



# wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 12:33 PM EST

PDB ID : 3J2A  
EMDB ID : EMD-5502  
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 : 13.10 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.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

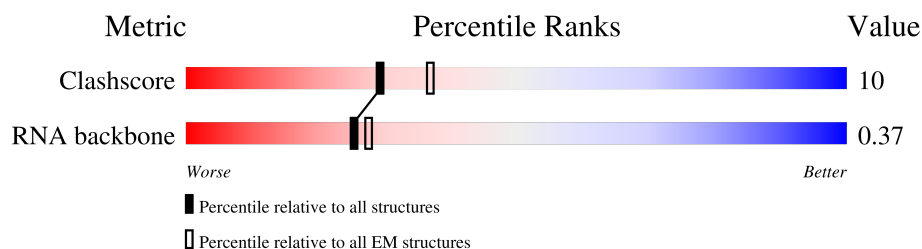
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 13.10 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.

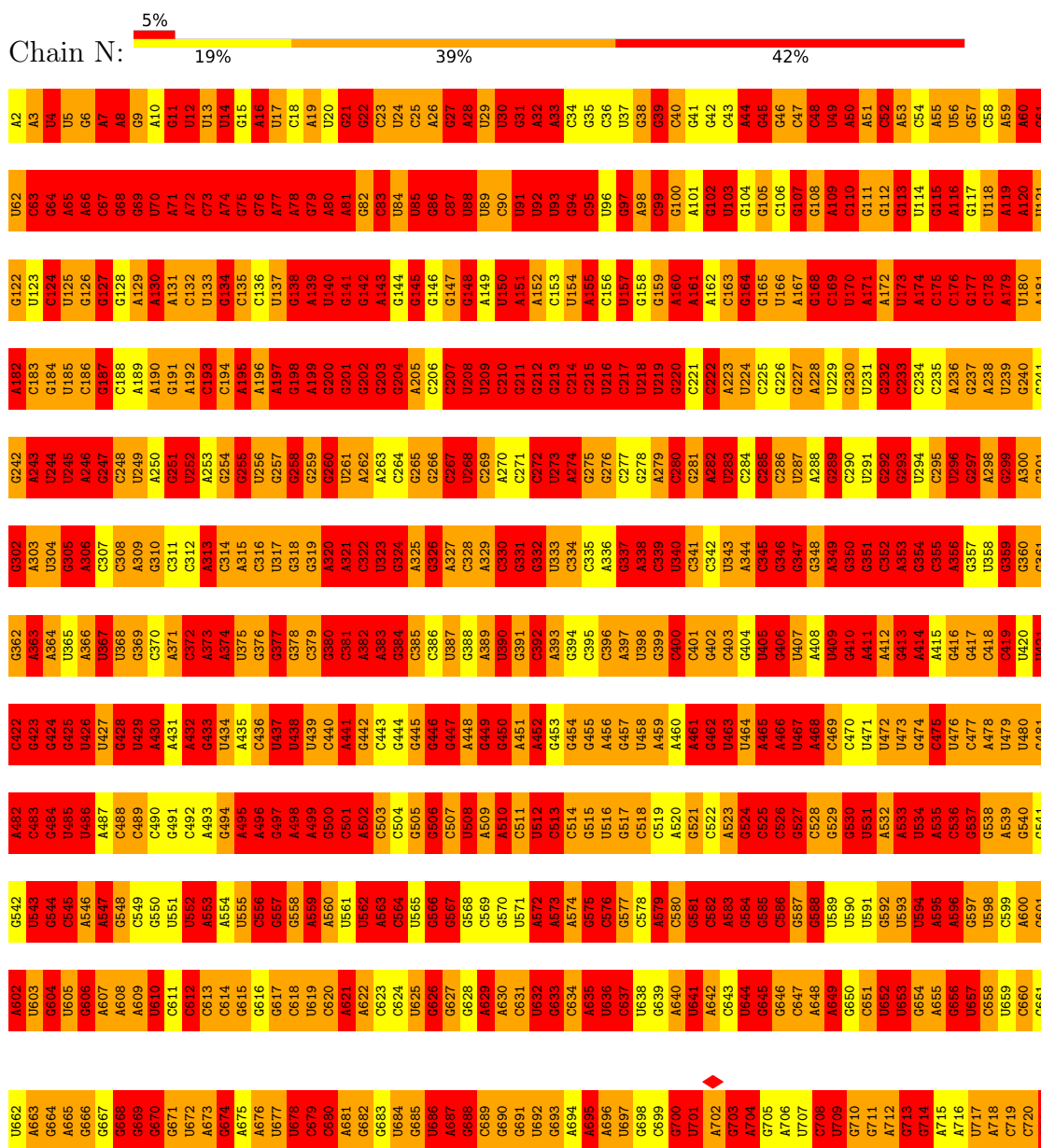
- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
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	U1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	A1324	G1144	G1084	G1024	A964	U904	G844	A784	G724
G1505	U1445	C1325	A1145	U1085	U1025	U965	U905	A845	G785	G725
U1506	A1446	U1326	G1146	G1086	G1026	G966	A906	G846	G786	C726
A1507	A1447	C1327	C1147	U1087	C1027	C967	A907	G847	G787	G727
A1508	C1448	U1328	U1148	G1088	G1028	A968	A908	C848	U788	A728
C1509	C1389	A1329	C1149	G1089	U1029	A969	A909	G849	U789	A729
C1510	U1390	U1330	A1150	U1090	U1030	C970	C910	U850	A790	G729
G1511	U1391	G1331	A1151	U1091	G1031	G851	U911	G851	G791	G731
U1512	U1392	A1332	G1152	A1092	G1032	C972	C912	G852	A792	C732
A1513	U1393	C1333	G1153	A1093	G1033	G973	A913	C853	G793	G733
G1514	A1394	G1334	C1214	G1094	G1034	A974	A914	U854	A794	G734
G1515	C1395	U1335	A1155	U1095	A1035	A975	A915	U855	C795	C735
G1516	A1396	C1336	G1156	C1096	A1036	G976	U916	C856	G796	C736
G1517	C1397	G1337	A1157	U1097	C1037	A977	G917	C857	C797	C737
A1518	G1454	G1338	G1158	C1098	C1038	C978	A918	G858	U798	C738
A1519	G1455	A1398	U1159	U1099	G1039	C979	A919	G859	G799	C739
C1520	G1456	C1399	C1219	G1100	U1040	U980	U920	A860	G800	U740
C1521	G1457	A1340	G1160	C1100	G1041	U981	U921	C861	U801	G741
U1522	G1458	U1341	C1161	A1101	A1042	U982	G922	C862	A802	G742
G1523	C1459	C1342	U1162	A1102	G1043	A983	A923	U863	G803	A743
C1524	C1460	G1343	G1163	C1103	A1044	C984	C924	A864	U804	C744
G1525	G1461	C1344	U1164	G1104	A1045	G985	G925	A865	C805	G745
G1526	C1462	A1345	G1165	A1105	C1045	U986	G926	C866	C806	A746
U1527	U1463	U1346	G1166	G1106	A1046	G987	G927	C867	A807	A747
U1528	U1464	G1347	A1167	C1107	G1047	G988	G928	C868	G808	G748
G1529	A1465	U1348	U1168	G1108	G1048	U989	G929	G869	G809	A749
G1530	A1466	A1349	A1169	C1109	U1049	C990	C930	U870	C810	C750
A1531	C1467	C1350	U1170	A1110	G1050	U991	C931	U871	C811	U751
U1532	C1468	U1351	C1171	G1111	C1051	U992	G932	A872	G812	G752
C1533	A1469	C1352	U1172	C1112	U1052	G993	G933	C873	U813	A753
A1534	C1469	G1353	U1173	C1113	G1053	C994	C934	A874	A814	C754
	U1470	U1354	G1174	C1114	A1054	A995	A935	U875	A815	G755
	U1471	G1355	U1175	U1115	A1055	A996	C936	C876	C816	C756
	U1472	A1356	G1176	U1116	U1056	G997	A937	A877	G817	U757
	G1473	C1357	U1177	A1117	G1057	C998	A938	A878	G818	C758
	U1474	U1358	G1178	U1118	C1058	C999	G939	C879	A819	A759
	G1475	C1359	A1179	C1119	C1059	A1000	C940	C880	U820	G760
	A1476	A1360	G1180	C1120	U1060	G1001	G941	G881	G821	G761
	U1477	G1361	U1181	U1121	U1061	G1002	G942	C882	U822	U762
	U1478	C1362	G1182	U1122	U1062	G1003	U943	C883	C823	G763
	U1479	U1363	U1183	U1123	C1063	A1004	G944	G884	G824	C764
	A1480	G1364	G1184	G1124	G1064	A1005	G945	G885	A825	G765
	U1481	C1365	U1185	U1125	C1065	G1006	A946	G886	C826	A766
	G1482	C1366	G1186	U1126	C1066	U1007	G947	G887	U827	A767
	A1483	C1367	U1187	C1127	G1067	A1008	C948	G888	U828	A768
	U1484	A1368	A1188	U1128	G1068	A949	A949	A889	G829	G769
	U1485	U1369	U1189	C1129	C1069	U1009	U950	G890	G830	G770
	G1486	G1370	G1190	A1130	U1070	C1011	G951	U891	A831	G771
	U1487	A1371	U1191	G1131	C1071	A1012	U952	A892	G832	U772
	G1488	U1372	C1192	C1132	G1072	G1013	G953	C893	G833	G773
	A1489	G1373	G1193	U1133	U1073	A1014	G954	G894	U834	G774
	U1490	A1374	U1194	G1134	G1074	G1015	U955	G895	U835	G775
	G1491	C1375	U1195	U1135	U1075	A1016	U956	C896	G836	G776
	A1492	U1376	A1196	C1136	G1076	U1017	U957	U897	G837	A777
	U1493	A1377	U1197	G1137	G1077	G1018	A898	C898	G838	G778
	G1494	C1378	G1198	U1138	U1078	A1019	A959	C899	C839	C779
	U1495	A1379	U1199	G1139	G1079	A1020	U960	A900	A780	G779
	G1496	C1380	C1200	C1140	A1080	A1021	U961	C841	G781	A781
	U1497	U1381	A1201	C1141	A1081					
	A1498									
	U1499									
	A1500									
	C1501									

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30262	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	4.176	Depositor
Minimum map value	-6.630	Depositor
Average map value	-3.903	Depositor
Map value standard deviation	0.568	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	3.48	5331/36831 (14.5%)	4.00	9667/57458 (16.8%)

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	937

The worst 5 of 5331 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1299	A	N7-C5	-19.75	1.27	1.39
1	N	787	A	N7-C5	-16.87	1.29	1.39
1	N	1367	C	N1-C6	16.52	1.47	1.37
1	N	1504	G	C6-N1	16.46	1.51	1.39
1	N	854	U	N3-C4	16.35	1.53	1.38

The worst 5 of 9667 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1225	A	N1-C6-N6	28.69	135.81	118.60
1	N	438	U	P-O3'-C3'	28.20	153.54	119.70
1	N	1130	A	N1-C6-N6	26.64	134.58	118.60
1	N	889	A	N1-C6-N6	25.22	133.73	118.60
1	N	748	G	N1-C6-O6	25.02	134.91	119.90

There are no chirality outliers.

5 of 937 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	11	G	Sidechain
1	N	12	U	Sidechain
1	N	4	U	Sidechain
1	N	7	A	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	16528	504	0
All	All	32892	16554	16528	504	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 504 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:928:G:H21	1:N:1533:C:H42	1.24	0.85
1:N:67:C:H2'	1:N:68:G:C8	2.13	0.83
1:N:50:A:H1'	1:N:52:C:C6	2.23	0.73
1:N:1266:G:H21	1:N:1269:A:H8	1.39	0.70
1:N:1394:A:H3'	1:N:1395:C:H5'	1.74	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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	1532/1533 (99%)	460 (30%)	145 (9%)

5 of 460 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 145 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1228	C
1	N	1530	G
1	N	1282	C
1	N	1363	A
1	N	430	A

## 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.

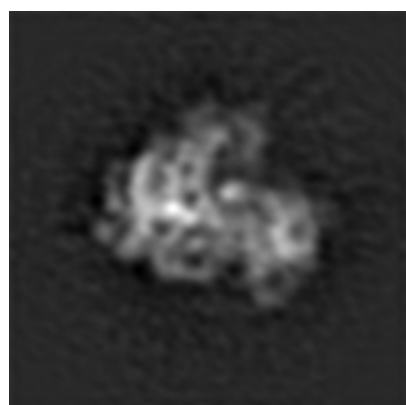
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5502. These allow visual inspection of the internal detail of the map and identification of artifacts.

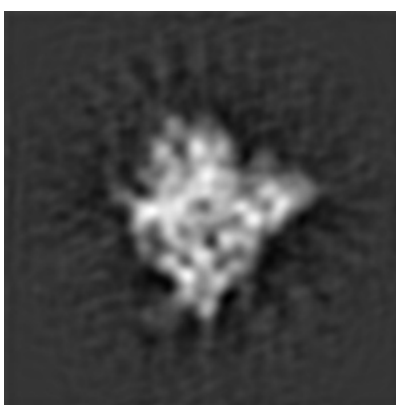
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

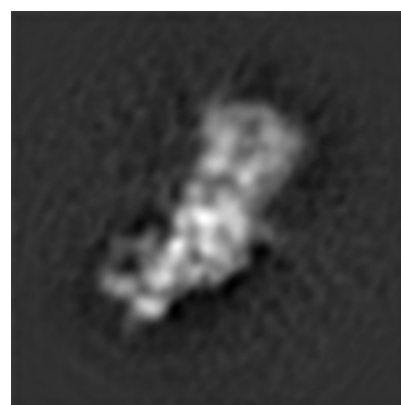
#### 6.1.1 Primary map



X



Y

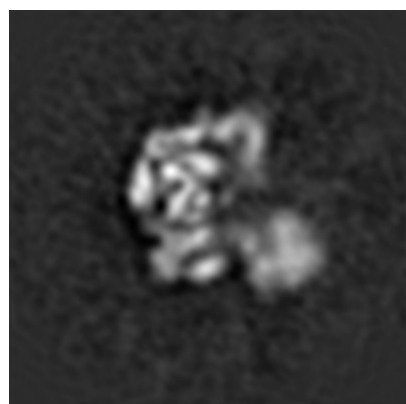


Z

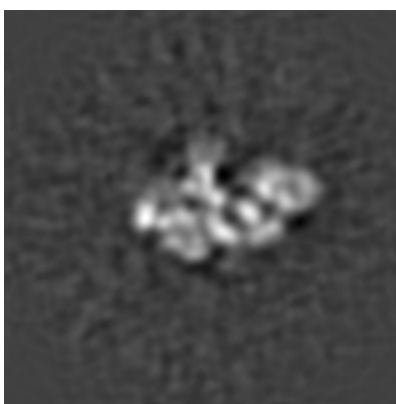
The images above show the map projected in three orthogonal directions.

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

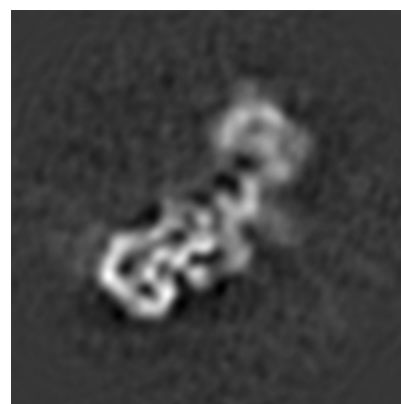
#### 6.2.1 Primary map



X Index: 62



Y Index: 62

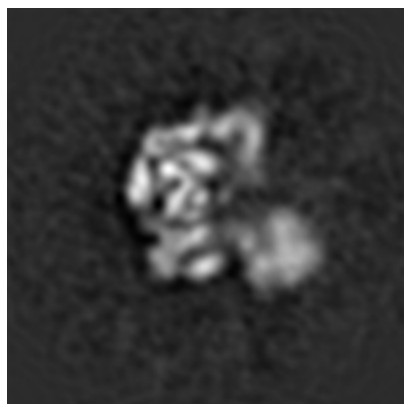


Z Index: 62

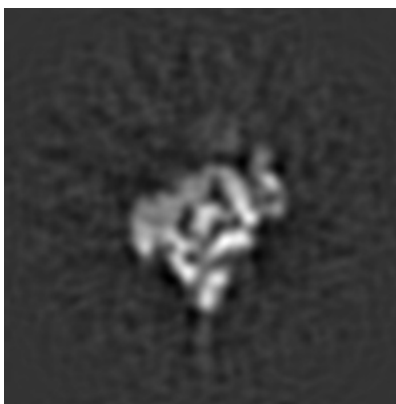
The images above show central slices of the map in three orthogonal directions.

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

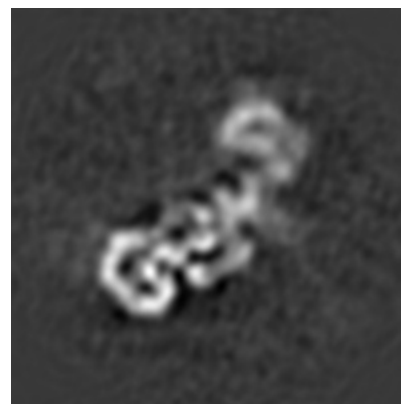
### 6.3.1 Primary map



X Index: 62



Y Index: 51

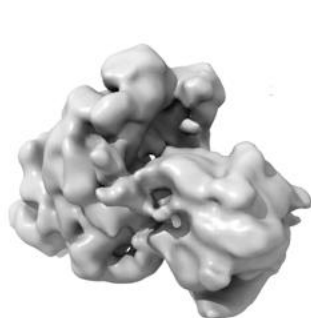


Z Index: 63

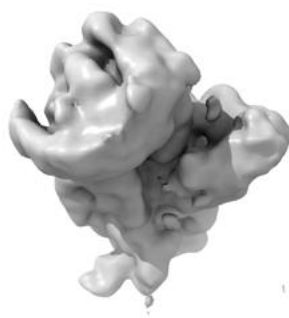
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

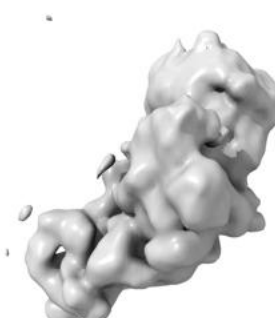
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level - 2.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

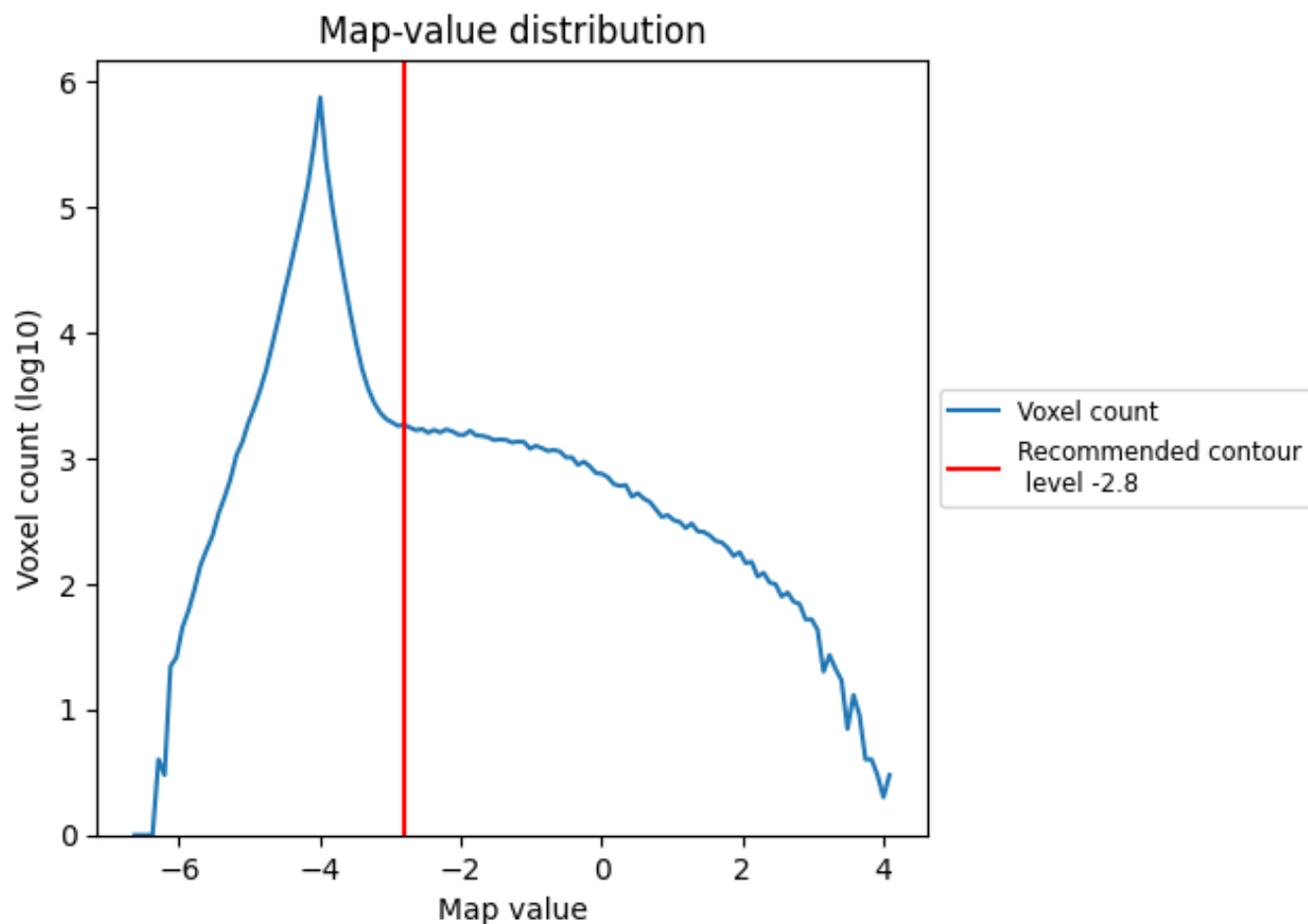
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

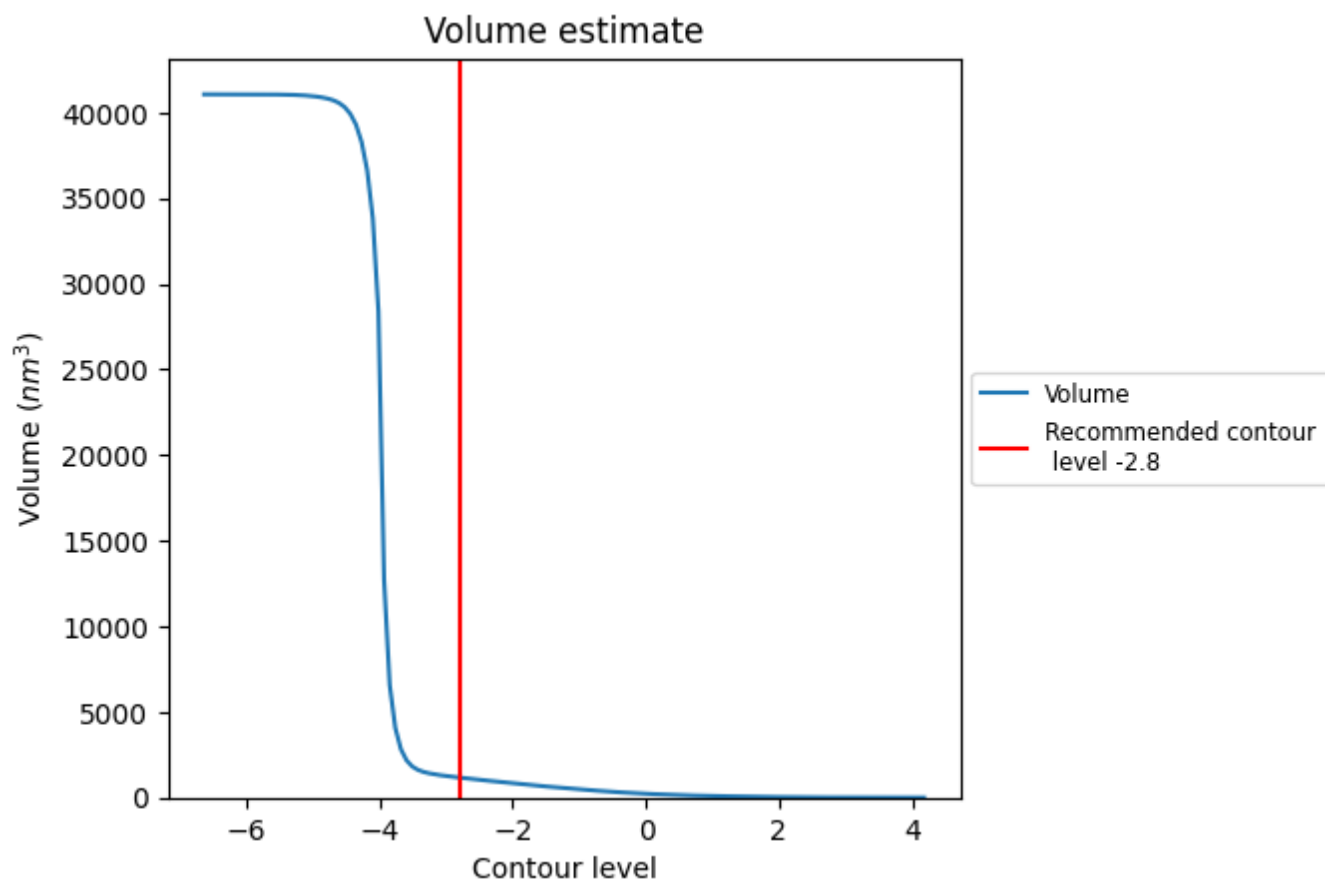
This section contains the results of statistical analysis of the map.

### 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.

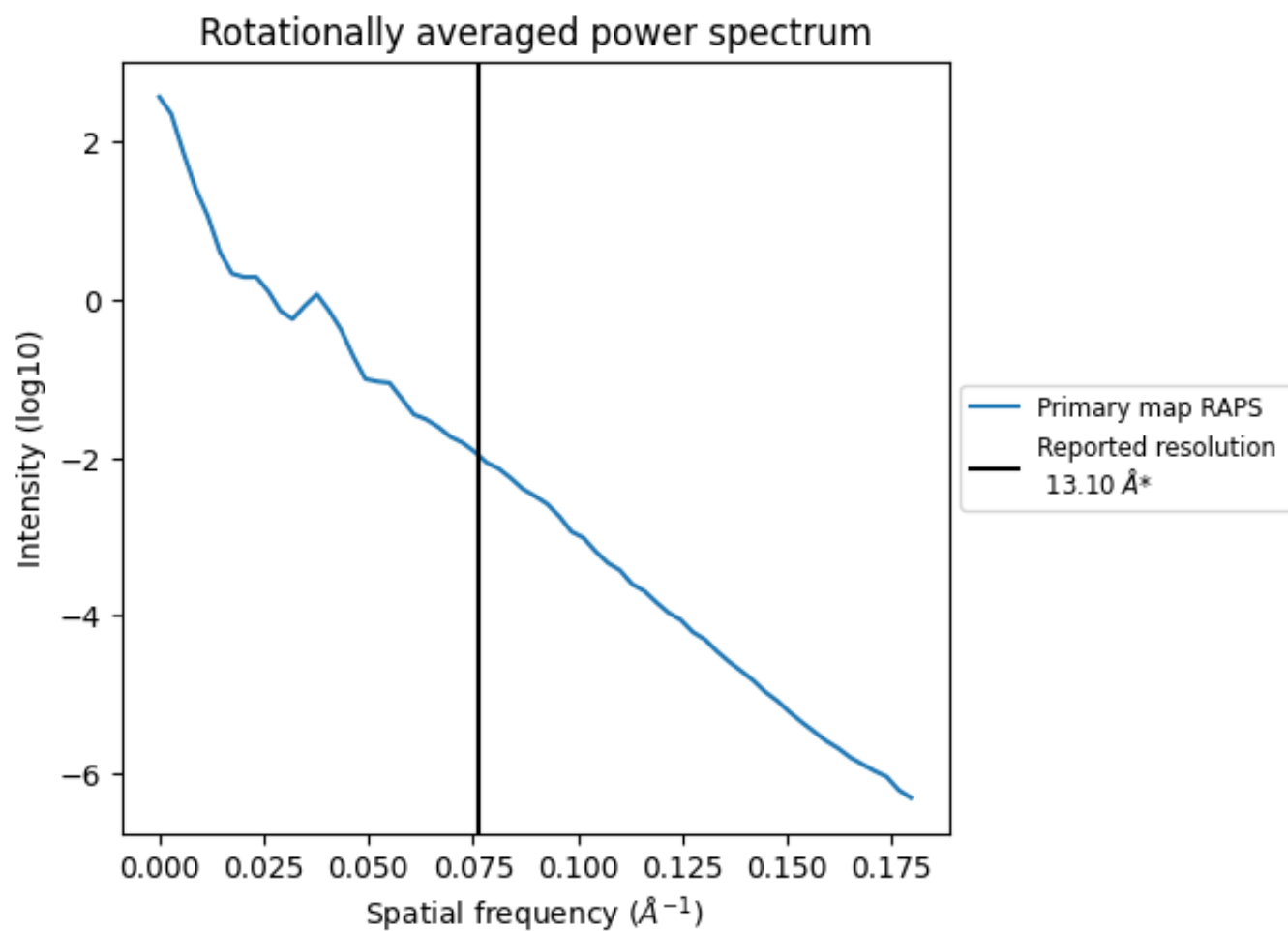
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1168 nm<sup>3</sup>; this corresponds to an approximate mass of 1055 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 0.076 Å<sup>-1</sup>



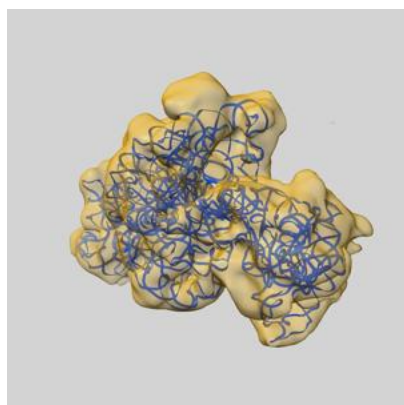
## 8 Fourier-Shell correlation

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

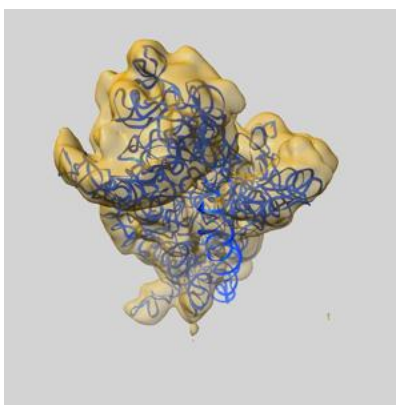
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5502 and PDB model 3J2A. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

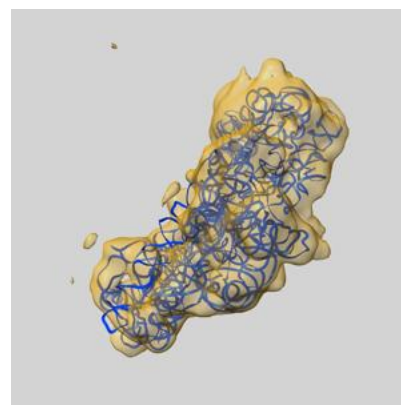
### 9.1 Map-model overlay [i](#)



X



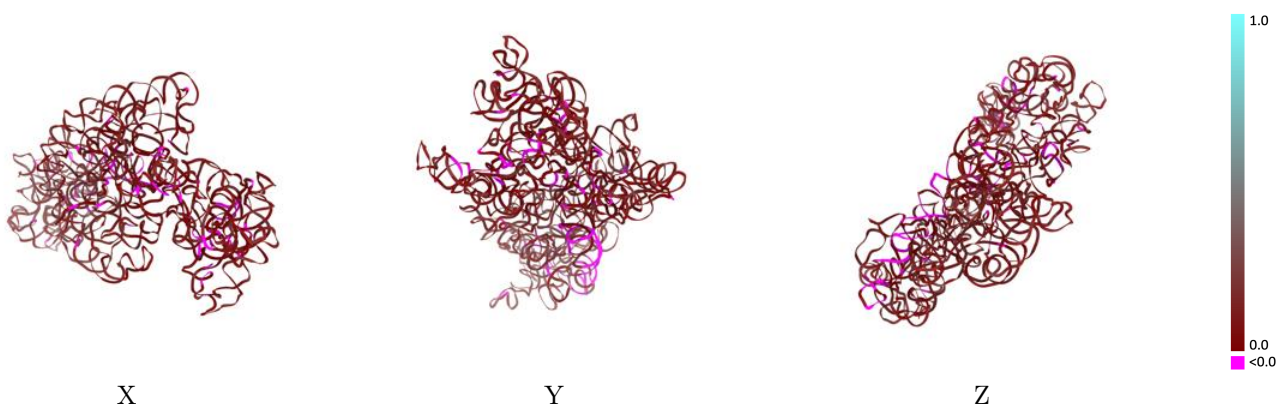
Y



Z

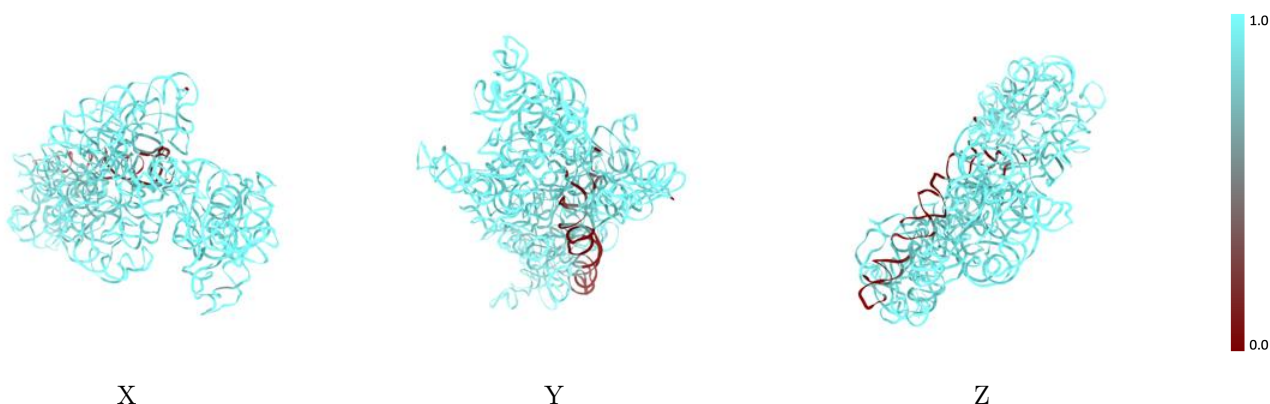
The images above show the 3D surface view of the map at the recommended contour level -2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



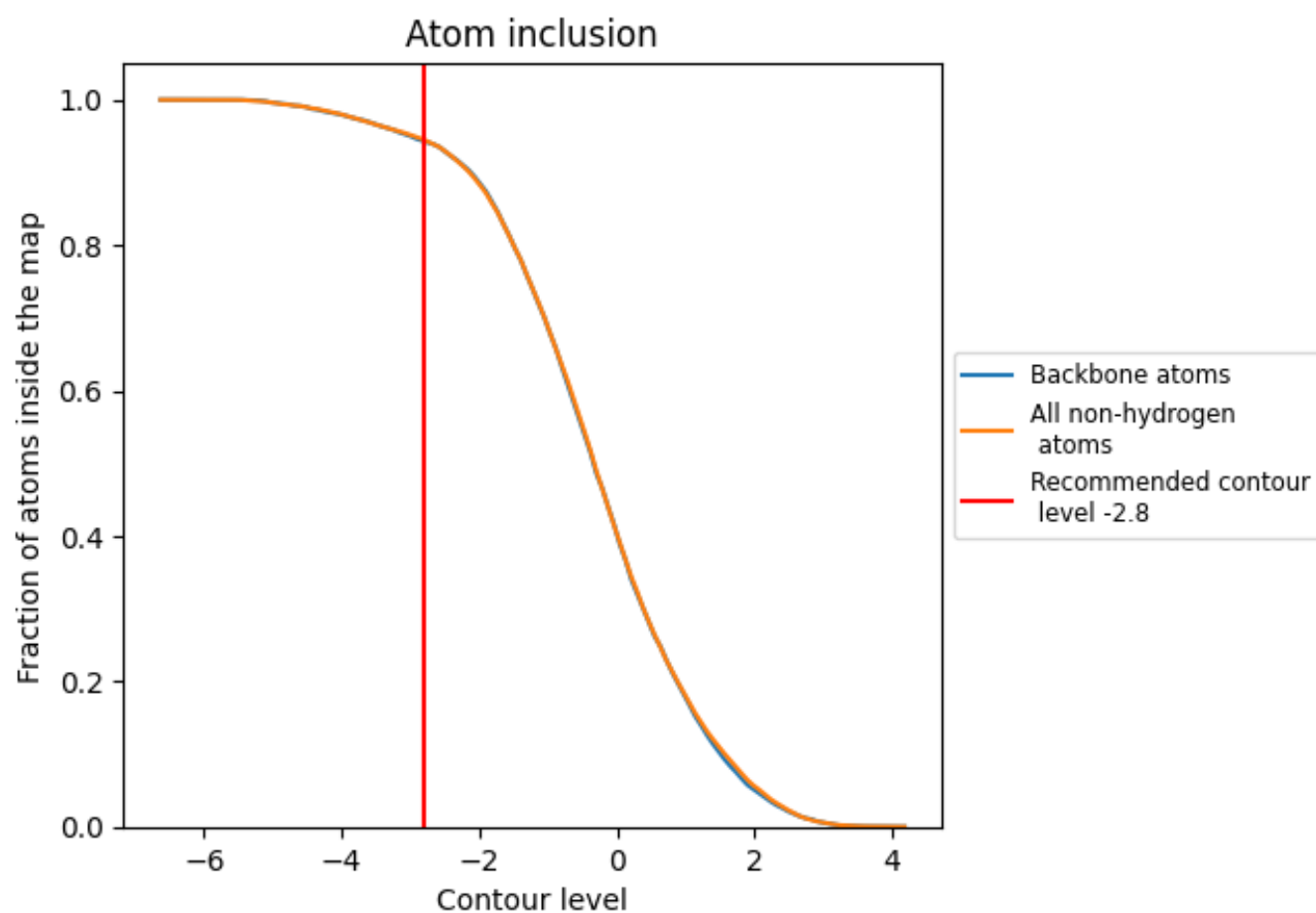
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 94% 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 (-2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9448	<div><div></div></div> 0.0980
N	<div><div></div></div> 0.9447	<div><div></div></div> 0.0980

