



## wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 12:55 PM JST

PDB ID : 3J2B  
EMDB ID : EMD-5503  
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 : 13.60 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](mailto: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>.

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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

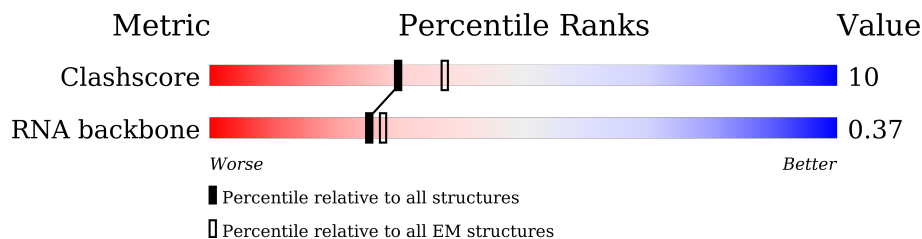
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 13.60 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  $\geq 3$ , 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.

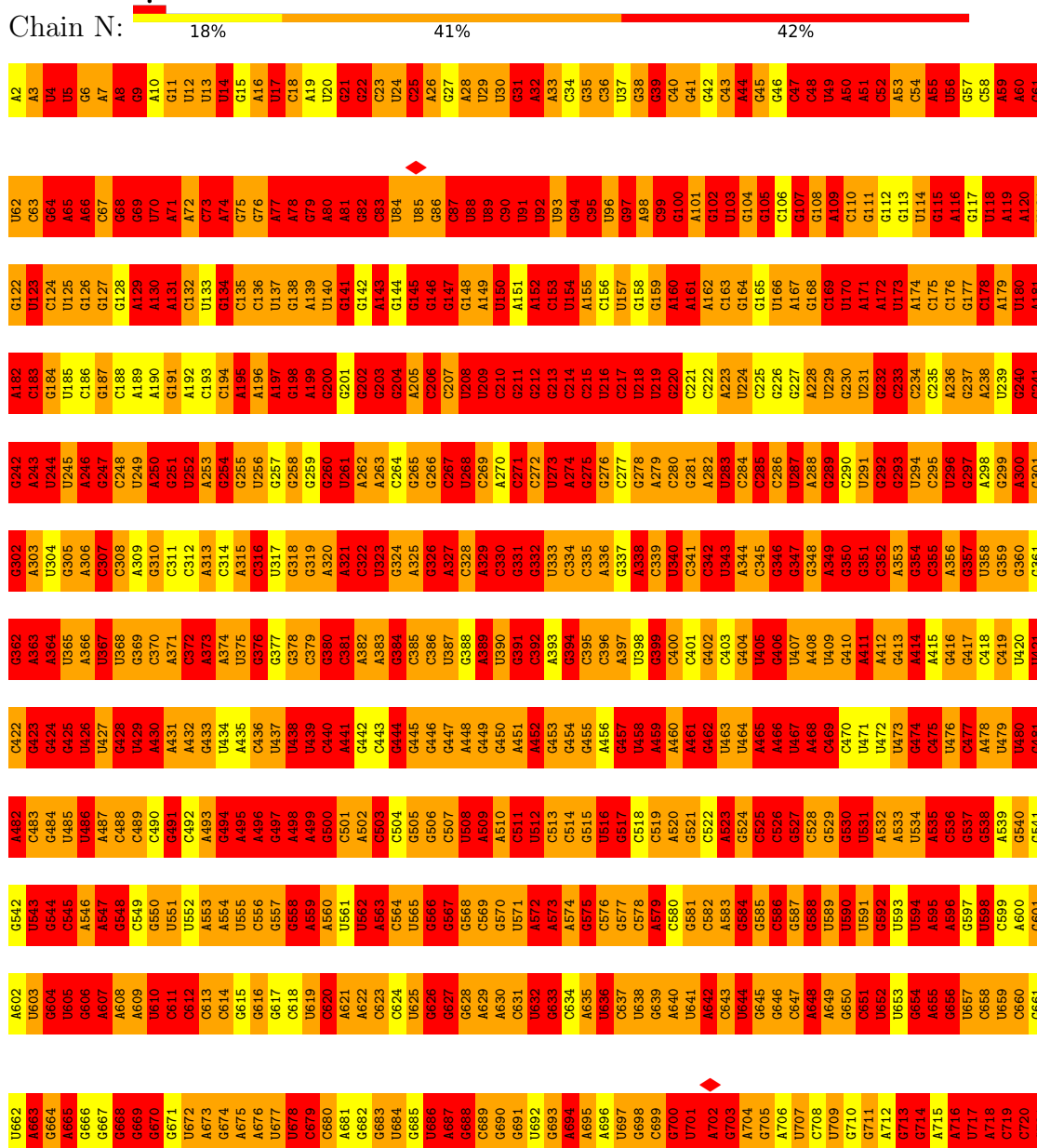
- Molecule 1 is a RNA chain called 16S rRNA.

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	G1522	C1262	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	G1523	C1263	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	C1384	A1324	A1204	A1144	U1084	G1024	A964	U904	G844	A784	G724
G1505	U1444	C1385	C1325	U1205	A1145	U1085	U1025	U965	U905	G845	A785	G725
U1506	U1445	G1386	G1266	G1206	G1146	U1086	G1026	G966	A906	G846	G786	G726
A1466	A1446	G1387	U1327	G1207	C1147	G1088	C1027	G967	A907	G847	A787	G727
A1508	C1447	C1388	C1328	C1208	U1148	G1088	U1028	A968	A908	C848	U788	A728
C1509	C1448	A1389	A1209	C1209	C1149	G1089	U1029	A969	A909	C849	U789	A729
C1510	C1449	G1390	G1270	C1210	A1150	G1090	U1030	C970	C910	U850	A790	G730
G1511	U1450	G1331	G1271	U1211	A1151	U1091	C1031	G971	U911	G851	G731	A731
A1513	U1451	A1332	A1272	U1212	A1152	A1092	G1032	C972	C912	G852	A792	C732
G1514	C1452	C1273	A1213	A1213	G1153	A1093	G1033	G973	A913	C853	U793	G733
G1515	C1453	A1274	G1214	C1214	G1154	G1094	G1034	A974	A914	U854	A794	G734
G1516	G1453	A1275	G1215	G1215	A1155	U1095	A1035	A975	A915	U855	C785	C735
G1517	C1454	G1276	A1216	C1216	G1156	C1096	A1036	G976	U916	C856	C796	C736
G1518	G1455	C1277	A1217	C1217	A1157	C1097	C1037	G977	U917	C857	C797	A737
A1456	A1456	G1338	G1278	A1218	U1158	C1098	C1038	A978	A918	G858	U788	C738
A1519	C1399	A1339	A1219	A1219	U1159	G1099	G1039	C979	A919	G859	C799	C739
G1457	G1457	A1340	A1220	G1220	G1160	C1100	U1040	C980	U920	A860	G800	U740
G1458	U1463	C1281	G1221	G1221	C1161	A1101	G1041	U981	U921	C861	U801	G741
C1460	C1460	C1282	G1222	G1222	C1162	A1102	A1042	U982	G922	C862	A802	G742
G1461	C1461	U1283	C1223	C1223	A1163	C1103	G1043	A983	A923	U863	G803	A743
G1524	C1403	C1284	U1224	U1224	G1164	G1104	A1044	C984	C924	A864	U804	C744
G1525	C1404	A1285	A1225	A1225	U1165	A1105	C1045	C985	G925	A865	C805	G745
G1526	G1405	U1286	C1226	C1226	G1166	G1106	A1046	U986	G926	C866	C806	G746
U1527	U1406	A1287	A1227	A1227	A1167	C1107	G1047	G987	G927	C867	A807	A747
U1528	U1464	U1288	C1228	C1228	U1168	G1108	U1048	G988	G928	C868	C808	G748
G1529	A1465	A1289	A1229	A1229	U1169	C1109	U1049	U989	G929	C869	G809	A749
A1531	C1466	A1350	G1230	C1230	U1170	A1110	G1050	C990	C930	U870	C810	C750
C1467	C1411	U1291	G1231	G1231	A1171	A1111	C1051	U991	C931	U871	C811	C751
A1468	C1412	U1292	U1232	U1232	C1172	C1112	U1052	U992	G932	A872	G812	G752
C1469	A1413	C1293	G1233	G1233	U1173	C1113	G1053	G993	C933	C873	U813	A753
U1470	U1414	G1294	C1234	C1234	G1174	C1114	C1054	A994	C934	G874	A814	C754
U1471	G1415	U1295	U1235	U1235	G1175	U1115	A1055	A995	A935	U875	A815	C755
G1472	G1416	C1296	U1236	U1236	U1176	U1116	U1056	A996	C936	C876	A816	C756
G1473	G1417	G1297	C1237	C1237	G1177	A1117	G1057	U997	A937	G877	C817	U757
U1474	A1418	U1298	A1238	A1238	U1178	U1118	G1058	C998	G938	C878	G818	C758
G1475	C1419	A1299	A1239	A1239	A1179	C1119	C1059	C999	C940	C880	A819	A759
A1476	U1420	G1300	U1240	U1240	U1180	C1120	U1060	C1000	G941	G881	U821	G761
U1477	U1421	U1301	G1241	G1241	G1181	U1121	G1061	C1001	G942	C882	U822	U762
U1478	G1422	C1302	C1242	C1242	U1182	U1122	U1062	G1002	U943	C883	G823	G763
C1479	G1423	C1303	C1243	C1243	U1183	U1123	C1063	G1003	G944	U884	G824	C764
A1480	G1424	G1304	G1244	G1244	G1184	U1124	G1064	A1004	G945	C885	A825	G765
U1481	U1425	A1305	C1245	C1245	G1186	U1126	C1066	G1006	A946	G886	C826	A766
G1482	G1426	U1307	U1247	U1247	G1187	G1127	A1067	U1007	G947	G887	U827	A767
A1483	G1427	U1308	A1248	A1248	A1188	C1128	G1068	G888	C948	U828	A768	G774
C1484	C1427	G1309	C1249	C1249	U1189	C1129	C1069	A889	A949	G829	G769	C770
U1485	A1428	A1310	A1250	A1250	G1190	A1130	U1070	U890	U950	G890	G830	C770
U1486	A1429	A1311	A1251	A1251	A1191	G1131	C1071	U891	G951	U891	A831	G771
G1487	A1430	C1312	A1252	A1252	C1192	C1132	G1072	A892	U952	G892	G832	U772
G1488	A1431	U1313	G1253	G1253	G1193	U1133	U1073	A893	G953	G893	G833	G773
U1489	G1432	U1314	A1254	A1254	U1194	G1134	G1074	U894	G954	U894	U834	G774
U1490	U1376	C1315	G1255	G1255	C1195	U1135	U1075	G895	U965	G895	U835	G775
G1491	A1377	G1316	A1256	A1256	A1196	C1136	U1076	G896	U967	C897	U837	A777
U1492	A1378	A1317	A1257	A1257	U1197	C1137	G1077	G898	U968	G898	G838	G778
A1493	A1433	A1318	G1258	G1258	C1198	G1138	U1078	A899	A969	C899	C839	C779
G1494	A1434	A1319	C1259	C1259	U1199	G1139	G1079	U900	A970	C900	A840	A780
G1495	U1440	A1320	G1260	G1260	C1200	C1140	A1080	G1020	U961	C901	C841	A781
C1496	A1441	U1321	U1261	U1261	A1201	A1141	A1081	A1021				

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30892	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	80000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	5.345	Depositor
Minimum map value	-7.752	Depositor
Average map value	-4.176	Depositor
Map value standard deviation	0.605	Depositor
Recommended contour level	-2.8	Depositor
Map size ( $\text{\AA}$ )	345.0, 345.0, 345.0	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.76, 2.76, 2.76	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	3.50	5275/36831 (14.3%)	3.96	9425/57458 (16.4%)

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	935

The worst 5 of 5275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	205	A	N7-C5	-20.49	1.26	1.39
1	N	499	A	N7-C5	-19.93	1.27	1.39
1	N	923	A	N7-C5	-19.93	1.27	1.39
1	N	3	A	N3-C4	-18.54	1.23	1.34
1	N	549	C	N3-C4	17.73	1.46	1.33

The worst 5 of 9425 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1519	A	N1-C6-N6	26.47	134.48	118.60
1	N	376	G	N1-C6-O6	26.45	135.77	119.90
1	N	832	G	C5-C6-O6	-25.79	113.13	128.60
1	N	722	G	N1-C6-O6	25.48	135.19	119.90
1	N	1261	A	N1-C6-N6	24.80	133.48	118.60

There are no chirality outliers.

5 of 935 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	11	G	Sidechain
1	N	4	U	Sidechain
1	N	5	U	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	16532	493	0
All	All	32892	16554	16532	493	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 10.

The worst 5 of 493 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:1123:U:H3	1:N:1150:A:H61	1.28	0.81
1:N:688:G:C8	1:N:688:G:H5''	2.18	0.78
1:N:1255:G:H2'	1:N:1279:G:H1	1.54	0.72
1:N:1240:U:C6	1:N:1241:G:H5'	2.24	0.71
1:N:50:A:H1'	1:N:52:C:C6	2.27	0.69

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%)	441 (28%)	162 (10%)

5 of 441 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	7	A

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1064	G
1	N	1331	G
1	N	1129	C
1	N	1197	A
1	N	1364	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.

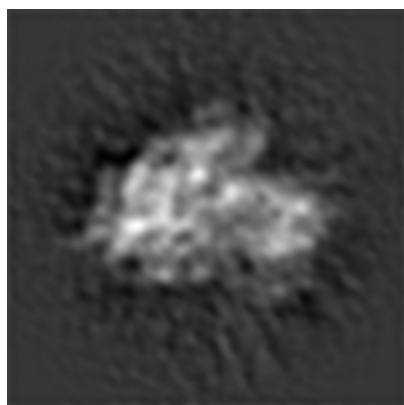
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5503. These allow visual inspection of the internal detail of the map and identification of artifacts.

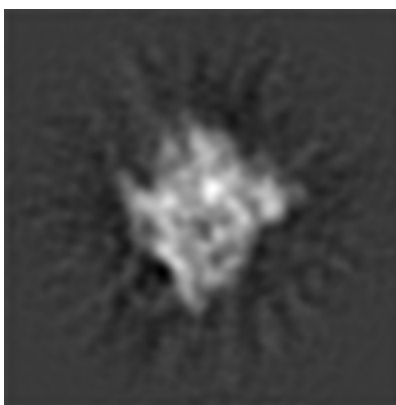
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

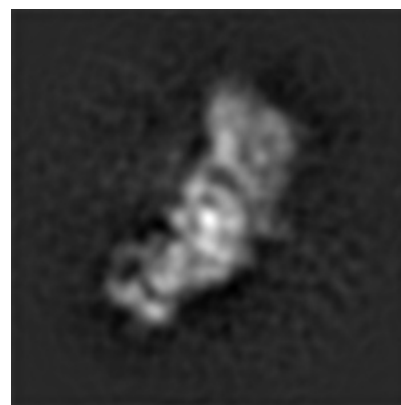
#### 6.1.1 Primary map



X



Y

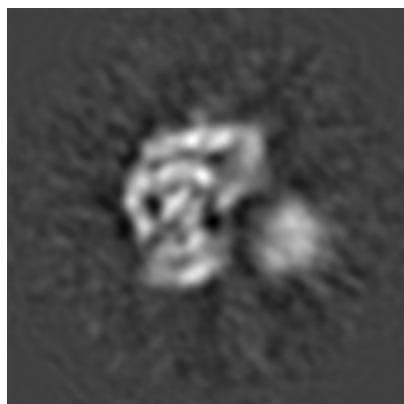


Z

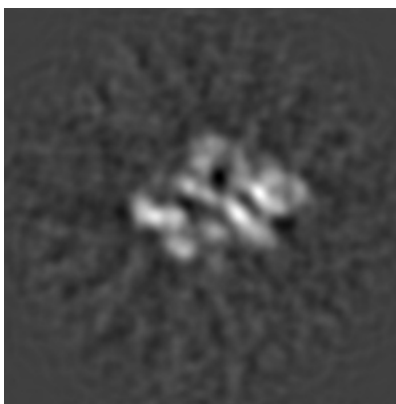
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

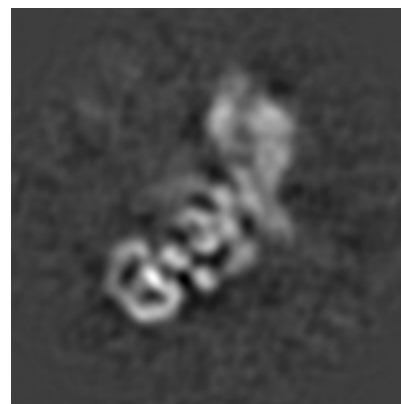
#### 6.2.1 Primary map



X Index: 62



Y Index: 62

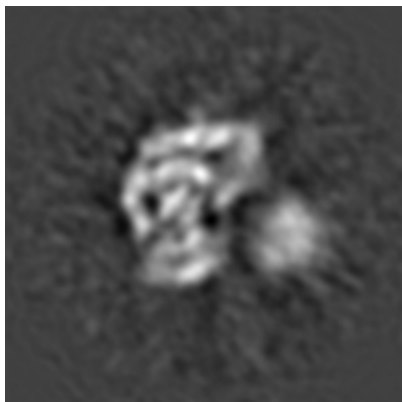


Z Index: 62

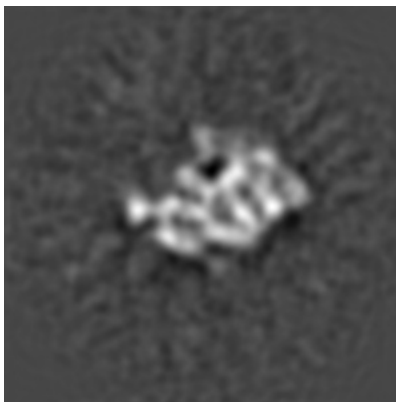
The images above show central slices of the map in three orthogonal directions.

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

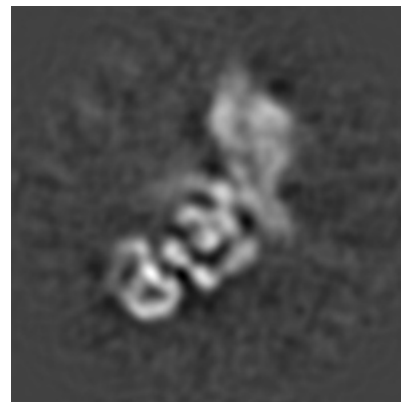
### 6.3.1 Primary map



X Index: 62



Y Index: 58

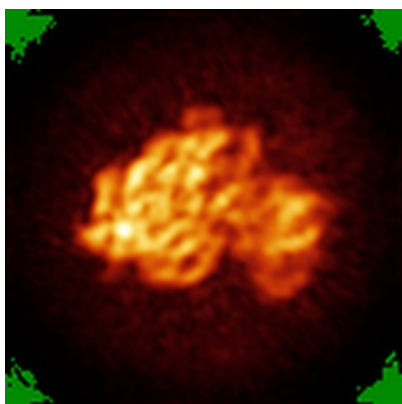


Z Index: 63

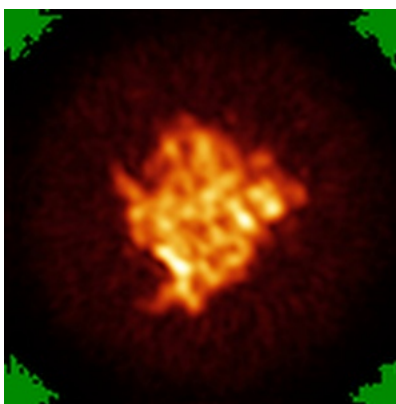
The images above show the largest variance slices of the map in three orthogonal directions.

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

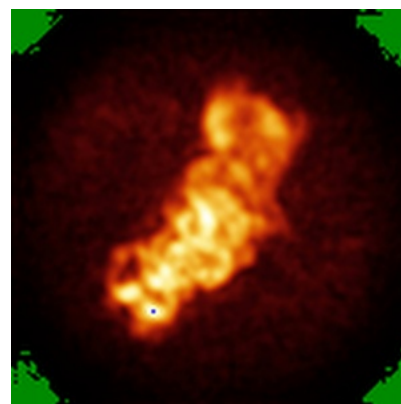
### 6.4.1 Primary map



X



Y

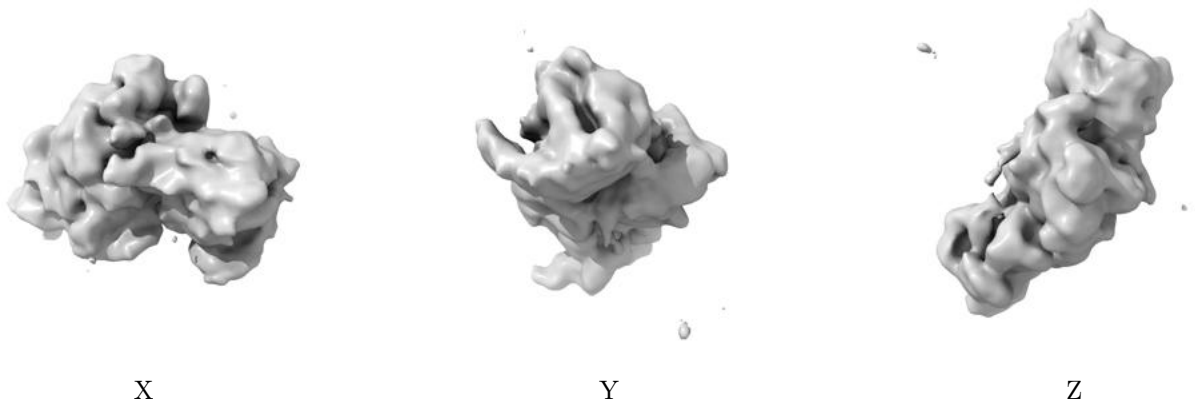


Z

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.

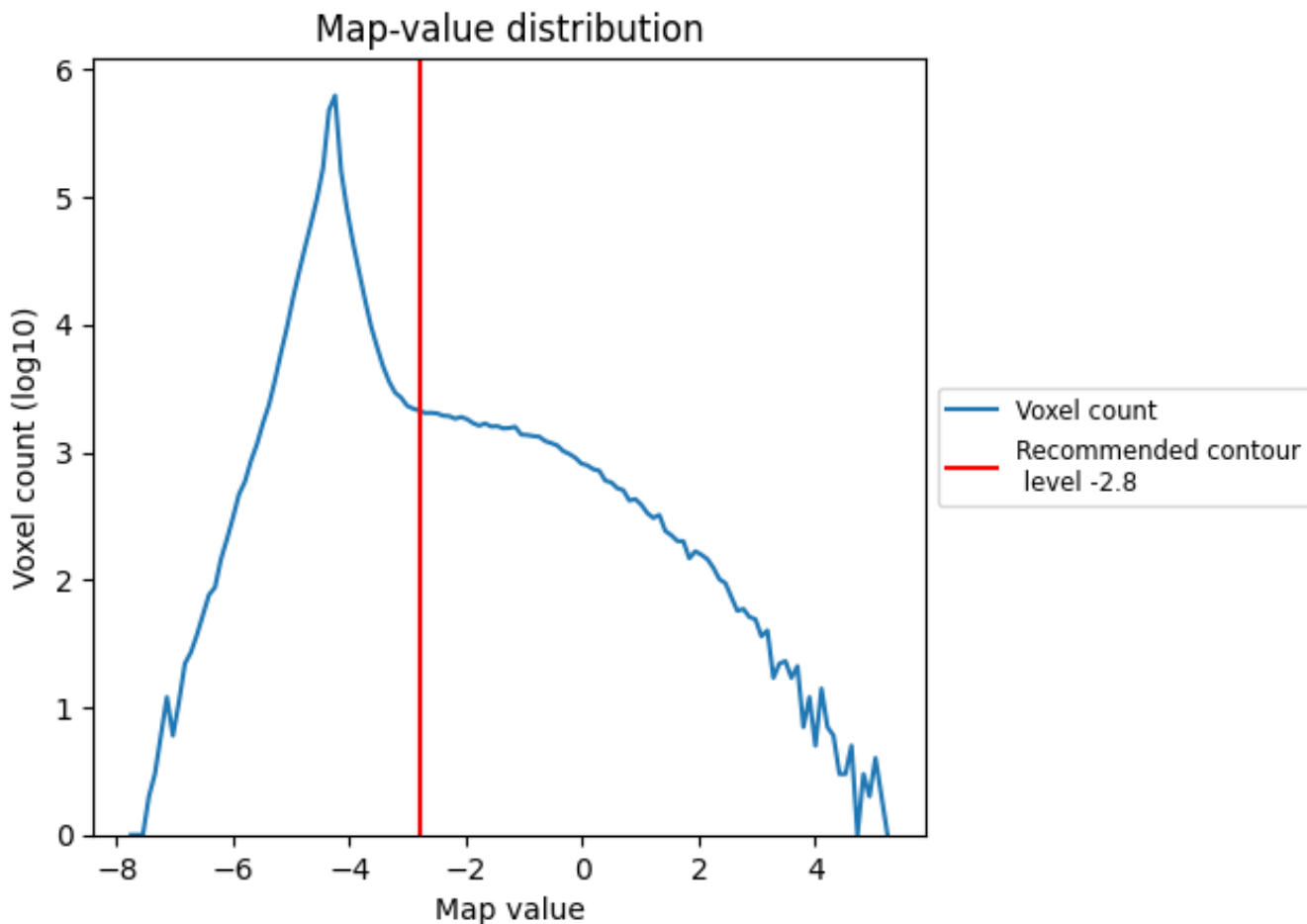
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

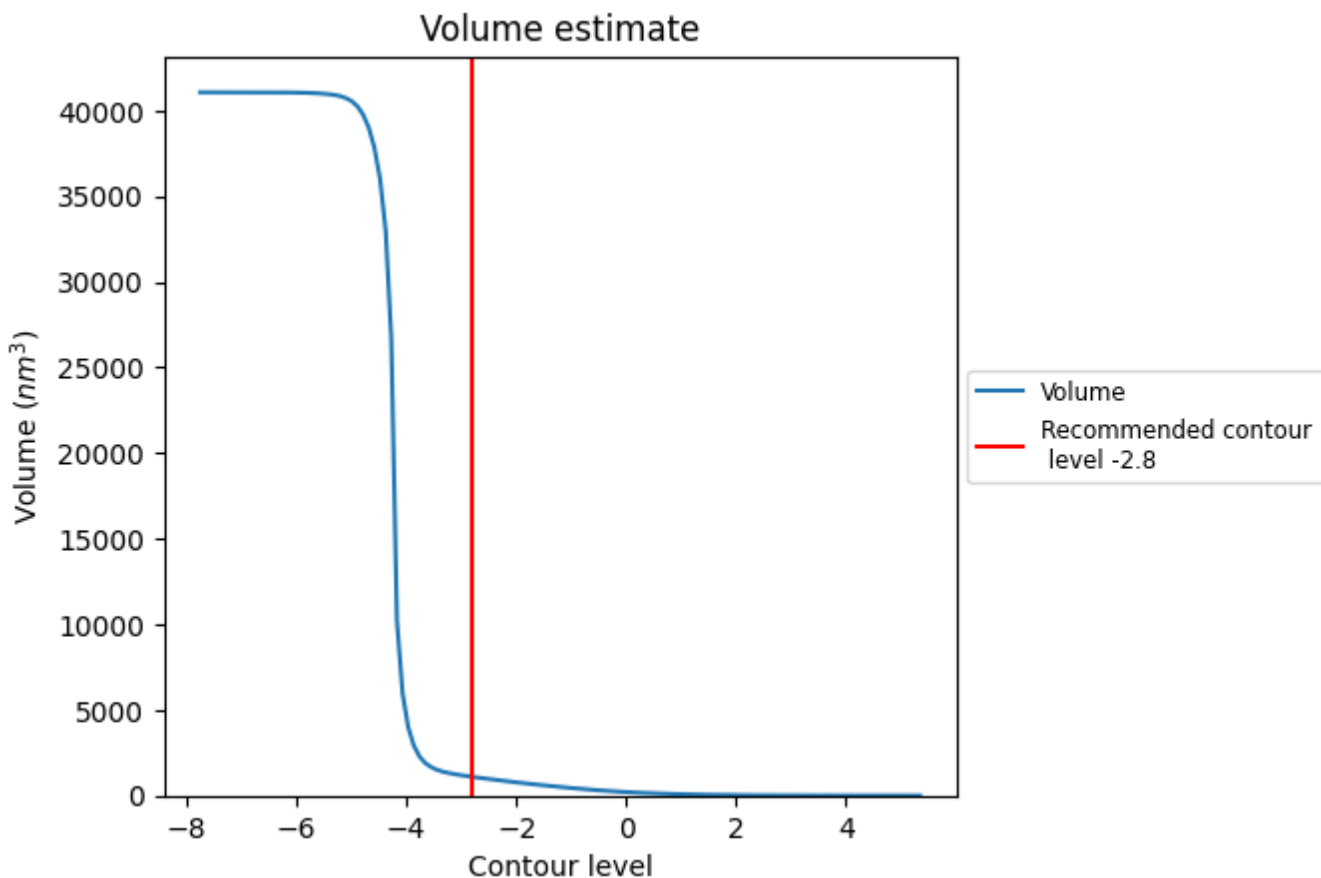
This section contains the results of statistical analysis of the map.

### 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.

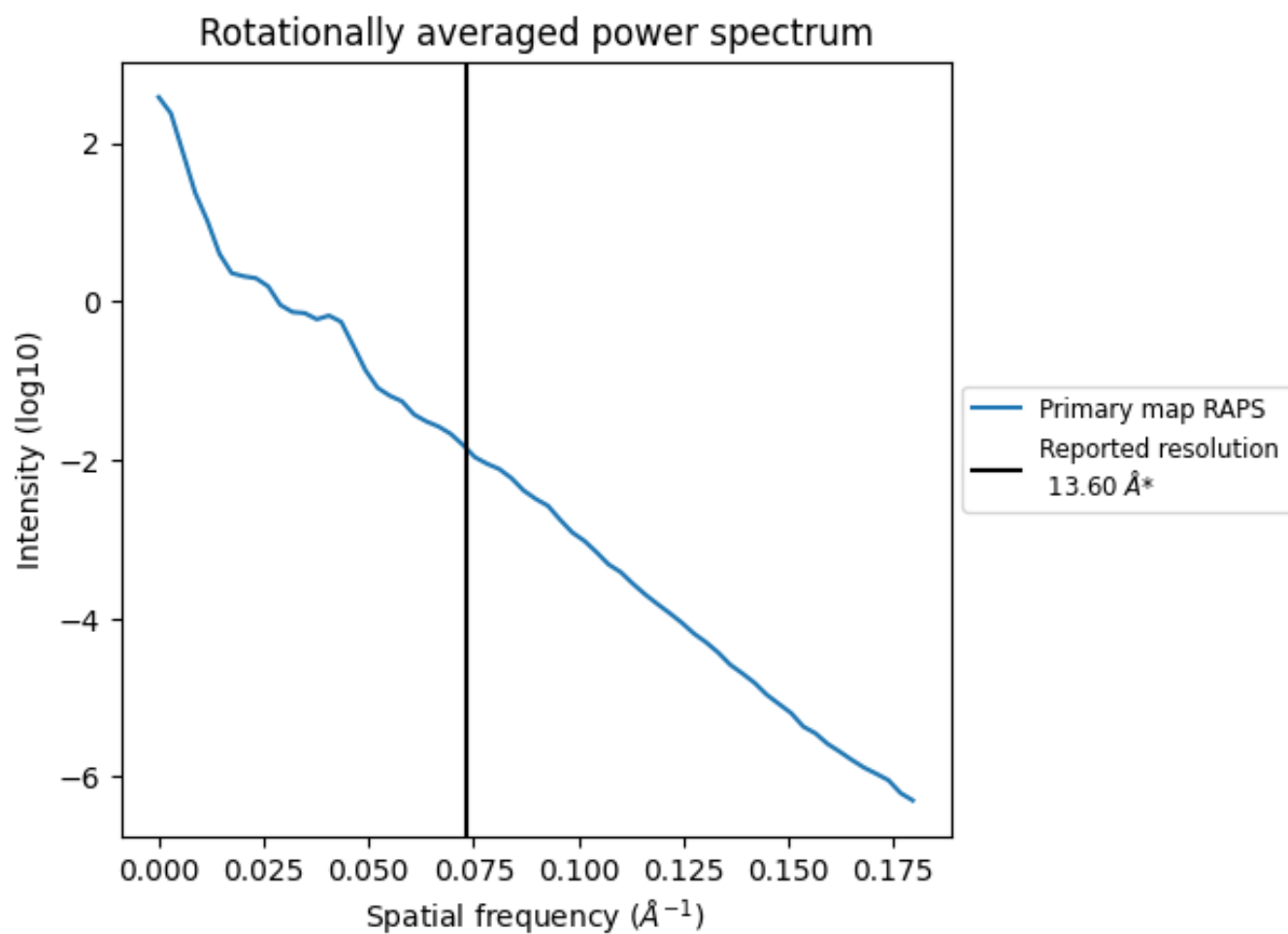
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $1092 \text{ nm}^3$ ; this corresponds to an approximate mass of 986 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 0.074 Å<sup>-1</sup>



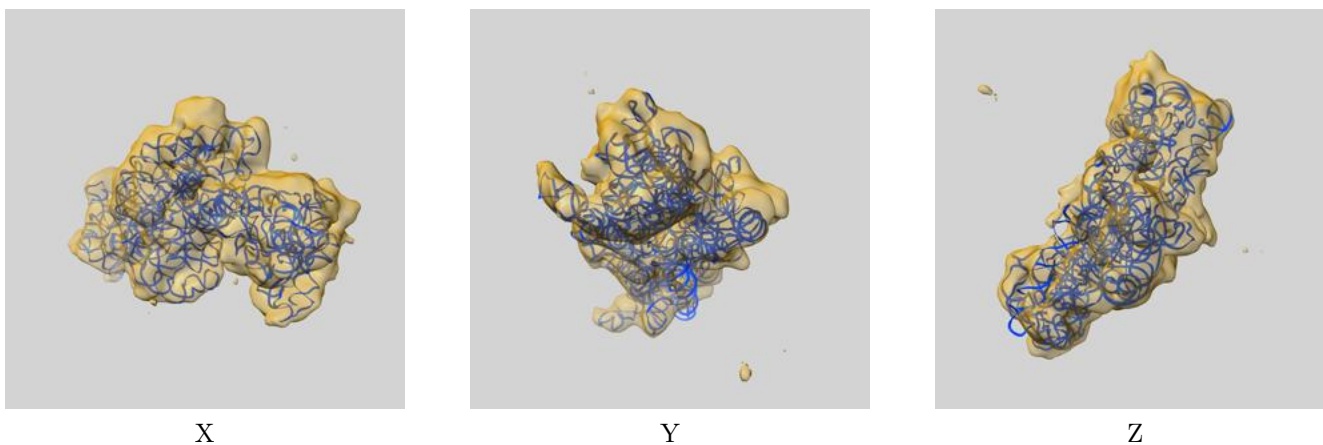
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

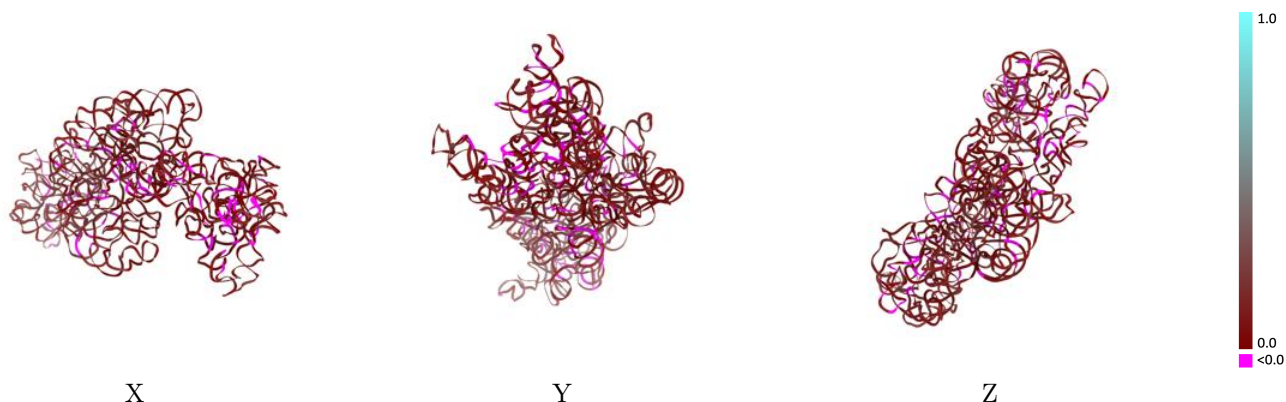
This section contains information regarding the fit between EMDB map EMD-5503 and PDB model 3J2B. Per-residue inclusion information can be found in section 3 on page 4.

### 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](#)



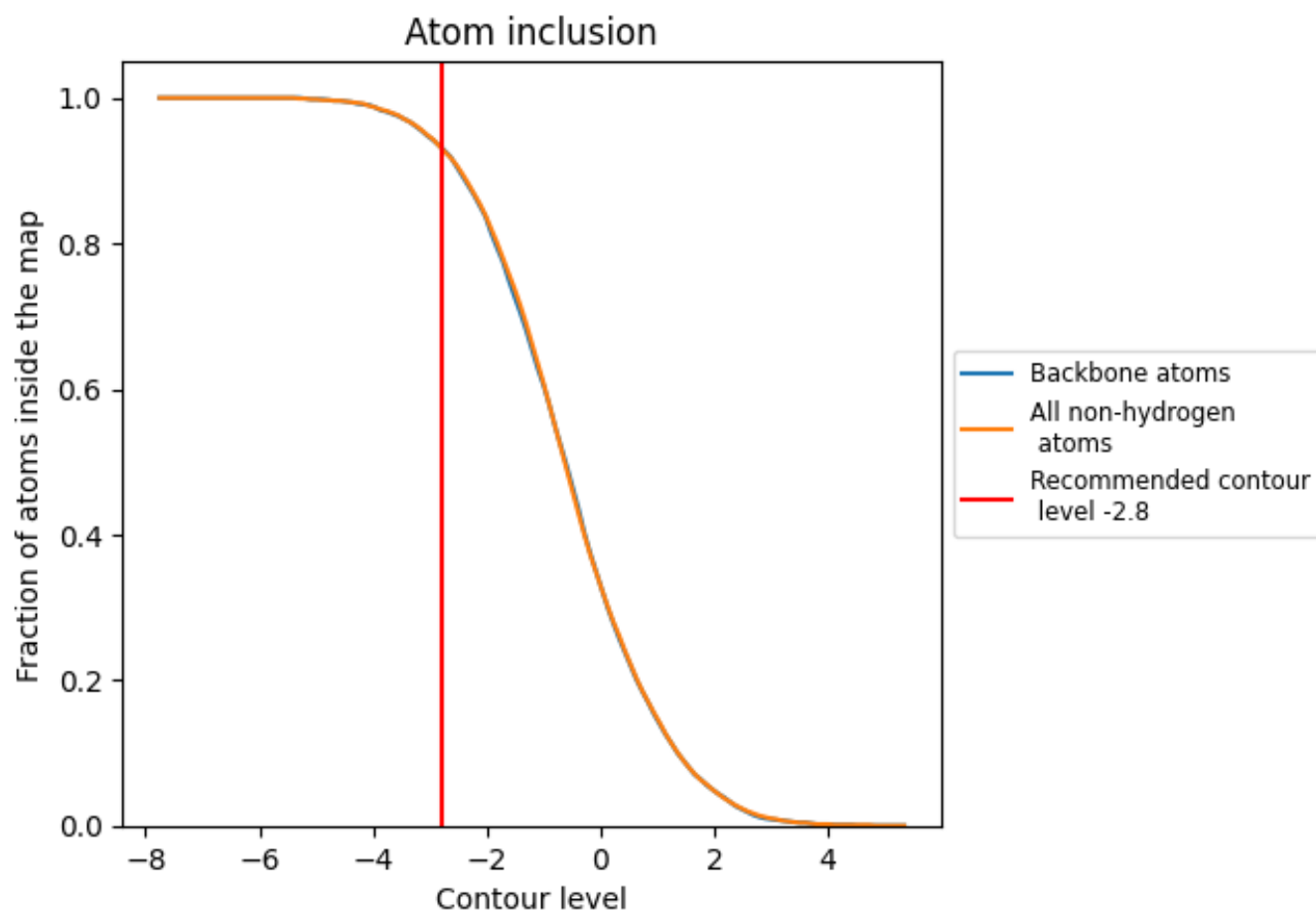
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 93% 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	 0.9310	 0.0880
N	 0.9310	 0.0880

