



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 01:56 PM EST

PDB ID : 3J2H
EMDB ID : EMD-5510
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 : 18.80 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

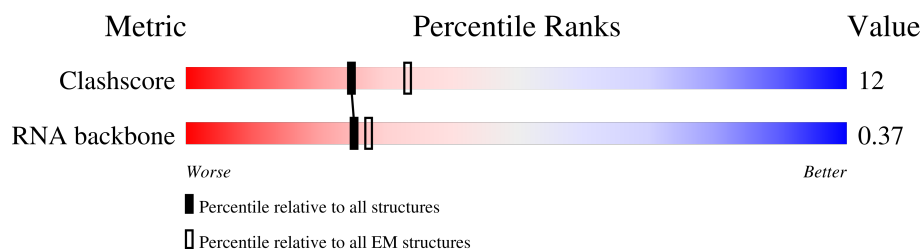
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 18.80 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.

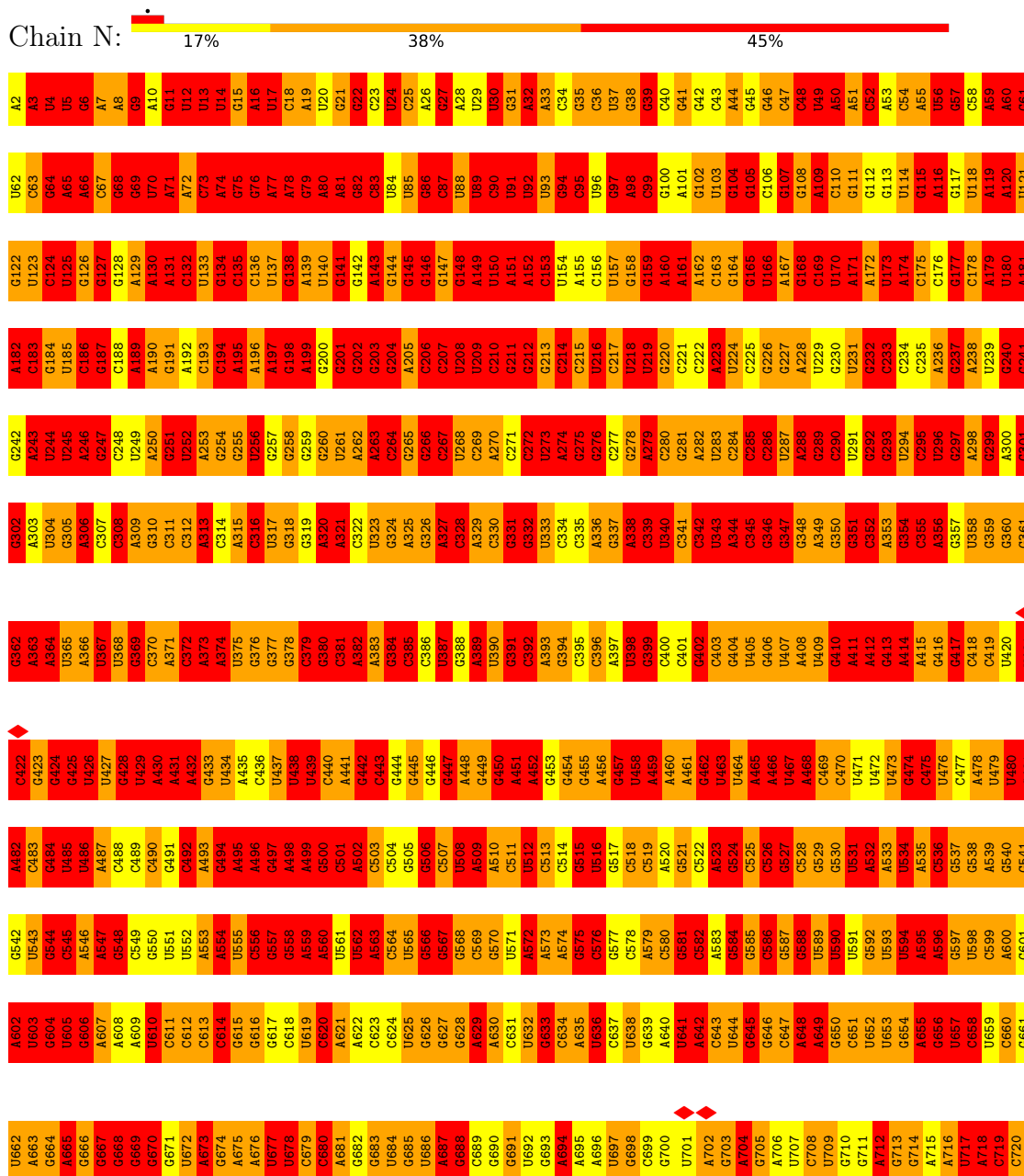
- Molecule 1 is a RNA chain called 16S rRNA.

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	U1202	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	C1203	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	C1384	A1204	G1144	G1084	G1024	A964	U904	A844	A784	G724
G1505	U1445	C1385	U1205	A1145	U1085	G1025	U965	U905	A845	G785	G725
A1506	U1446	C1386	G1206	A1146	U1086	U1026	G966	A906	G846	G786	G726
A1507	G1387	G1266	G1207	C1147	U1087	G1027	C967	A907	G847	A787	G727
A1508	C1388	C1267	C1208	U1148	G1088	C1028	A968	A908	C848	U788	A728
A1509	C1389	G1268	C1209	C1149	U1089	C1029	A969	A909	G849	U789	A729
C1510	U1390	A1269	C1210	A1150	U1090	U1029	C970	C910	U850	A790	G730
U1511	G1391	G1270	C1211	A1151	U1091	U1030	G971	U911	G851	G731	G731
U1512	A1392	A1271	U1212	A1152	A1092	C1031	C972	C912	G852	A792	C732
A1513	U1393	G1272	U1213	G1153	A1093	G1032	G973	A913	C853	U793	G733
G1514	C1394	C1273	A1214	G1154	G1094	G1033	A974	U854	A794	C734	G734
G1515	C1395	C1273	C1214	A1155	U1095	G1033	A975	U855	C735	C735	G735
G1516	A1396	A1274	G1215	G1156	C1096	G1034	G976	C856	G736	G736	G736
G1517	C1397	A1275	A1216	A1157	C1097	A1035	A977	G917	C737	C737	G737
A1518	G1397	G1276	C1217	U1158	C1098	A1036	A978	G858	U738	C738	G738
A1519	A1398	G1277	C1218	U1159	G1099	C1037	C979	G859	G739	G739	G739
C1520	C1399	C1278	A1219	C1160	C1100	C1038	C980	U920	A860	G800	U740
C1521	G1400	G1279	G1220	C1161	A1101	C1039	U981	U921	C861	U801	G741
C1522	G1401	A1280	G1221	C1162	A1102	U1040	U982	G922	C862	A802	G742
C1523	G1343	C1281	G1222	G1163	C1103	G1041	C983	A923	U863	G803	A743
C1524	C1344	C1282	C1223	U1164	G1104	A1042	C984	C924	A864	U804	C744
G1525	U1345	U1283	U1224	U1165	A1105	G1043	C985	G925	A865	C805	G745
G1526	A1346	C1284	C1225	G1166	A1106	A1044	U986	G926	C866	C806	A746
U1527	G1347	A1285	C1226	A1167	C1107	C1045	C987	C927	C867	A807	A747
U1528	U1348	U1286	A1227	U1168	G1108	A1046	G988	G928	C868	C808	G748
U1529	A1349	A1287	C1228	U1169	C1109	G1047	U989	G929	G869	G809	A749
G1530	C1409	A1288	A1229	A1170	C1110	G1048	C990	C930	U870	C810	C750
A1531	A1410	A1289	C1230	A1171	A1111	U1049	U991	C931	U871	C811	G751
C1532	C1411	G1290	G1231	C1172	C1112	G1050	U992	G932	A872	G812	G752
C1533	G1412	U1291	U1232	U1173	C1113	C1051	G993	C933	A873	U813	A753
A1534	A1413	C1292	C1233	G1174	C1114	U1052	A994	C934	G874	A814	C754
	U1414	G1293	C1234	G1175	U1115	G1053	C995	A935	U875	A815	G755
	G1415	C1294	U1235	A1176	C1054	C1054	A996	G936	C876	A816	C756
	G1416	U1295	A1236	G1177	A1117	A1055	U997	A937	G877	C817	U757
	A1417	C1296	C1237	U1178	C1118	U1056	C998	A938	A878	G818	C758
	A1418	G1297	A1238	A1179	C1119	G1057	C999	G939	C879	A819	A759
	G1419	U1298	A1239	A1180	C1120	G1058	A1000	C940	C880	U820	G760
	U1420	A1299	U1240	G1181	U1121	C1059	C1001	G941	G881	G761	G761
	G1421	G1300	G1241	U1182	U1122	U1060	G1002	G942	C882	U822	U762
	G1422	U1301	G1242	U1183	U1123	G1061	G1003	U943	C883	G823	G763
	C1423	C1302	C1243	G1184	G1124	C1062	A1004	G944	U884	G824	G764
	U1424	G1303	G1244	G1185	U1125	C1063	A1005	G945	G885	A825	G765
	U1425	C1304	C1245	G1186	U1126	G1064	A1006	A946	G886	C826	A766
	G1426	G1305	A1246	G1187	G1127	U1065	G1006	G947	C887	U827	A767
	C1427	A1306	U1247	A1188	C1128	C1066	U1007	C948	G888	U828	A768
	A1428	U1307	A1248	U1189	C1129	A1067	A889	A949	G889	G829	G769
	A1429	U1308	C1249	G1190	C1130	G1068	U1008	G950	G890	G830	C770
	A1430	G1309	A1250	A1191	G1131	C1069	U1009	G951	U891	A831	G771
	A1431	C1310	A1251	C1192	C1132	U1070	U1010	U952	A892	C832	U772
	G1432	A1311	A1252	G1193	G1133	C1071	C1011	G953	C893	G833	G773
	A1433	G1312	G1253	U1194	G1134	G1072	A1012	G954	G894	U834	G774
	G1434	U1313	A1254	C1195	U1135	U1073	G1013	U955	G895	U835	G775
	A1435	C1314	G1255	C1196	C1136	G1074	A1014	U956	C896	G836	G776
	A1436	U1315	A1256	A1197	C1137	U1075	G1015	U957	C897	U837	A777
	G1437	G1316	A1257	G1198	G1138	U1076	A1016	A898	G898	G838	G778
	U1438	C1317	G1258	U1199	G1139	G1077	U1017	A959	C899	C839	C779
	A1439	A1318	C1259	C1200	C1140	U1078	G1018	U960	A900	A780	A780
	U1440	C1319	C1260	A1201	C1141	G1079	G1019	U961	A901	C841	A781
	A1441	C1320	A1261			A1080	G1020				
		U1381				A1081	A1021				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11474	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	4.629	Depositor
Minimum map value	-7.414	Depositor
Average map value	-4.262	Depositor
Map value standard deviation	0.653	Depositor
Recommended contour level	-2.3	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)	3.0, 3.0, 3.0	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	3.47	5192/36831 (14.1%)	3.99	9508/57458 (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	978

The worst 5 of 5192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	815	A	N7-C5	-18.92	1.27	1.39
1	N	435	A	N7-C5	-18.59	1.28	1.39
1	N	572	A	N7-C5	-18.24	1.28	1.39
1	N	367	U	C2-N3	17.85	1.50	1.37
1	N	202	G	N7-C5	16.97	1.49	1.39

The worst 5 of 9508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	567	G	C5-C6-O6	-27.97	111.82	128.60
1	N	184	G	N1-C6-O6	26.91	136.04	119.90
1	N	184	G	C5-C6-O6	-26.87	112.48	128.60
1	N	567	G	N1-C6-O6	25.95	135.47	119.90
1	N	713	G	N1-C6-O6	24.64	134.69	119.90

There are no chirality outliers.

5 of 978 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	3	A	Sidechain
1	N	4	U	Sidechain
1	N	5	U	Sidechain
1	N	6	G	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	16521	571	0
All	All	32892	16554	16521	571	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 12.

The worst 5 of 571 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:32:A:H4'	1:N:48:C:H42	1.50	0.75
1:N:594:U:C4	1:N:595:A:C6	2.74	0.75
1:N:338:A:H61	1:N:351:G:H1	1.36	0.73
1:N:116:A:H61	1:N:313:A:H1'	1.53	0.73
1:N:197:A:H2	1:N:198:G:C4	2.08	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%)	449 (29%)	152 (9%)

5 of 449 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 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1189	U
1	N	1432	G
1	N	1224	U
1	N	1319	A
1	N	1532	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.

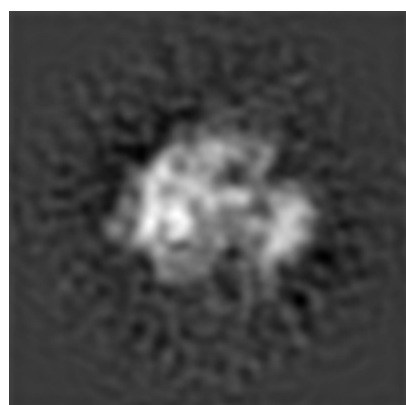
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5510. These allow visual inspection of the internal detail of the map and identification of artifacts.

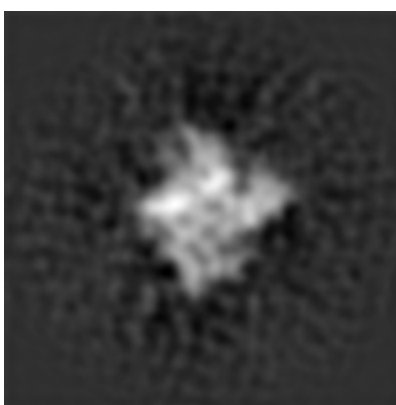
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

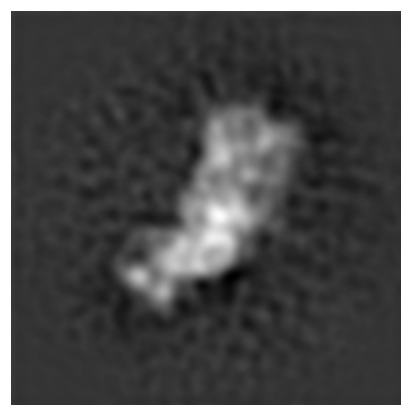
6.1.1 Primary map



X



Y

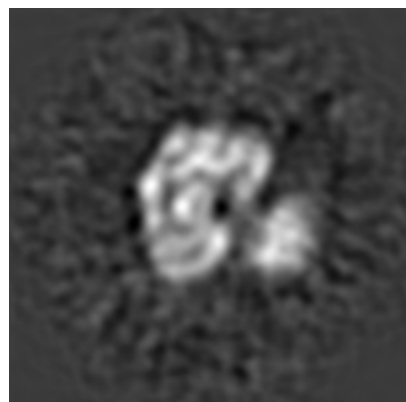


Z

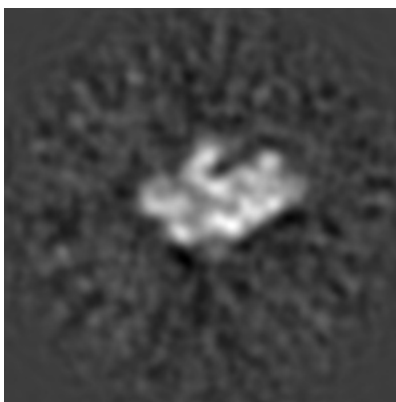
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

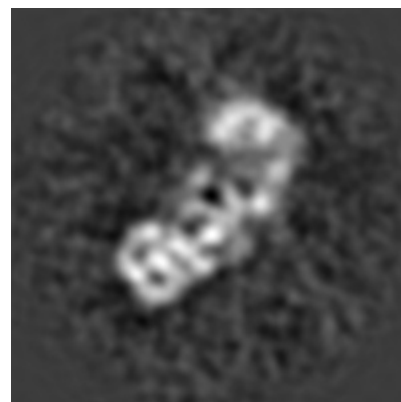
6.2.1 Primary map



X Index: 62



Y Index: 62

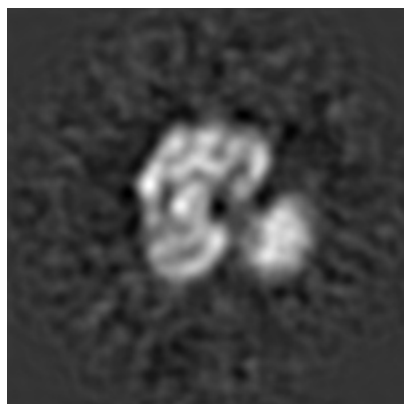


Z Index: 62

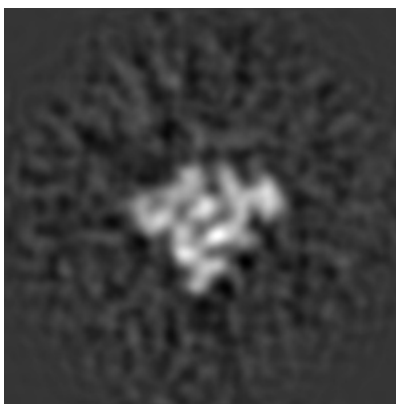
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

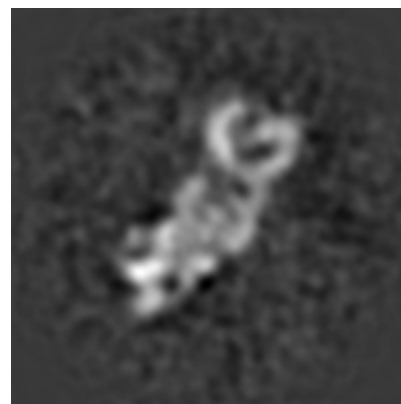
6.3.1 Primary map



X Index: 63



Y Index: 53

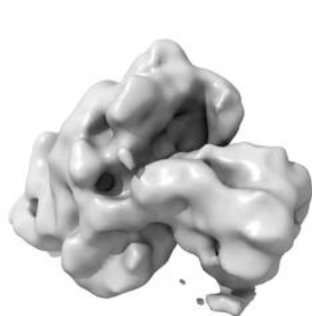


Z Index: 58

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

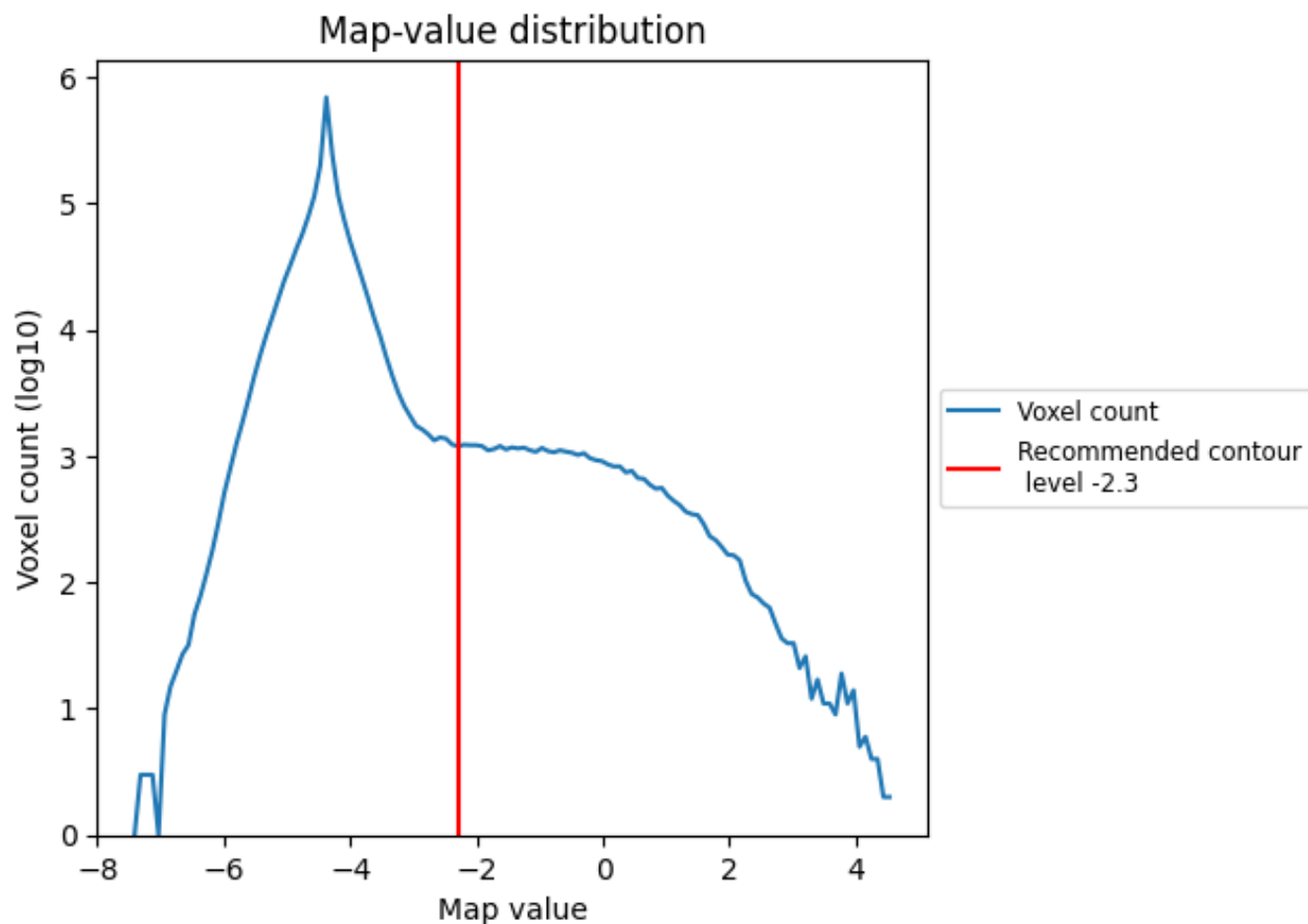
6.5 Mask visualisation

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

7 Map analysis [i](#)

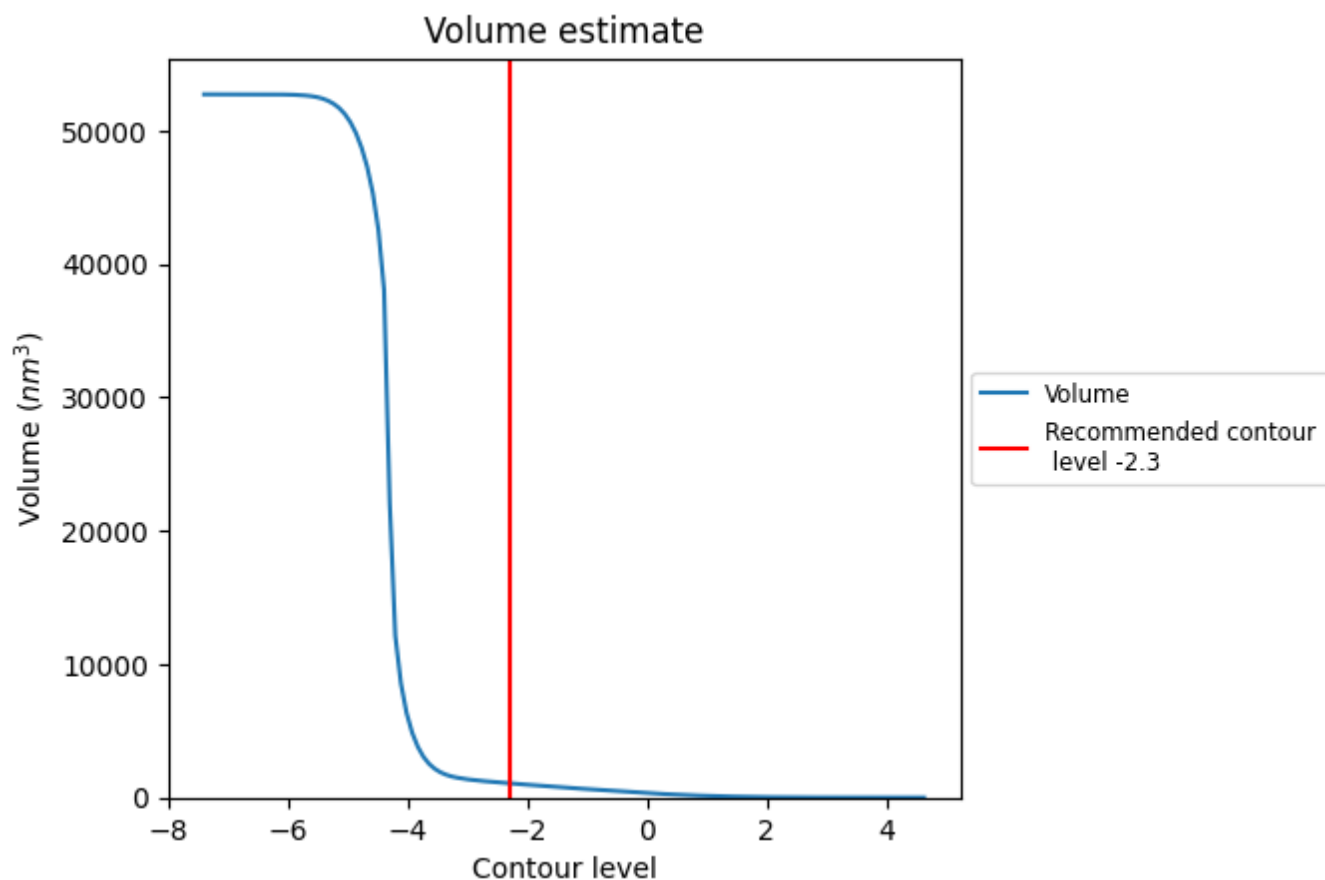
This section contains the results of statistical analysis of the map.

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.

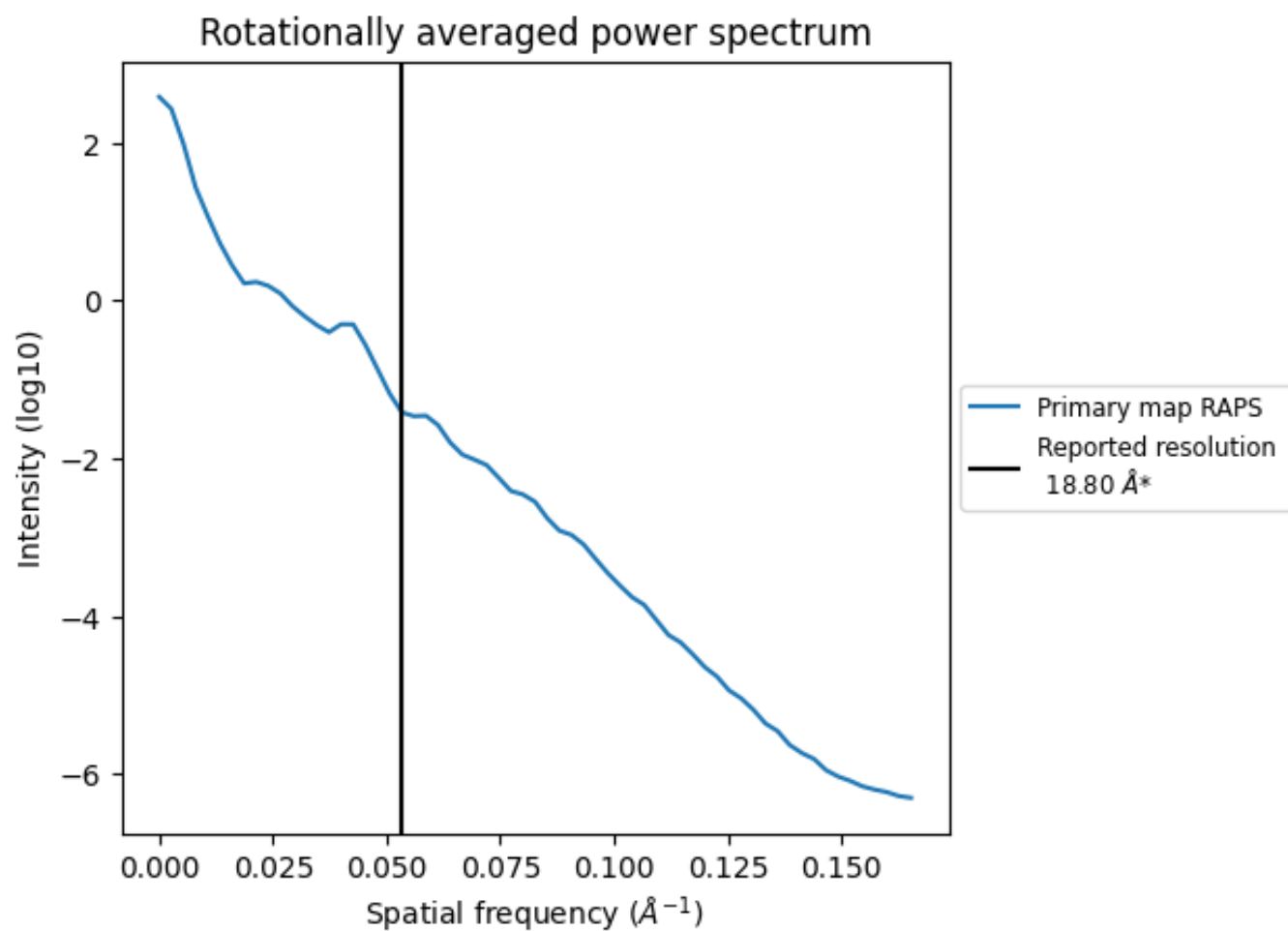
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1065 nm³; this corresponds to an approximate mass of 962 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 0.053 Å⁻¹

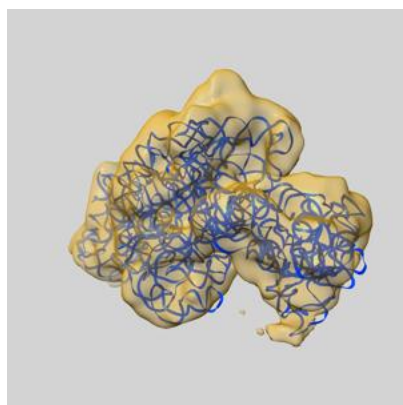
8 Fourier-Shell correlation

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

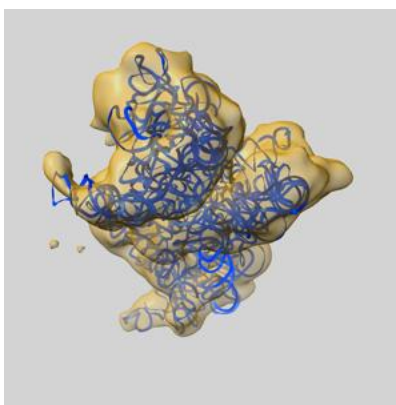
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5510 and PDB model 3J2H. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

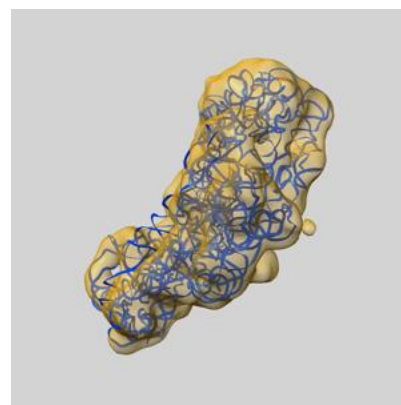
9.1 Map-model overlay [i](#)



X



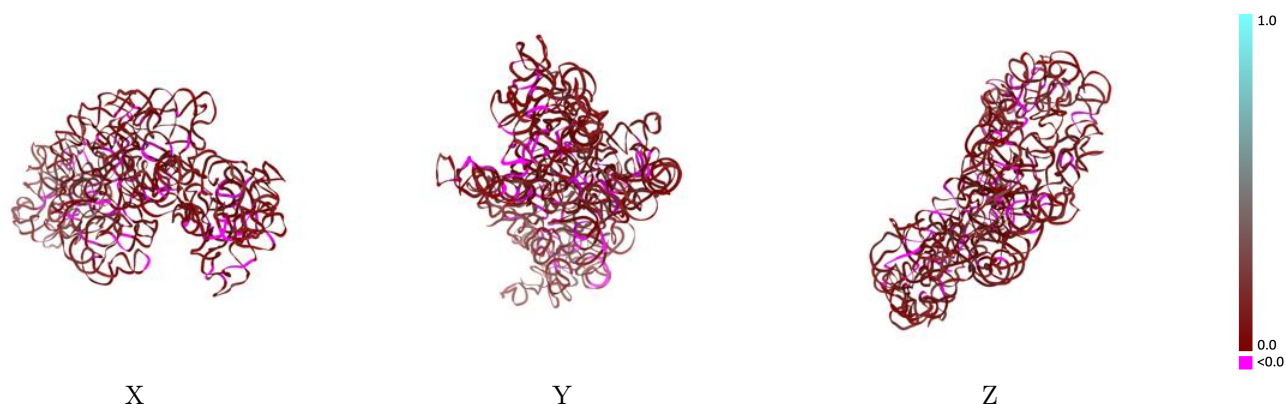
Y



Z

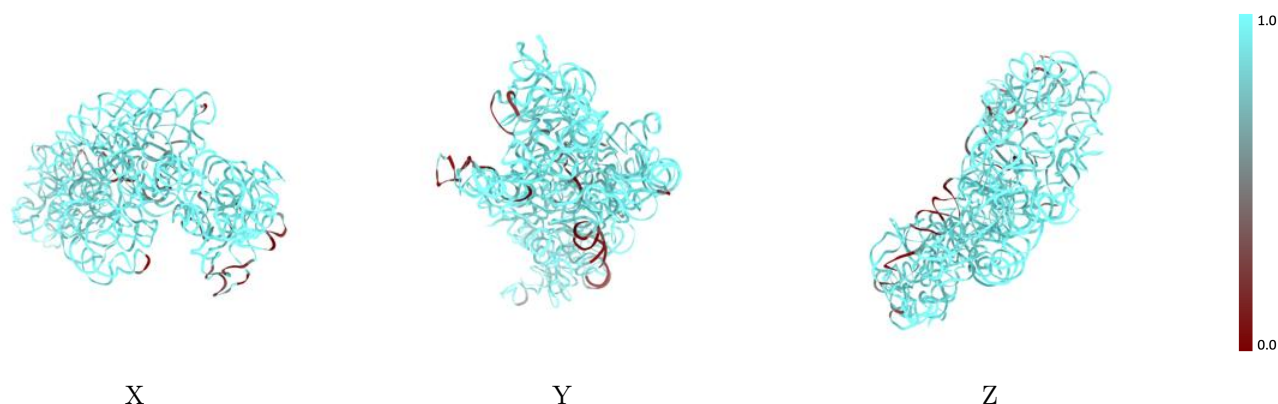
The images above show the 3D surface view of the map at the recommended contour level -2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



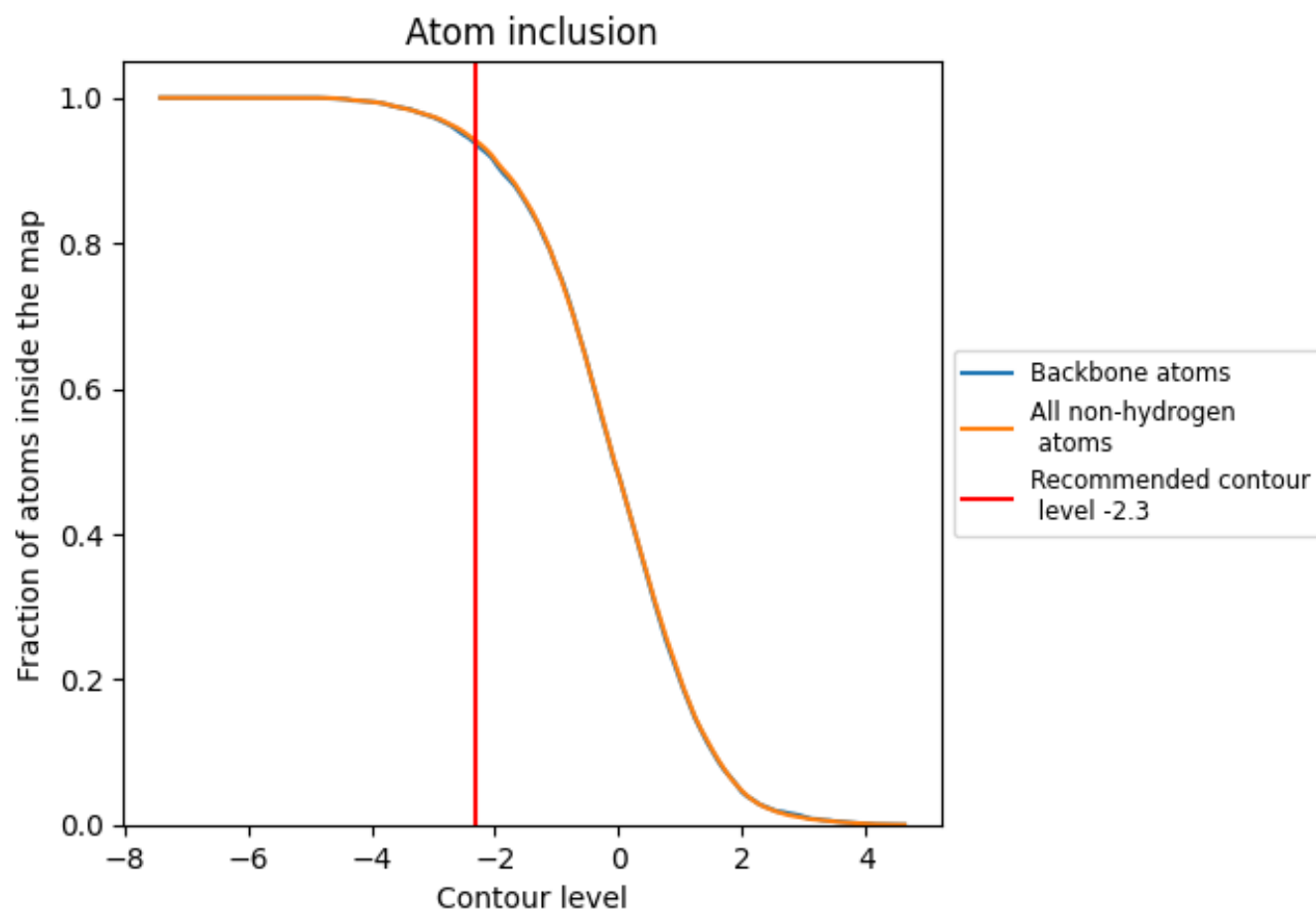
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (-2.3).

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 (-2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9407	<div></div> 0.0780
N	<div></div> 0.9416	<div></div> 0.0780

