U1091	U1029	C970	U911	G851	G791	G731
A1513	U1451	G1392	A1152	A1092	U1030	C971	C912	G852	A792	G732
G1514	C1452	U1393	G1153	A1093	U1031	C972	A913	C853	U793	G733
G1515	A1384	C1273	A1213	G1094	C1031	G973	A914	U854	A794	G734
G1516	C1385	C1274	A1155	U1095	G1032	A974	A915	U855	C795	C735
G1517	G1386	A1275	G1156	C1096	G1033	A975	U916	C856	C796	C736
G1518	C1387	G1276	A1157	C1097	G1034	G976	G917	C857	C797	C737
A1519	G1388	C1277	U1158	C1098	A1035	A977	A918	G858	U798	C738
C1520	C1389	G1278	C1159	G1099	A1036	C979	A919	G859	G799	C739
C1521	U1340	G1279	G1160	C1100	U1037	C980	U920	A860	G800	U740
G1522	U1341	A1280	C1161	A1101	C1037	C981	U921	C861	U801	G741
C1523	C1342	C1281	C1162	A1102	U1038	U981	G922	C862	A802	G742
C1524	G1343	U1282	A1163	C1103	G1039	U982	A923	U863	G803	A743
G1525	C1344	U1283	G1164	G1104	U1040	A983	C924	A864	U804	C744
G1526	U1345	U1284	U1165	A1105	G1041	C984	G925	A865	C805	G745
G1527	A1346	A1285	G1166	G1106	A1042	C985	G926	C866	C806	G746
U1528	G1347	U1286	A1167	C1107	G1043	U986	G927	C867	A807	A747
G1529	U1348	A1287	U1168	G1108	A1044	G987	G928	C868	C808	G748
A1530	A1408	C1288	A1169	C1109	C1045	U989	G929	G869	G809	A749
G1531	C1409	A1289	A1170	A1110	U1046	C990	C930	U870	C810	C750
A1531	A1410	U1351	A1171	C1230	A1047	C991	C931	U871	C811	U751
C1467	C1411	U1291	C1172	C1112	G1048	U991	C932	A872	G812	G752
C1468	C1412	G1292	U1173	C1113	U1049	U992	C933	A873	U813	A753
C1469	A1413	C1293	G1174	C1114	G1050	G993	C934	G874	A814	G754
U1470	A1414	G1294	G1175	U1115	C1051	A994	A935	U875	A815	G755
U1471	G1415	U1295	A1176	U1116	C1052	C995	C936	C876	A816	C756
U1472	G1416	A1296	G1177	A1117	U1053	A996	A937	G877	C817	U757
G1473	G1417	G1297	U1178	U1118	C1054	C997	A938	A878	G818	C758
U1474	A1418	U1298	A1179	C1119	C1055	C998	C939	C879	A819	A759
G1475	G1419	U1299	U1180	C1120	A1056	C999	C940	C880	U820	G760
A1476	U1420	C1300	G1181	U1121	G1057	A1000	G941	G881	G821	G761
U1477	G1421	U1301	U1182	U1122	C1058	C1001	G942	C882	U822	U762
U1478	G1422	C1302	U1183	U1123	C1059	G1002	U943	C883	C823	G763
C1479	G1423	G1303	G1184	G1124	U1060	G1003	G944	U884	G824	C764
A1480	U1424	G1304	U1185	U1125	G1061	A1004	G945	G885	A825	G765
U1481	U1425	G1305	G1186	U1126	U1062	A1005	A946	G886	C826	A766
G1426	G1426	A1306	U1187	G1127	C1063	G1006	G947	G887	U827	A767
C1427	U1427	U1307	A1188	C1128	G1064	A888	C948	G888	U828	A768
A1483	C1427	G1309	U1189	C1129	U1065	A889	U950	G889	G829	G769
C1484	A1428	U1310	G1190	A1130	C1066	U890	G951	G890	G830	C770
U1485	A1429	U1311	A1191	G1131	A1067	U891	U952	U891	A831	G771
G1486	A1430	G1312	C1192	C1132	G1068	A892	G953	A892	C832	U772
G1487	A1431	U1313	G1193	G1133	C1069	G893	G954	C893	G833	G773
G1488	G1432	C1314	C1195	U1135	U1070	C1011	G955	G894	U834	G774
G1489	A1433	U1315	A1196	U1136	C1071	A1012	U956	G895	U835	G775
U1490	A1434	G1316	A1197	C1137	G1072	G1013	U957	C896	G836	G776
G1491	U1379	C1317	G1198	C1138	U1073	A1014	U958	U897	U837	A777
A1492	U1380	A1318	U1199	G1139	G1074	A1015	A959	C898	C838	G778
A1493	G1435	A1319	C1200	C1140	U1075	A1016	U960	C899	C839	C779
U1494	U1436	U1320	A1201	C1141	G1076	G1017	A900	A900	A900	A780
U1496	U1437	C1320	A1201	C1141	G1077	A1019	G1018	A901	C841	A781
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A1500	A1499	A1500	A1501	A1502	A1503	A1504	A1505	A1506	A1507	A1508
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A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535
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A1556	A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566
A1557	A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567
A1558	A1559	A1560	A1561	A1562	A1563	A1564	A1565	A1566	A1567	A1568
A1559	A1560									

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 ⓘ

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

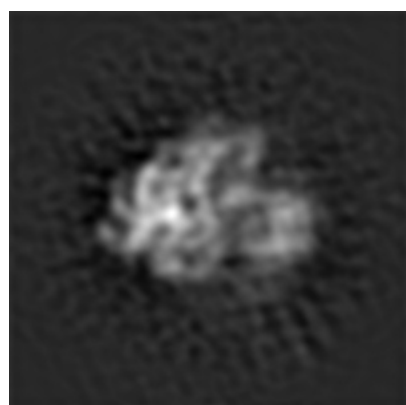
6 Map visualisation [i](#)

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.

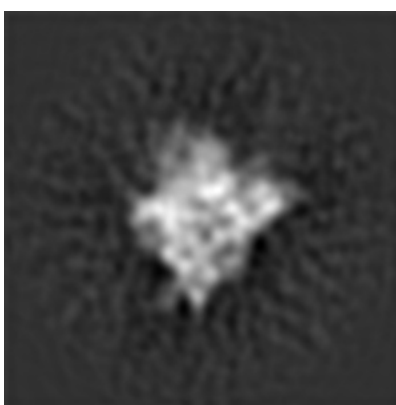
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

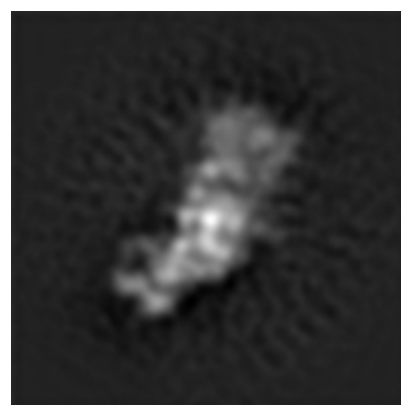
6.1.1 Primary map



X



Y

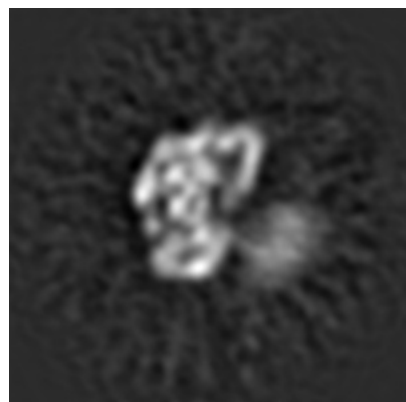


Z

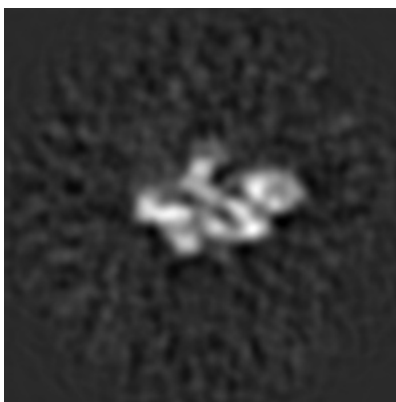
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

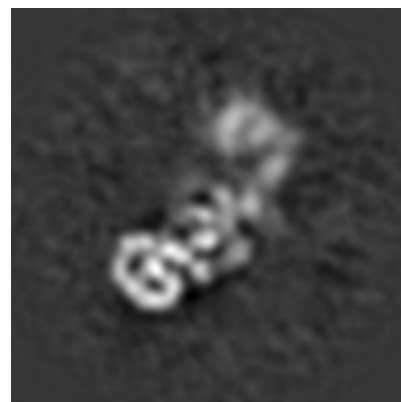
6.2.1 Primary map



X Index: 62



Y Index: 62

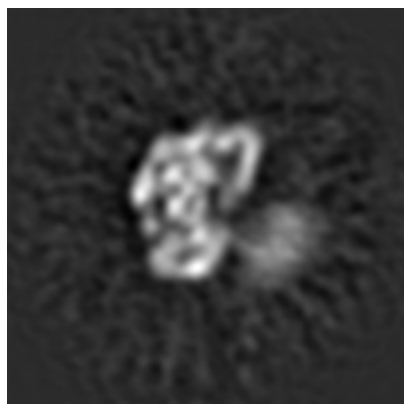


Z Index: 62

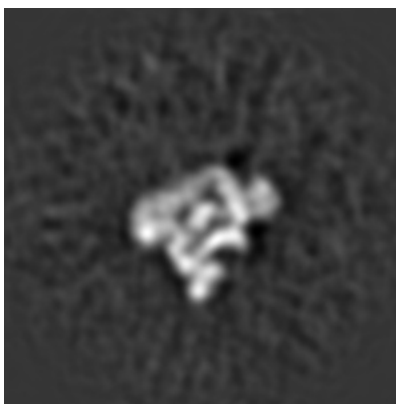
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

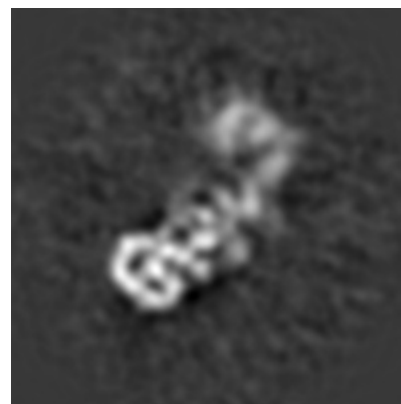
6.3.1 Primary map



X Index: 62



Y Index: 51

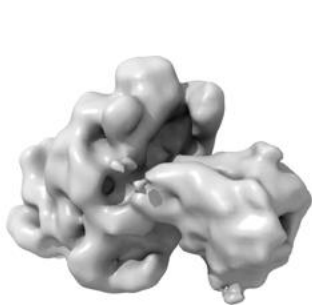


Z Index: 61

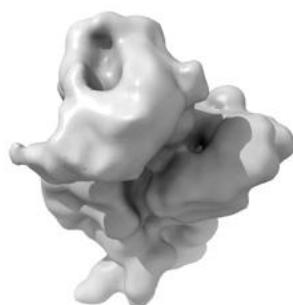
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

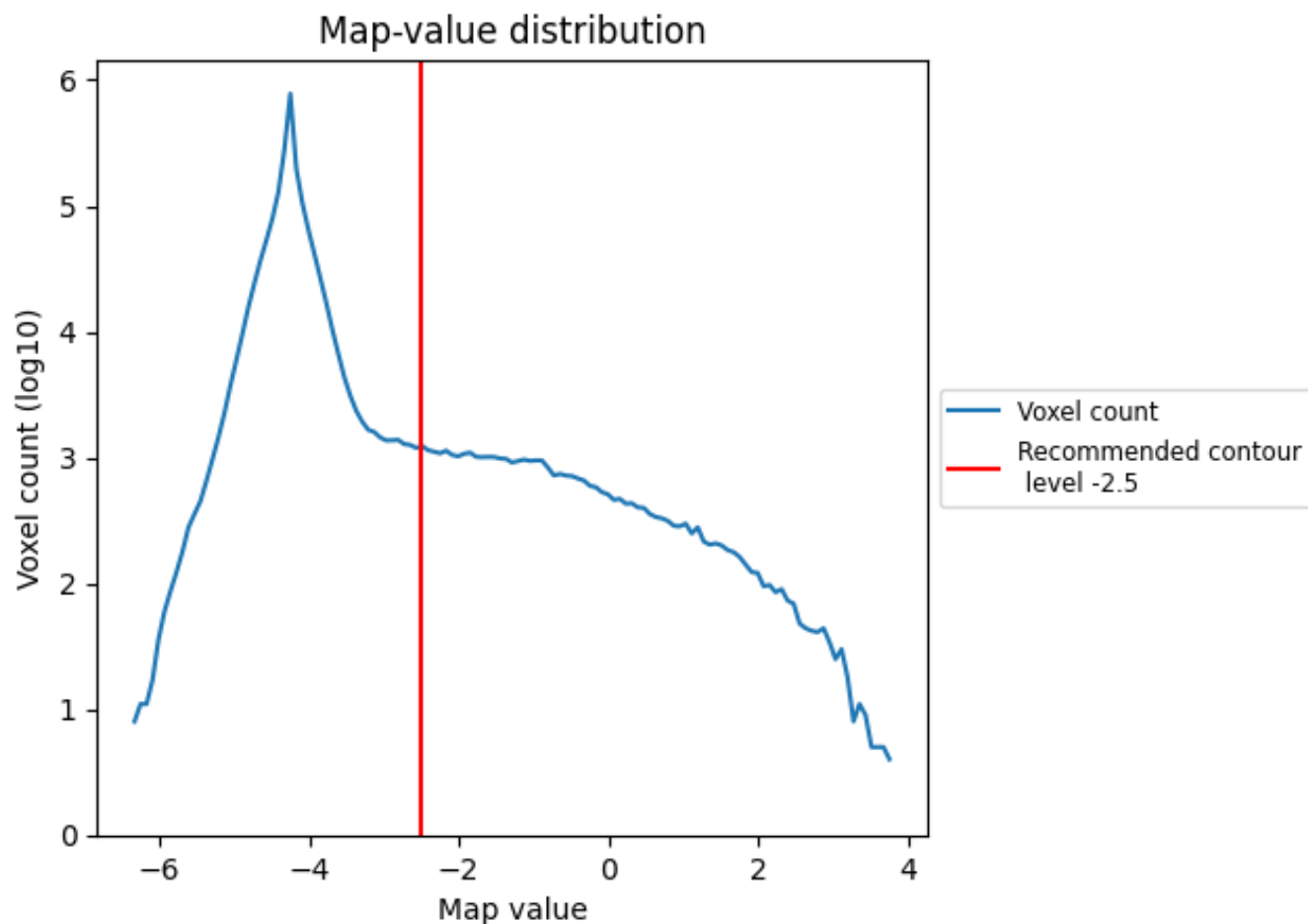
6.5 Mask visualisation

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

7 Map analysis [i](#)

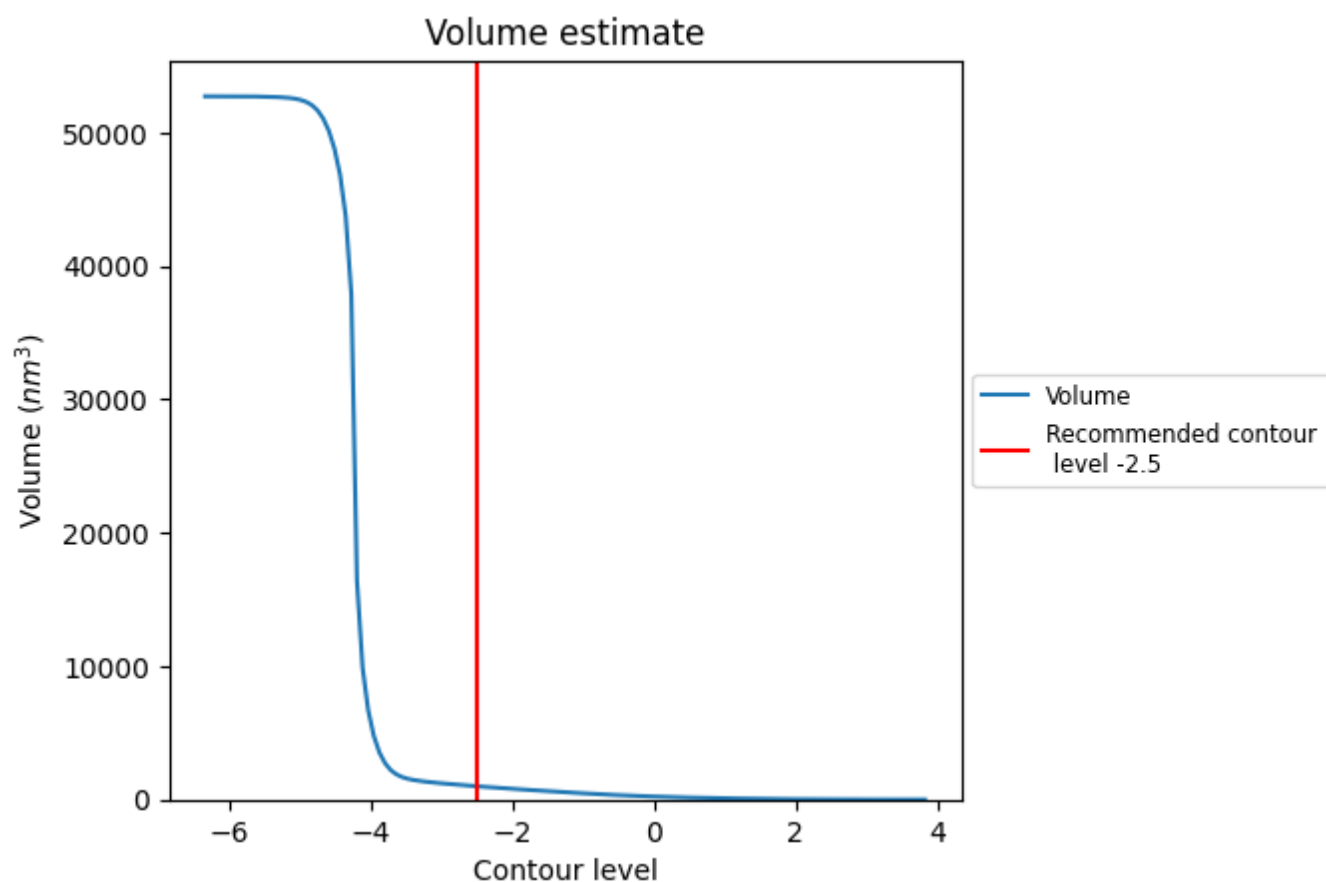
This section contains the results of statistical analysis of the map.

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.

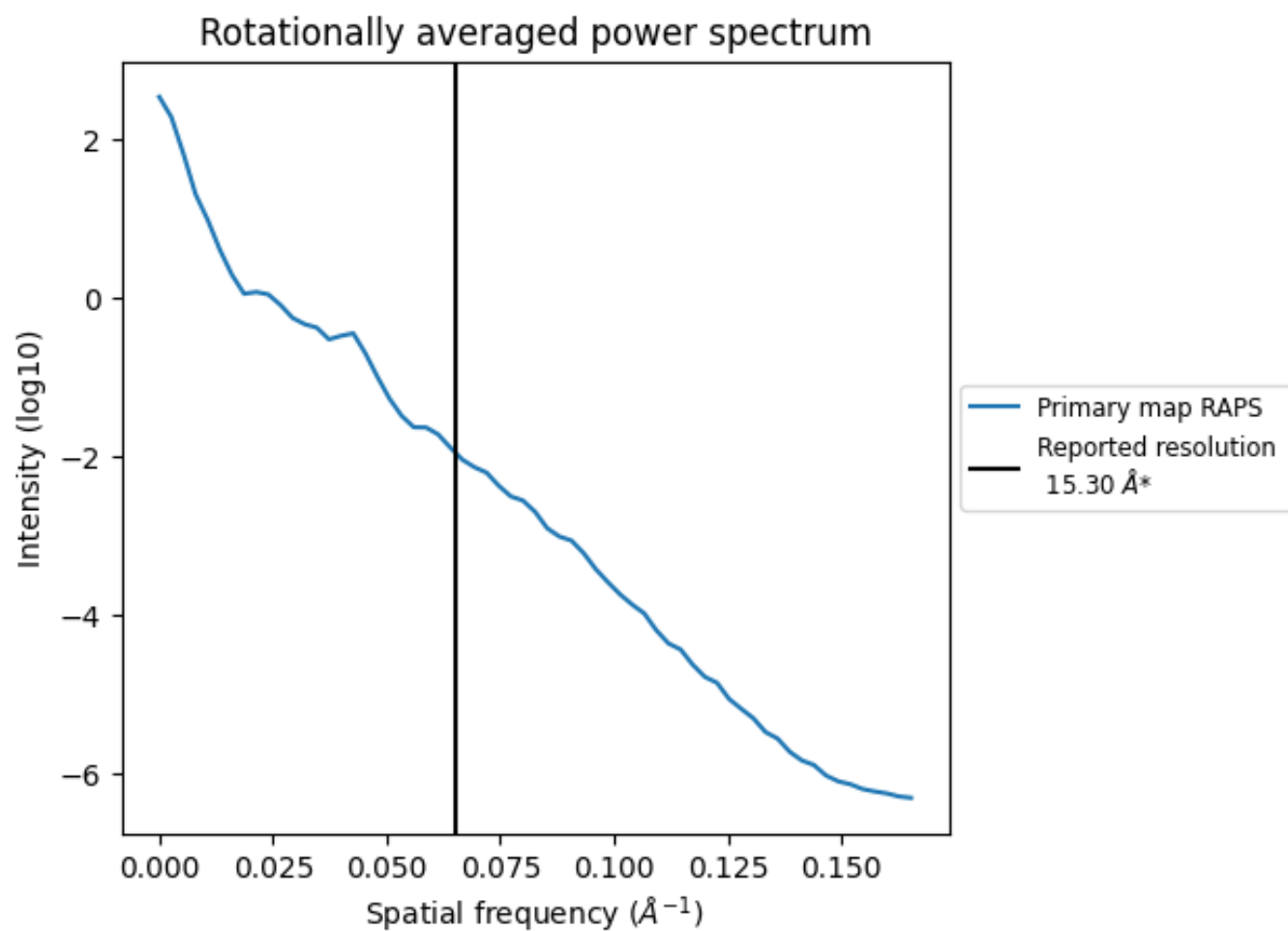
7.2 Volume estimate [i](#)



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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.065 Å⁻¹

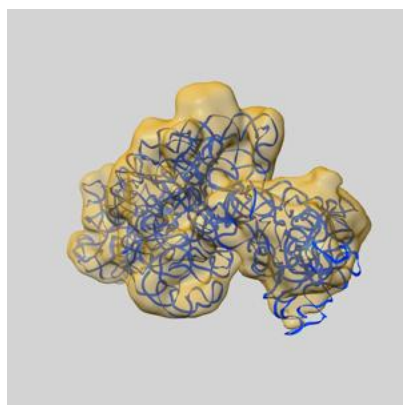
8 Fourier-Shell correlation

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

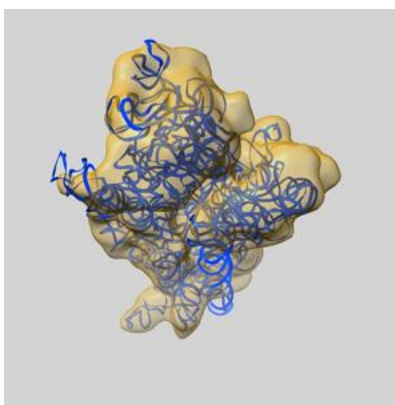
9 Map-model fit [i](#)

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](#).

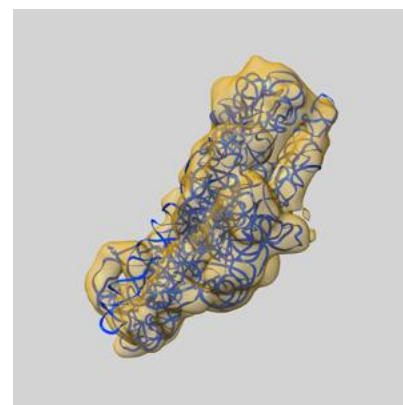
9.1 Map-model overlay [i](#)



X



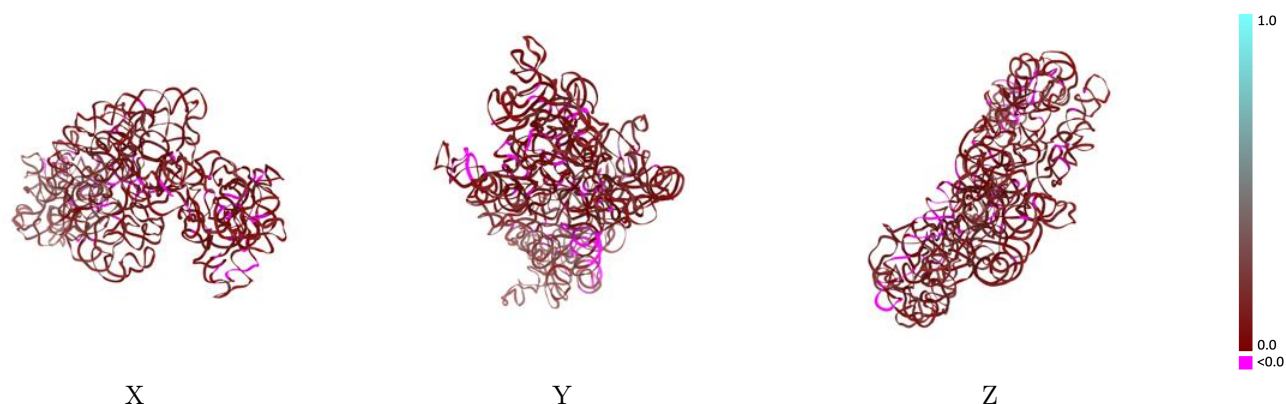
Y



Z

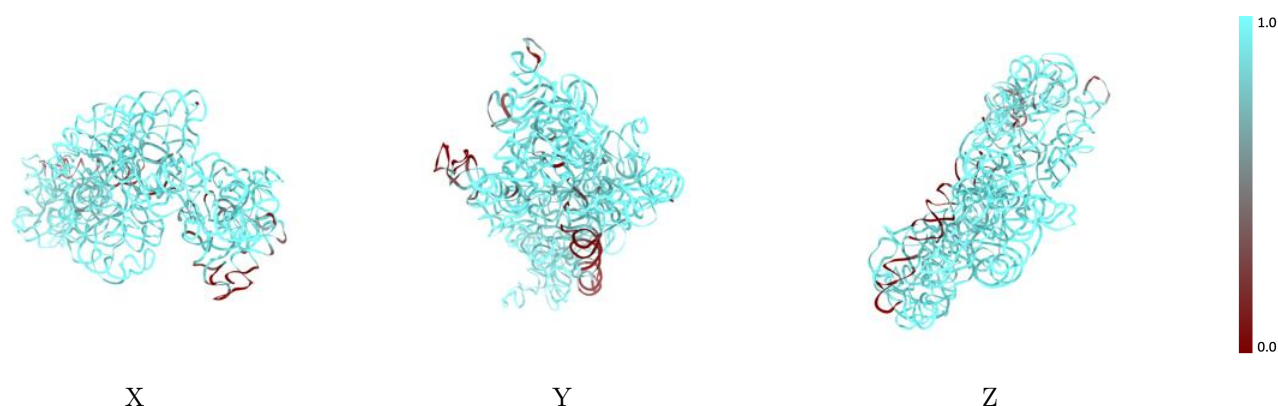
The images above show the 3D surface view of the map at the recommended contour level -2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



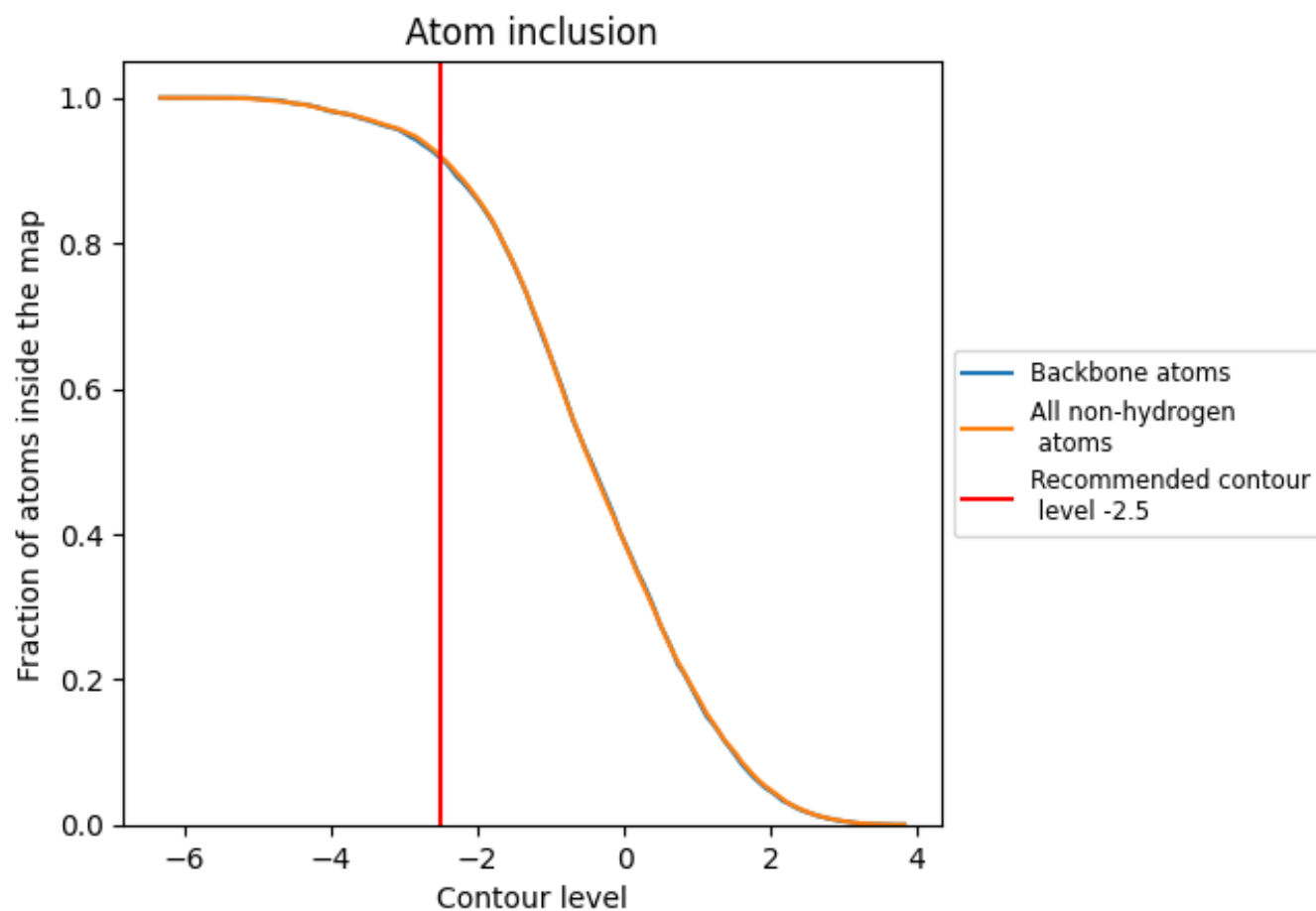
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	<div><div></div></div> 0.9190	<div><div></div></div> 0.0900
N	<div><div></div></div> 0.9189	<div><div></div></div> 0.0900

