



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 12:28 PM EST

PDB ID : 3J29
EMDB ID : EMD-5501
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 : 14.00 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.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

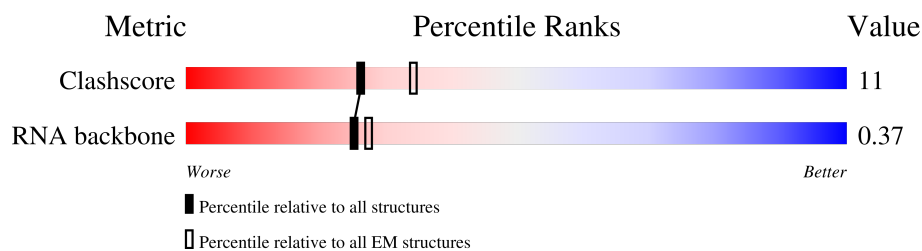
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 14.00 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.

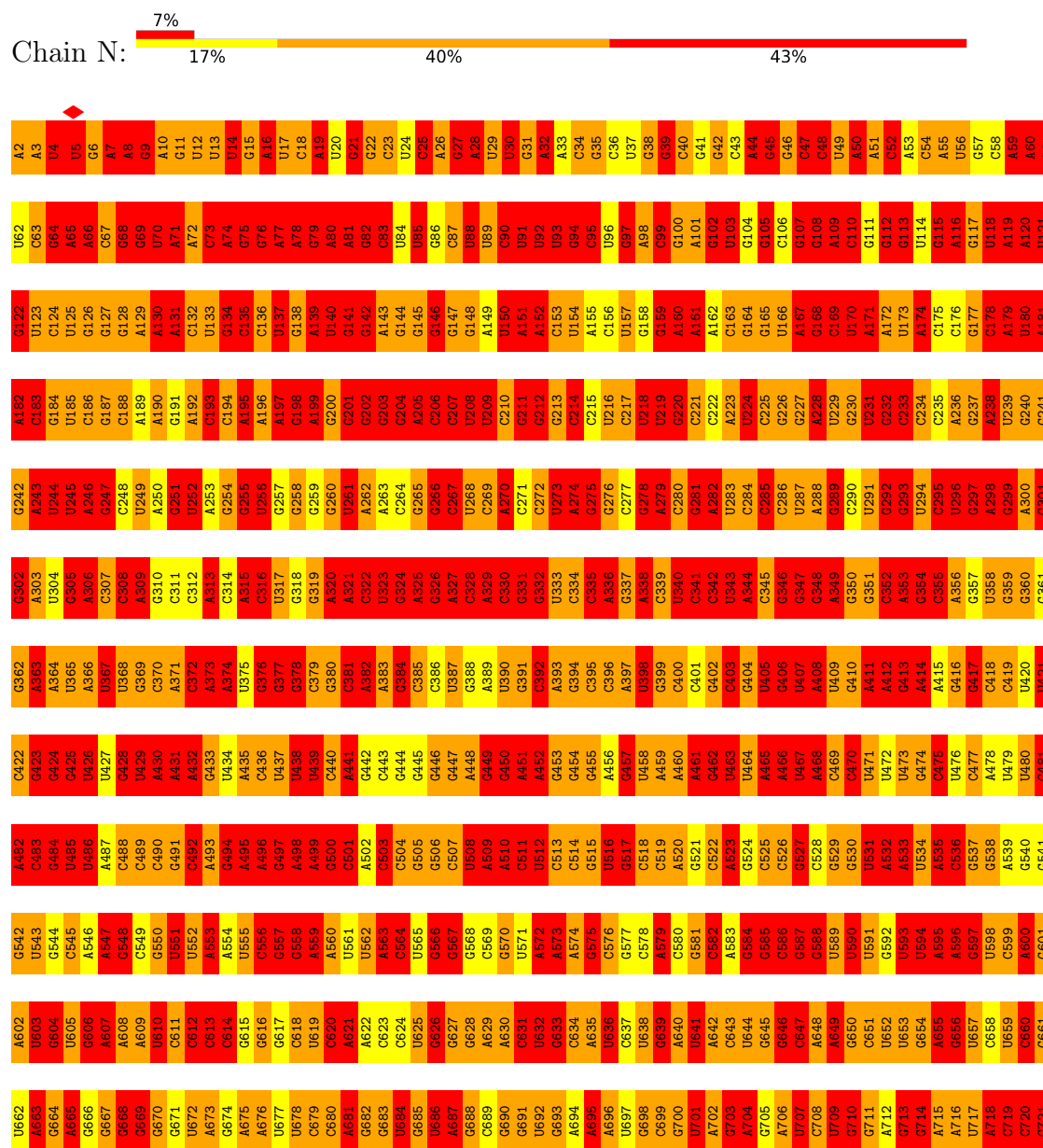
- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
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	G1522	C1262	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	G1523	C1263	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	C1444	C1384	A1324	U1264	G1144	U1084	G1024	A964	U904	G844	C784	U724
G1505	U1444	G1385	C1325	C1265	A1145	U1085	G1025	U965	U905	A845	G785	G725
U1506	U1445	G1386	G1326	C1266	A1146	U1086	U1026	G966	A906	G846	G786	G726
A1507	A1446	G1387	G1327	C1267	G1147	U1087	C1027	C967	A907	G847	A787	G727
A1508	A1447	C1388	C1328	G1268	U1148	U1088	G1028	A968	A908	C848	U788	A728
C1448	C1448	C1389	A1329	G1269	C1149	U1089	C1028	U969	A909	C849	U789	A729
C1449	U1390	U1390	U1330	G1270	A1151	U1090	C1028	A969	C910	U850	G790	G730
C1510	U1391	G1331	A1332	A1271	A1152	U1091	U1029	C970	U911	G851	G791	G731
U1450	U1451	G1392	A1332	U1212	A1153	U1092	U1030	C971	C912	G852	A792	C732
A1512	U1452	U1393	G1333	A1213	G1153	A1093	G1031	C972	A913	C853	U793	G733
A1513	C1453	A1394	C1334	C1214	G1154	G1094	C1032	A973	A914	U854	A794	G734
G1514	G1454	A1396	A1275	G1215	A1155	U1095	G1033	A974	A915	U855	C795	G735
G1515	C1396	G1276	G1276	A1216	G1156	C1096	G1034	A975	U916	C856	C796	C736
G1516	C1397	C1277	C1277	C1217	A1157	C1097	G1035	A976	G917	C857	C797	C737
G1517	A1455	A1398	G1337	C1218	U1158	C1098	A1036	A977	A918	G858	U798	G738
A1518	A1456	C1399	A1339	G1219	U1159	G1099	A1035	A978	A919	G859	G799	C739
A1519	G1457	G1400	A1340	A1220	G1160	C1100	A1036	C979	U920	C860	G800	U740
C1520	G1458	G1401	U1341	G1221	C1161	A1101	C1037	U980	U921	C861	U801	G741
C1521	C1402	C1402	C1342	G1222	C1162	A1102	C1038	U981	G922	C862	A802	G742
U1522	C1403	C1403	G1343	C1223	A1163	C1103	G1039	U982	A923	U863	G803	A743
G1523	C1404	C1404	U1344	U1224	G1164	G1104	G1040	A983	C924	A864	U804	C744
C1524	G1461	G1405	U1345	A1225	U1165	A1105	U1040	C984	G925	A865	C805	G745
G1525	U1462	A1406	A1346	C1226	G1166	G1106	G1041	C985	G926	C866	C806	A746
G1526	U1463	C1407	G1347	A1227	A1167	C1107	G1042	U986	G927	C867	A807	A747
U1527	U1464	A1408	A1348	C1228	U1168	G1108	A1043	C987	G928	C868	C808	G748
U1528	A1465	A1409	A1349	A1229	A1169	C1109	A1044	G988	G929	C869	G809	A749
G1529	C1466	C1410	A1350	C1230	A1170	C1110	C1045	U989	C930	U870	C810	C750
G1530	C1467	C1411	U1351	G1231	A1171	A1111	G1046	C990	C931	U871	C811	U751
A1531	A1468	C1412	G1352	U1232	C1172	C1112	U1047	U991	G932	A872	G812	G752
U1532	C1469	A1413	U1354	C1233	U1173	G1113	G1048	U992	G933	A873	U813	A753
C1533	U1470	A1414	G1355	G1234	G1174	C1114	U1049	G993	C934	A874	A814	C754
A1534	U1471	G1415	G1356	U1235	G1175	U1115	G1050	A994	A935	U875	A815	G755
			G1357	A1236	A1176	U1116	C1051	C995	C936	C876	A816	C756
			A1357	C1237	G1177	A1117	U1052	A996	A937	G877	C817	U757
			U1358	A1238	U1178	U1118	C1053	U997	A938	A878	G818	C758
			C1359	U1239	A1179	C1119	C1054	C998	G939	C879	A819	A759
			A1360	U1240	A1180	C1120	C1055	C999	C940	C880	U820	G760
			G1361	G1241	G1181	U1121	U1056	A1000	G941	G881	G821	G761
			A1362	C1242	U1182	U1122	G1057	U1000	G942	C882	U822	U762
			C1363	C1243	U1183	U1123	G1058	C1001	U943	C883	C823	G763
			U1364	G1244	G1184	G1124	G1059	G1002	G944	U884	G824	C764
			G1365	G1245	G1185	U1125	U1060	G1003	G945	G885	A825	G765
			C1366	A1246	U1186	U1126	G1061	A1004	A946	G886	C826	A766
			U1367	U1247	G1187	G1127	U1062	A1005	C947	G887	U827	A767
			A1368	A1248	A1188	C1128	C1063	G1006	A948	G888	U828	A768
			G1369	C1249	U1189	C1129	U1064	A889	A949	A889	G829	G770
			U1370	A1250	G1190	A1130	C1065	U1007	G951	G890	A831	G771
			A1371	A1251	A1191	G1131	C1066	U1008	U952	U891	C832	U772
			G1372	A1252	C1192	C1132	G1068	U1009	G953	C893	G833	G773
			U1373	U1253	G1193	G1133	C1069	U1010	G954	G894	U834	G774
			A1374	A1254	U1194	G1134	U1070	C1011	G895	G895	U835	G775
			C1375	G1255	C1195	U1135	C1071	A1012	U955	C896	G836	G776
			U1376	A1256	A1196	C1136	C1072	G1013	U956	C897	U837	A777
			A1377	C1317	A1197	C1137	G1073	A1014	U957	C898	G838	G778
			C1378	A1257	G1198	G1138	U1074	G1015	A958	C899	C839	G779
			U1379	C1258	U1199	G1139	G1075	G1016	A959	A900	A780	C780
			A1380	G1260	C1200	C1140	U1076	G1017	U960	A901	C841	A781
			C1381	A1261	A1201	C1141	U1077	A1018	U961			
							G1078	A1019				
							G1079	G1020				
							A1080	A1021				
							A1081					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26670	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	3.844	Depositor
Minimum map value	-6.202	Depositor
Average map value	-3.839	Depositor
Map value standard deviation	0.520	Depositor
Recommended contour level	-2.8	Depositor
Map size (\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 (\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	3.49	5233/36831 (14.2%)	3.97	9457/57458 (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	984

The worst 5 of 5233 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	331	G	N7-C5	-21.91	1.26	1.39
1	N	77	A	N7-C5	-19.35	1.27	1.39
1	N	885	G	N7-C5	-19.01	1.27	1.39
1	N	406	G	C6-N1	18.40	1.52	1.39
1	N	560	A	C6-N6	17.58	1.48	1.33

The worst 5 of 9457 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1299	A	N1-C6-N6	26.26	134.35	118.60
1	N	633	G	N1-C6-O6	25.68	135.31	119.90
1	N	1399	C	P-O3'-C3'	25.34	150.10	119.70
1	N	141	G	N1-C6-O6	24.86	134.81	119.90
1	N	207	C	C6-N1-C2	-24.71	110.42	120.30

There are no chirality outliers.

5 of 984 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	2	A	Sidechain
1	N	4	U	Sidechain
1	N	5	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	16524	547	0
All	All	32892	16554	16524	547	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 547 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:67:C:H2'	1:N:68:G:C8	2.21	0.76
1:N:664:G:H22	1:N:741:G:H1	1.34	0.76
1:N:858:G:H1	1:N:869:G:H2'	1.50	0.75
1:N:507:C:H3'	1:N:508:U:H5''	1.70	0.74
1:N:840:C:H1'	1:N:843:U:H3	1.51	0.74

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%)	446 (29%)	148 (9%)

5 of 446 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 148 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1191	A
1	N	1498	U
1	N	1228	C
1	N	1337	G
1	N	366	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-5501. These allow visual inspection of the internal detail of the map and identification of artifacts.

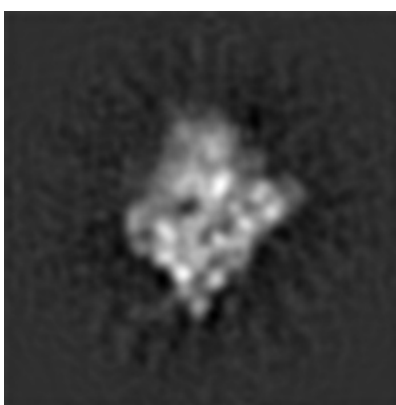
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

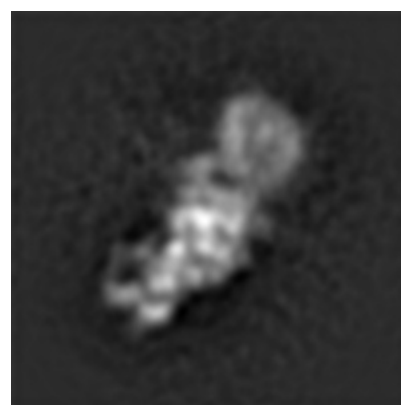
6.1.1 Primary map



X



Y

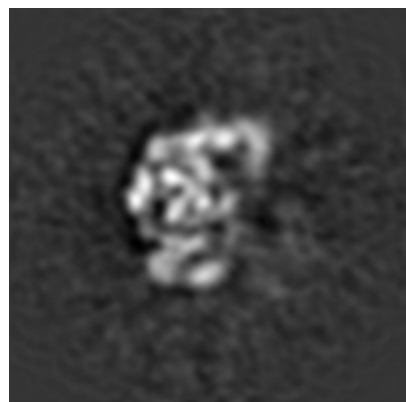


Z

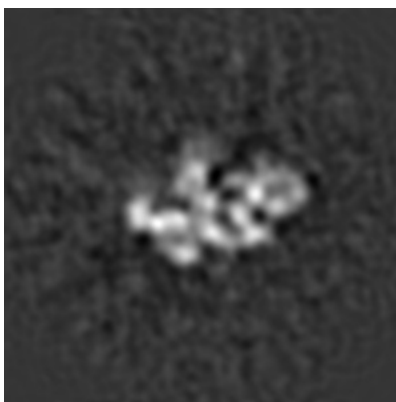
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

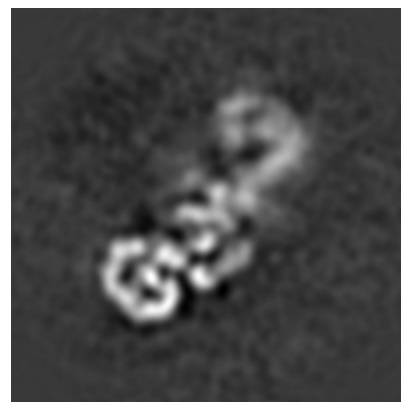
6.2.1 Primary map



X Index: 62



Y Index: 62

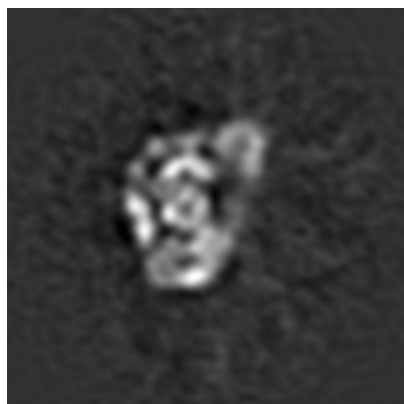


Z Index: 62

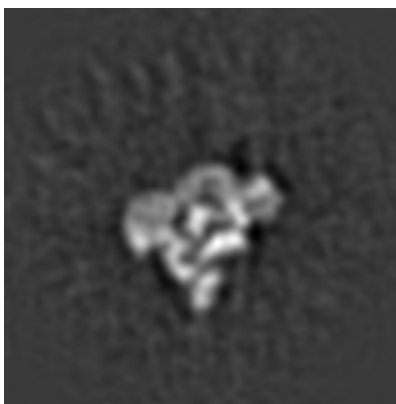
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

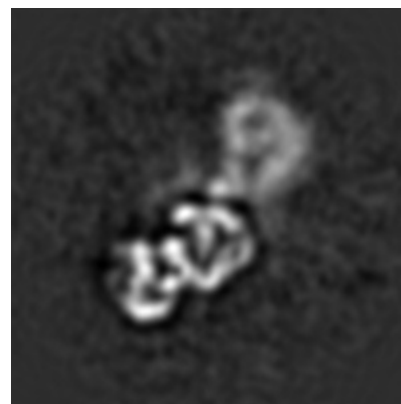
6.3.1 Primary map



X Index: 59



Y Index: 50

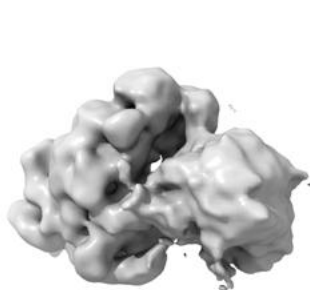


Z Index: 65

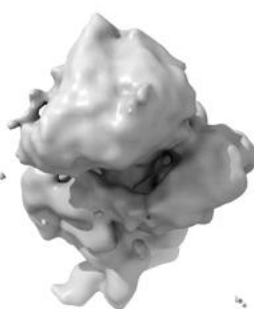
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

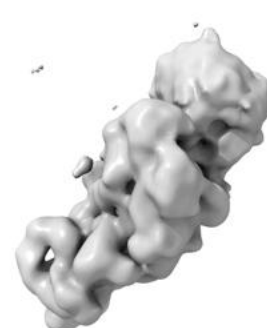
6.4.1 Primary map



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.

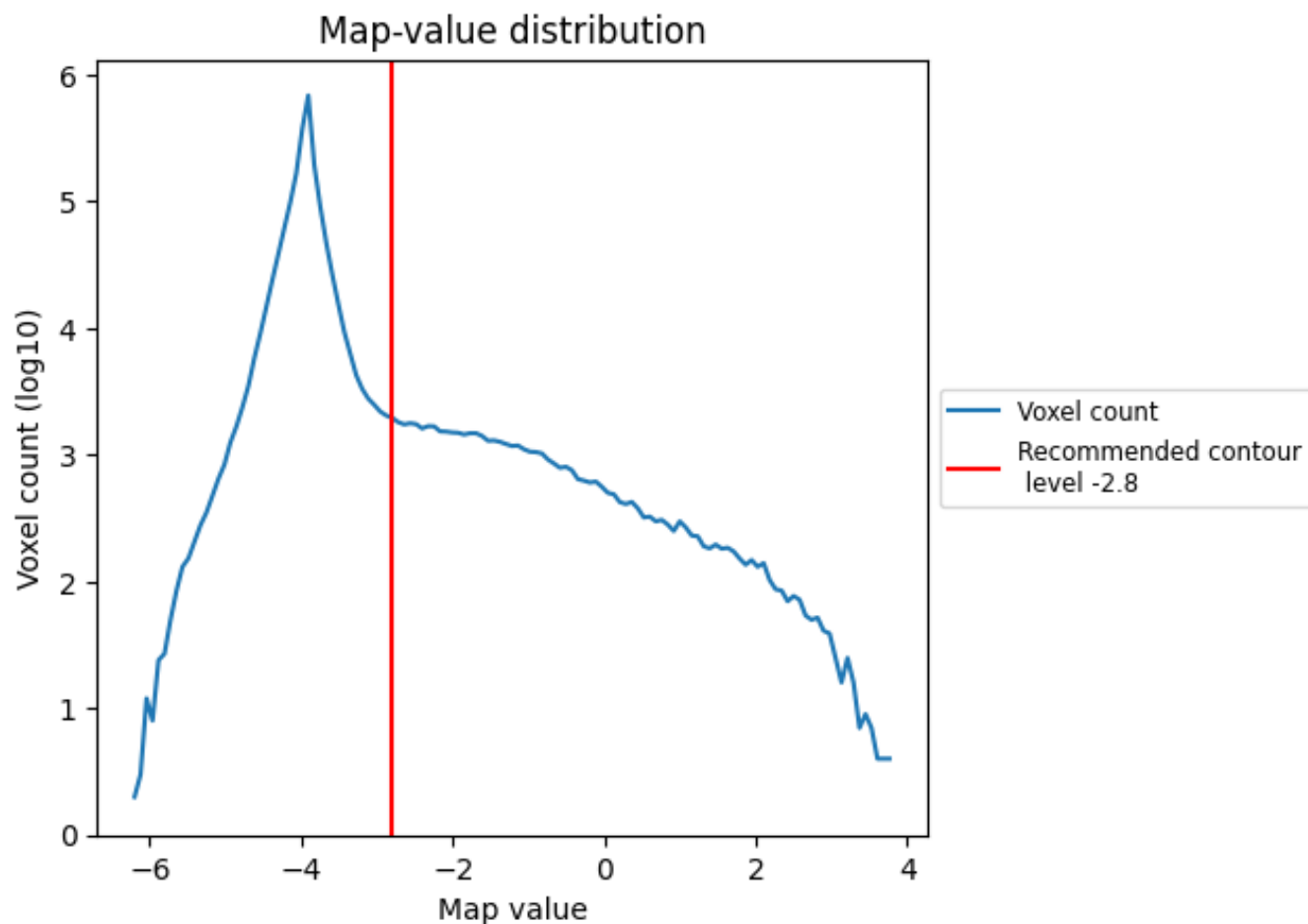
6.5 Mask visualisation

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

7 Map analysis [i](#)

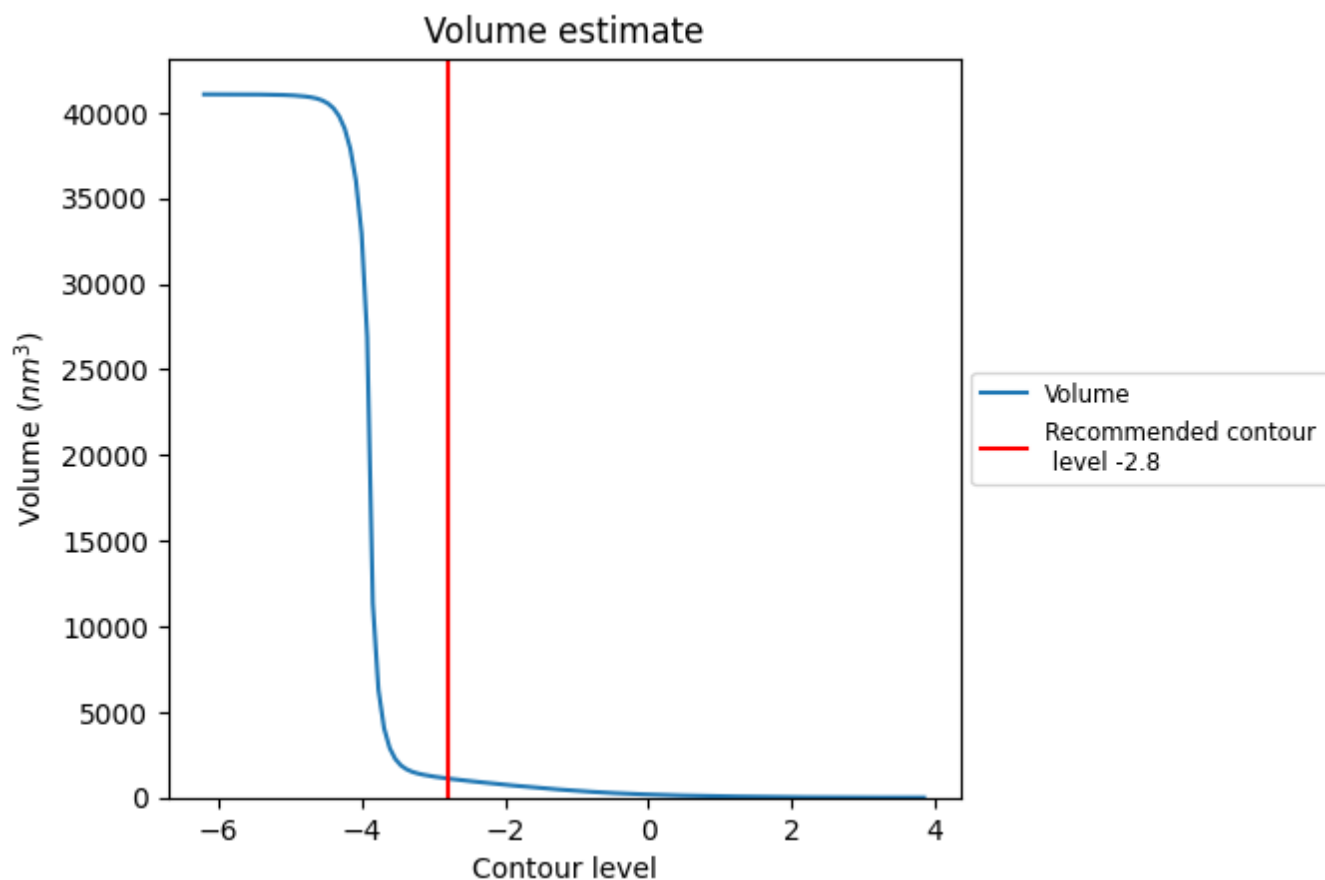
This section contains the results of statistical analysis of the map.

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.

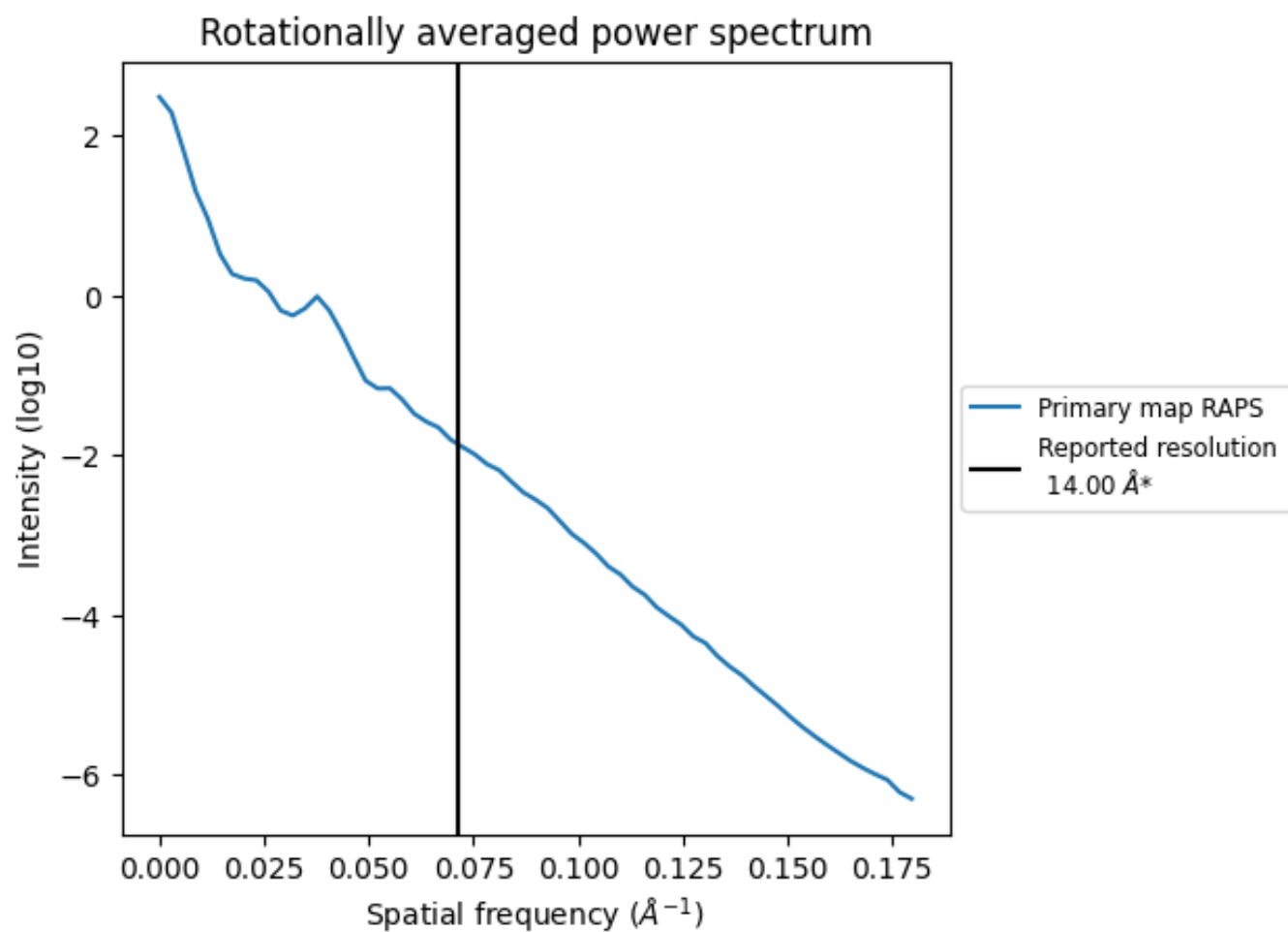
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1112 nm³; this corresponds to an approximate mass of 1005 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 0.071 Å⁻¹

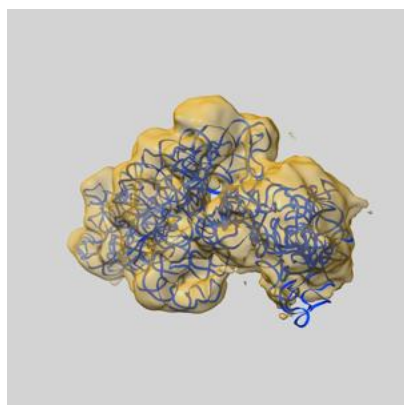
8 Fourier-Shell correlation

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

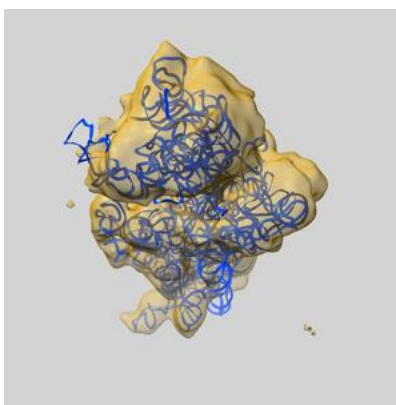
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5501 and PDB model 3J29. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

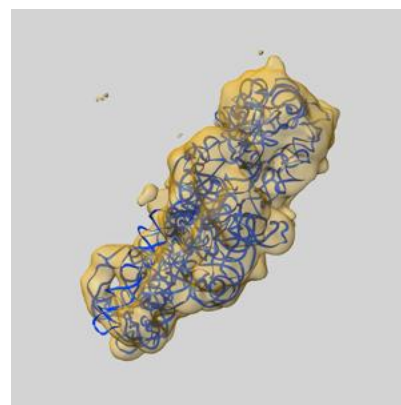
9.1 Map-model overlay [i](#)



X



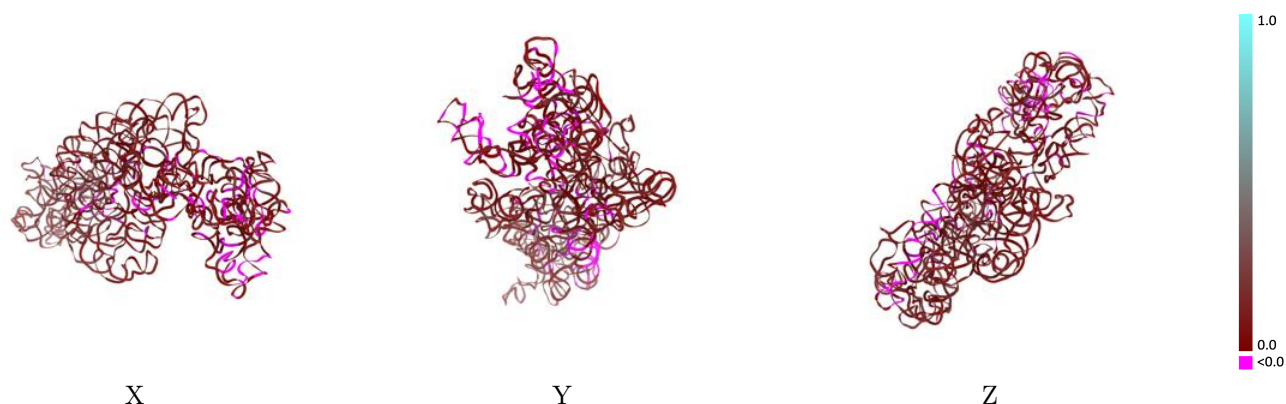
Y



Z

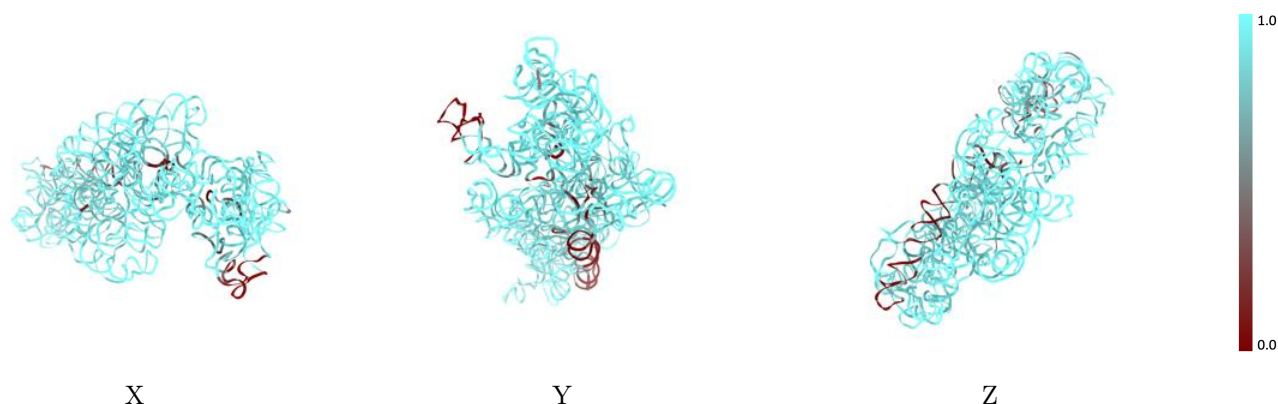
The images above show the 3D surface view of the map at the recommended contour level -2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



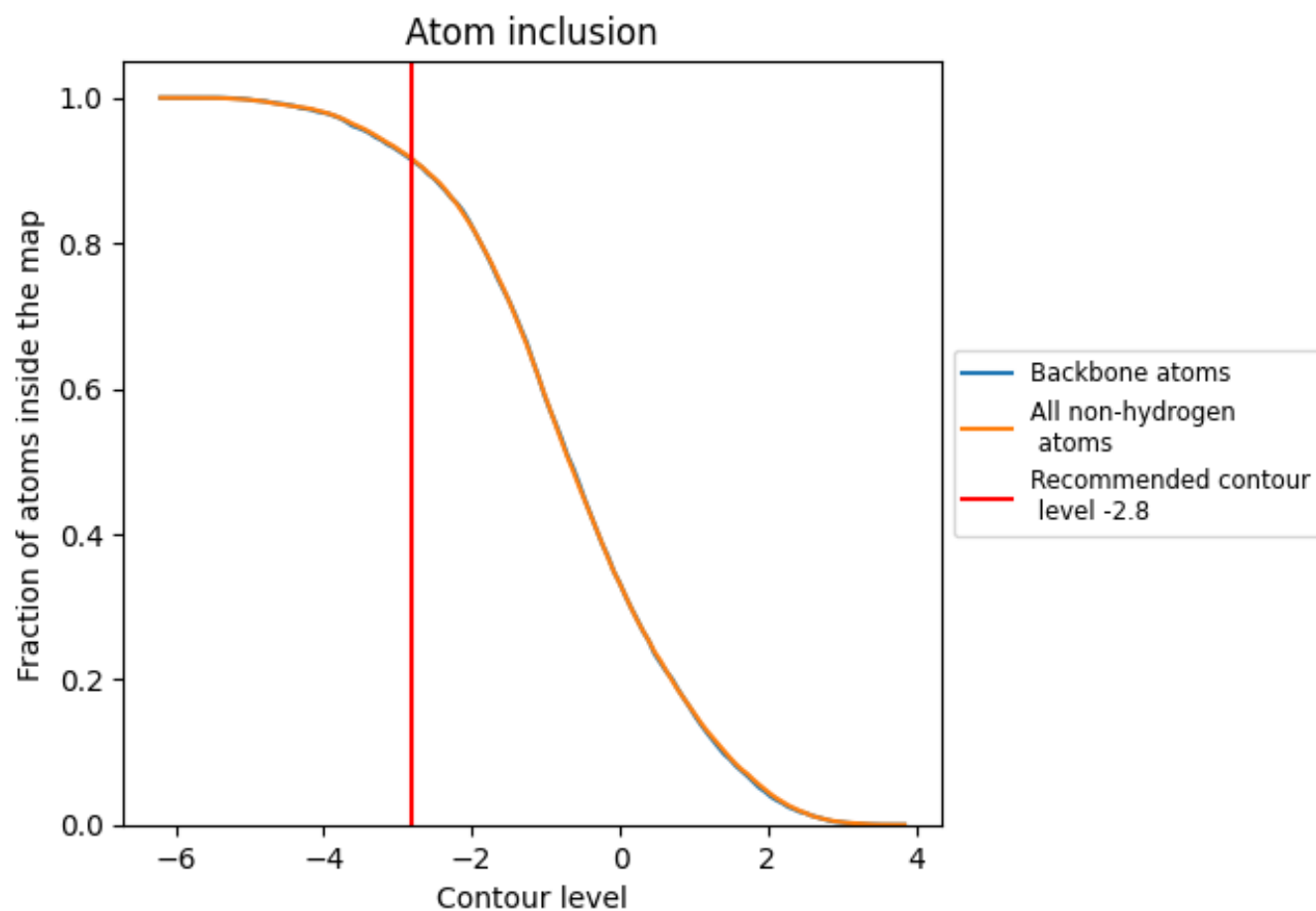
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% 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 (-2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9158	<div></div> 0.0890
N	<div></div> 0.9161	<div></div> 0.0890

