



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 01:34 PM EST

PDB ID : 3J2F
EMDB ID : EMD-5508
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 : 17.60 Å(reported)
Based on initial model : 3OFA

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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

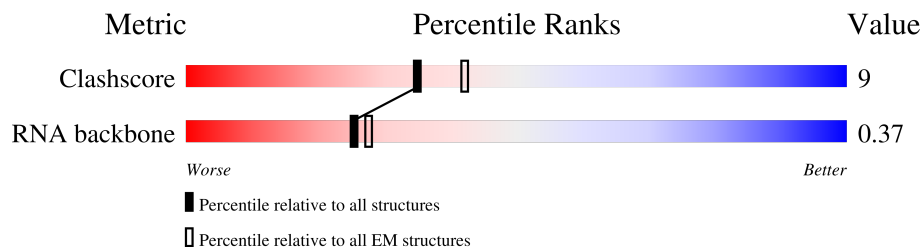
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 17.60 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 ≥ 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.

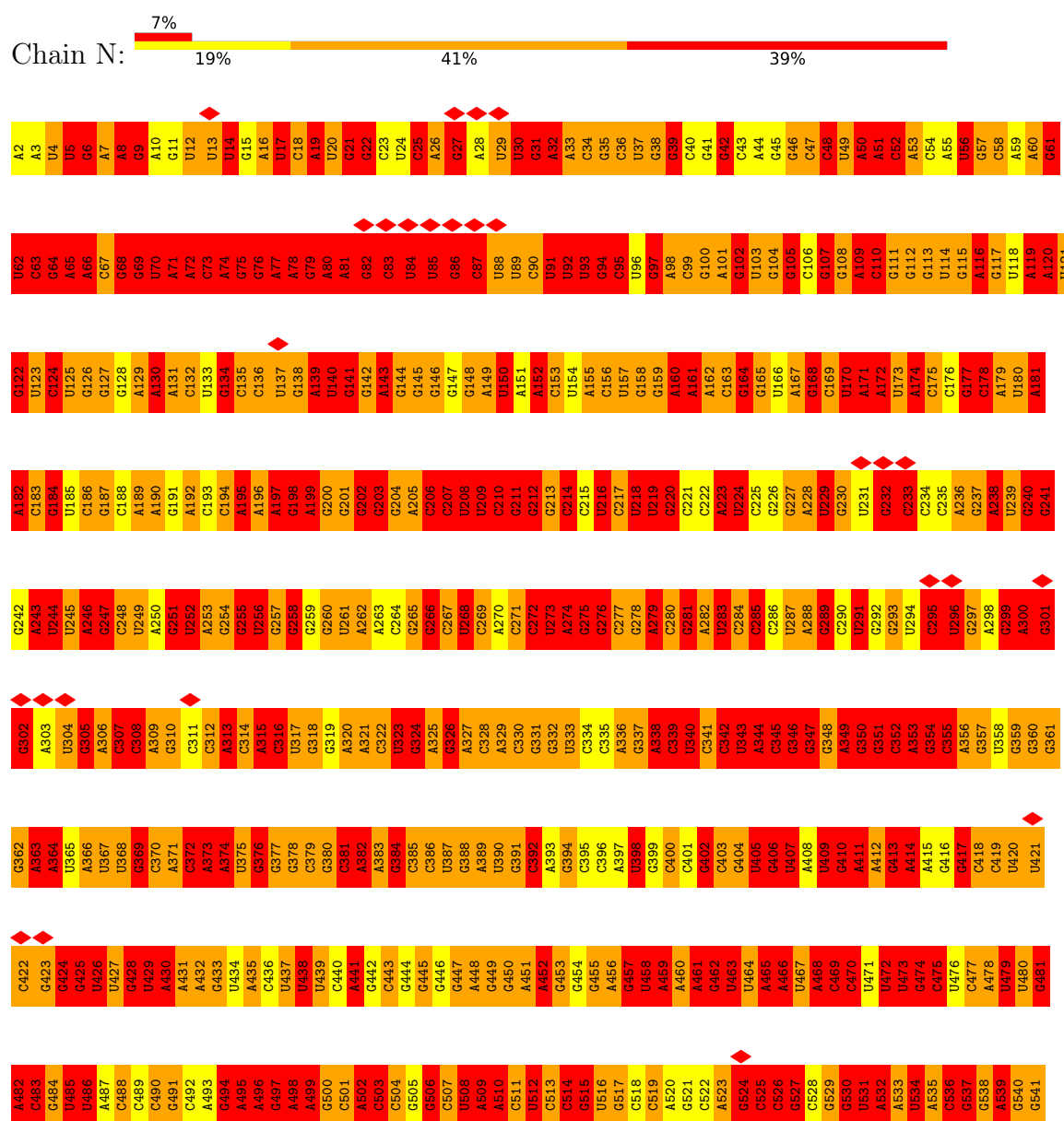
- Molecule 1 is a RNA chain called 16S rRNA.

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



G1322	C1262	G1142	A1082	A1022	C982	G902	U842	A782	G722	U662	A802	G542
G1323	C1263	G1143	U1083	U1023	G963	G903	U843	C783	U723	A663	A603	U543
A1324	U1264	G1144	U1084	G1024	A964	U904	A844	A784	G724	G664	U604	G544
C1325	C1265	A1145	U1085	U1025	U965	U905	A845	G785	G725	A665	U605	C545
U1326	U1266	A1146	U1086	G1026	G966	A906	G846	G786	G726	G666	G606	A546
C1327	G1267	G1147	G1087	C1027	C967	A907	G847	A787	G727	G667	A607	G547
C1328	U1268	U1148	U1088	C1028	A968	A908	C848	U788	A728	G668	A608	G548
A1329	A1269	C1149	G1089	U1029	A969	A909	G849	U789	A729	G669	A609	C549
U1330	G1270	C1150	U1090	U1030	C970	A910	U850	G790	A730	G670	U610	G550
G1331	A1271	A1151	U1091	C1031	G971	U911	G851	G791	G731	G671	C611	U551
A1332	C1272	A1152	A1092	G1032	C972	C912	G852	A792	C732	U672	C612	U552
G1333	G1273	G1153	A1093	G1033	G973	A913	G853	U793	G733	A673	C613	A553
A1334	A1274	G1154	U1094	U1034	A974	A914	U854	A794	G734	G674	C614	A554
U1335	A1275	A1155	U1095	G1035	A975	A915	U855	C795	C735	A675	G615	U555
C1336	G1276	G1156	C1096	A1036	A976	U916	C856	C796	G736	A676	G616	C556
G1337	C1277	A1157	C1097	A1037	A977	G917	C857	G797	C737	U677	G617	G557
G1338	G1278	C1158	U1098	C1038	A978	A918	G858	U798	C738	U678	C618	G558
A1339	U1279	U1159	G1099	G1039	C979	A919	G859	G799	G739	C679	U619	G559
A1340	A1280	G1160	C1100	G1040	C980	U920	A860	G800	U740	C680	C620	A560
U1341	C1281	C1161	U1101	U1041	U981	U921	C861	U801	G741	A681	A621	U561
C1342	G1282	C1162	A1102	G1042	U982	G922	C862	A802	G742	G682	A622	U562
G1343	U1283	A1163	U1103	A1043	C983	A923	U863	G803	A743	G683	C623	A563
C1344	C1284	G1164	G1104	G1044	C984	C924	A864	U804	C744	U684	C624	G564
A1345	A1285	U1165	A1105	A1045	C985	G925	A865	C805	G745	U685	G625	C564
A1346	U1286	G1166	G1106	C1046	U986	G926	C866	C806	A746	U686	G626	U565
G1347	A1287	A1167	C1107	A1047	C987	G927	C867	A807	A747	A687	G627	G566
U1348	U1288	U1168	G1108	G1048	G988	G928	C868	C808	G748	G688	G628	G567
A1349	A1289	C1169	C1109	U1049	U989	G929	G869	G809	A749	C689	A629	G568
A1350	G1290	A1170	A1110	C990	C990	C930	U870	C810	G750	G690	C630	C569
U1351	U1291	C1171	U1111	U1050	U991	C931	A872	G812	U751	G691	C631	G570
C1352	C1292	C1172	C1112	C1051	U992	G932	A873	U813	G752	U692	G632	U571
G1353	G1293	U1173	C1113	U1052	G993	C933	G874	U814	A753	G693	G633	A572
U1354	U1294	G1174	C1114	G1053	A994	C934	U875	A815	C754	A694	C634	A573
C1355	C1295	G1175	U1115	C1054	C995	A935	U876	A816	G755	A695	A635	A574
G1356	G1296	A1176	U1116	A1055	A996	C936	C877	C817	C756	A696	U636	G575
A1357	U1297	G1177	A1117	U1056	U997	A937	A878	G818	U757	U697	C637	C576
U1358	C1298	U1178	U1118	G1057	C998	A938	U879	A819	C758	G698	U638	G577
C1359	A1299	A1179	C1119	G1058	C999	G939	C880	A820	A759	C699	G639	C578
A1360	G1300	U1180	U1120	C1059	A1000	C940	G881	U821	G760	G700	A640	A579
G1361	U1301	G1181	U1121	U1060	C1001	G941	C882	U822	G761	U701	U641	C580
A1362	C1302	U1182	C1122	G1061	G1002	G942	C883	C823	U762	A702	A642	G581
C1363	G1303	U1183	U1123	U1062	G1003	U943	U884	G824	G763	G703	C643	C582
U1364	G1304	G1184	G1124	C1063	A1004	G944	G885	A825	C764	A704	U644	A583
G1365	C1305	U1185	U1125	U1064	A1005	G945	G886	C826	G765	G705	G645	G584
C1366	A1306	G1186	U1126	U1065	G1006	A946	G887	C827	A766	A706	G646	G585
U1367	U1307	G1187	G1127	C1066	U1007	G947	G888	U828	A767	U707	C647	C586
A1368	C1308	A1188	C1128	A1067	U1008	C948	A889	G829	C768	C708	A648	G587
C1369	U1309	U1189	U1129	U1068	U1009	A949	G890	G830	G769	U709	A649	G588
G1370	G1310	G1190	C1130	C1069	U1010	U950	U891	A831	C770	G710	G650	U589
U1371	A1311	A1191	G1131	U1070	U1011	G951	A892	G832	G771	G711	C651	U590
G1372	G1312	C1192	C1132	C1071	C1012	U952	G893	U833	U772	A712	U652	U591
A1373	U1313	G1193	G1133	G1072	A1013	G953	G894	U834	G773	G713	U653	G592
C1374	C1314	U1194	U1134	U1073	G1014	G954	G895	U835	G774	A715	A655	U593
U1375	U1315	C1195	U1135	U1074	A1015	U955	G896	G836	G775	A716	G556	U594
G1376	G1316	A1196	C1136	G1075	G1016	U956	C897	U837	G776	U717	C657	A595
A1377	C1317	U1197	C1137	U1076	A1017	U957	G898	G838	A777	U718	U657	A596
C1378	U1318	G1198	G1138	U1077	U1018	A958	C899	C839	G778	A718	C658	G597
G1379	A1319	U1199	G1139	G1078	A1019	U959	G900	C840	C779	C719	U659	U598
U1380	C1320	C1200	C1140	U1078	A1020	U960	A901	C841	A780	C720	C660	C599
C1381	U1321	A1201	G1141	G1079	G1021	U961			A781	G721	G661	A600
				A1080	A1021							G601
				A1081								

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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9609	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	6.063	Depositor
Minimum map value	-8.451	Depositor
Average map value	-4.957	Depositor
Map value standard deviation	0.711	Depositor
Recommended contour level	-2.8	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	5279/36831 (14.3%)	3.93	9337/57458 (16.3%)

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	941

The worst 5 of 5279 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	1299	A	N9-C4	19.01	1.49	1.37
1	N	250	A	N7-C5	-17.90	1.28	1.39
1	N	942	G	N7-C5	-17.43	1.28	1.39
1	N	1093	A	C6-N6	17.36	1.47	1.33
1	N	710	G	N7-C5	-17.22	1.28	1.39

The worst 5 of 9337 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1399	C	P-O3'-C3'	28.06	153.38	119.70
1	N	913	A	P-O3'-C3'	27.42	152.60	119.70
1	N	168	G	N1-C6-O6	27.05	136.13	119.90
1	N	1157	A	N1-C6-N6	26.02	134.21	118.60
1	N	168	G	C5-C6-O6	-25.86	113.09	128.60

There are no chirality outliers.

5 of 941 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	5	U	Sidechain
1	N	6	G	Sidechain
1	N	7	A	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	16526	428	0
All	All	32892	16554	16526	428	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 9.

The worst 5 of 428 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:203:G:H22	1:N:206:C:H41	1.34	0.73
1:N:594:U:C4	1:N:595:A:C6	2.77	0.73
1:N:67:C:H2'	1:N:68:G:C8	2.25	0.72
1:N:664:G:H22	1:N:741:G:H1	1.39	0.70
1:N:780:A:C2	1:N:801:U:C5	2.80	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 [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	1532/1533 (99%)	452 (29%)	147 (9%)

5 of 452 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	N	4	U
1	N	5	U
1	N	6	G
1	N	8	A
1	N	9	G

5 of 147 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1214	C
1	N	1502	A
1	N	1251	A
1	N	1345	U
1	N	372	C

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.

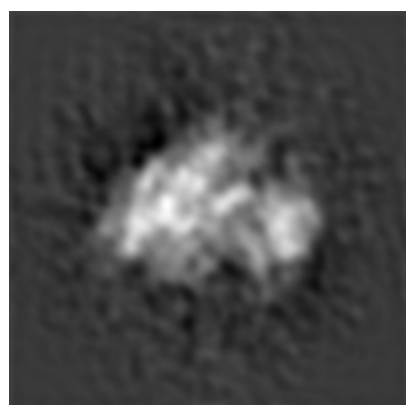
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5508. These allow visual inspection of the internal detail of the map and identification of artifacts.

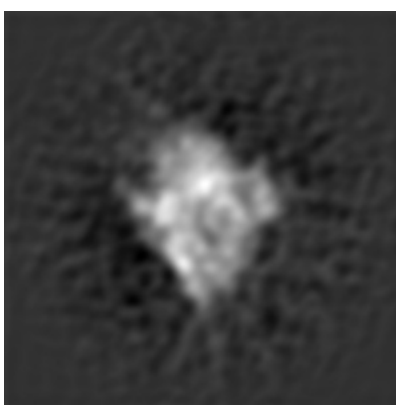
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

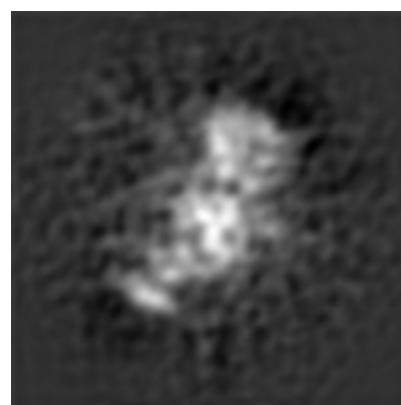
6.1.1 Primary map



X



Y

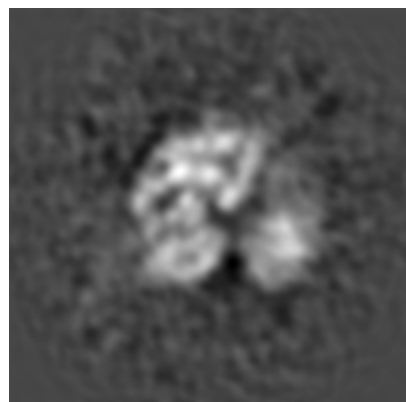


Z

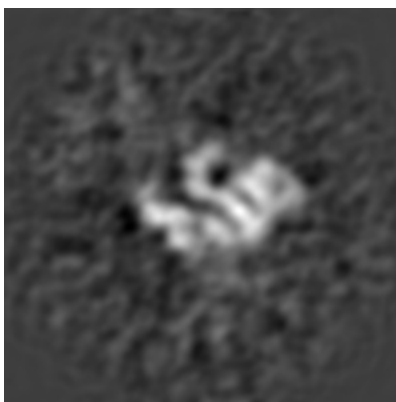
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

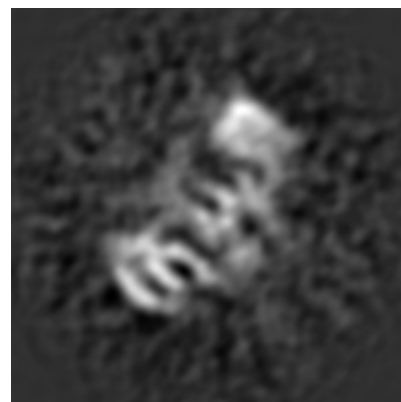
6.2.1 Primary map



X Index: 62



Y Index: 62

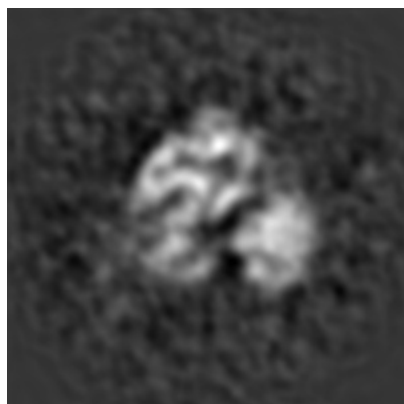


Z Index: 62

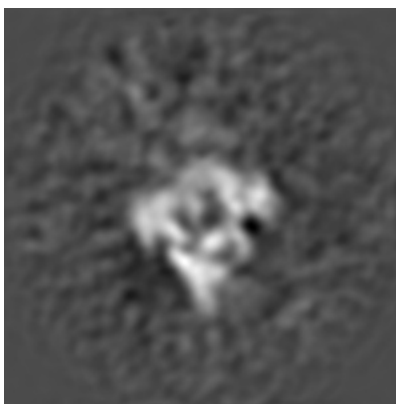
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

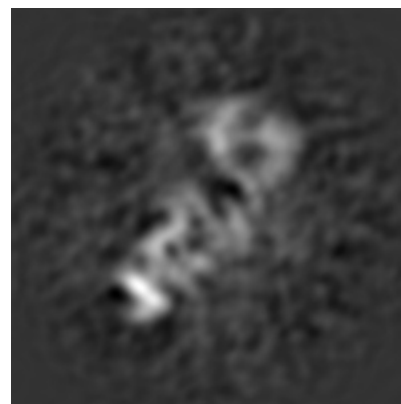
6.3.1 Primary map



X Index: 65



Y Index: 50

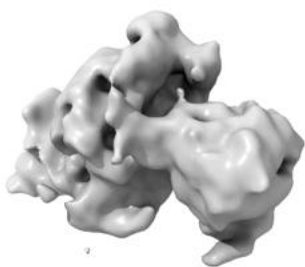


Z Index: 57

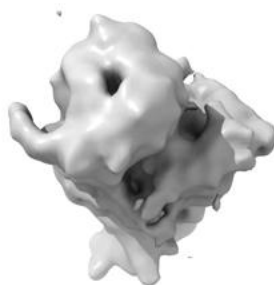
The images above show the largest variance slices of the map in three orthogonal directions.

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.

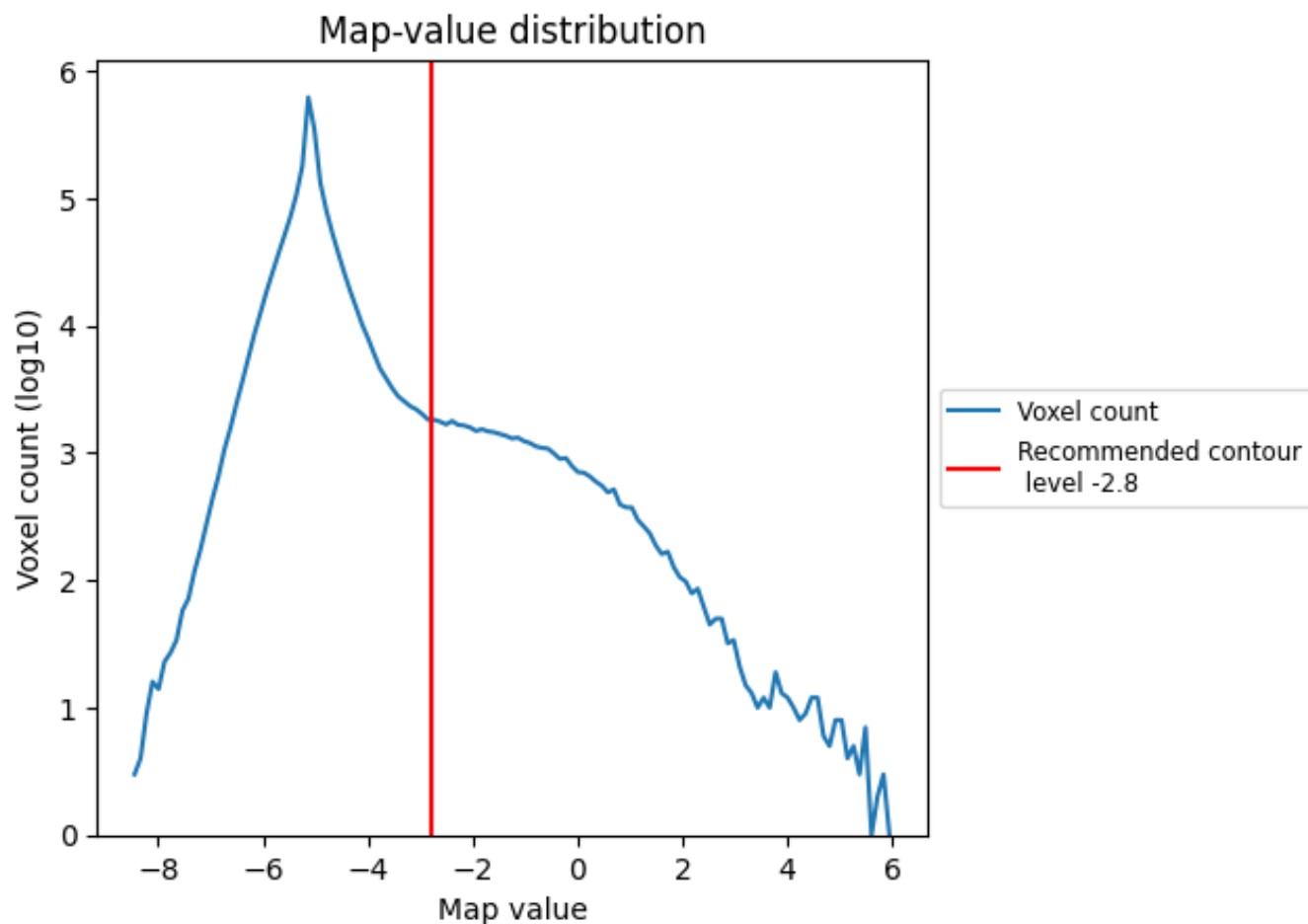
6.5 Mask visualisation

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

7 Map analysis [i](#)

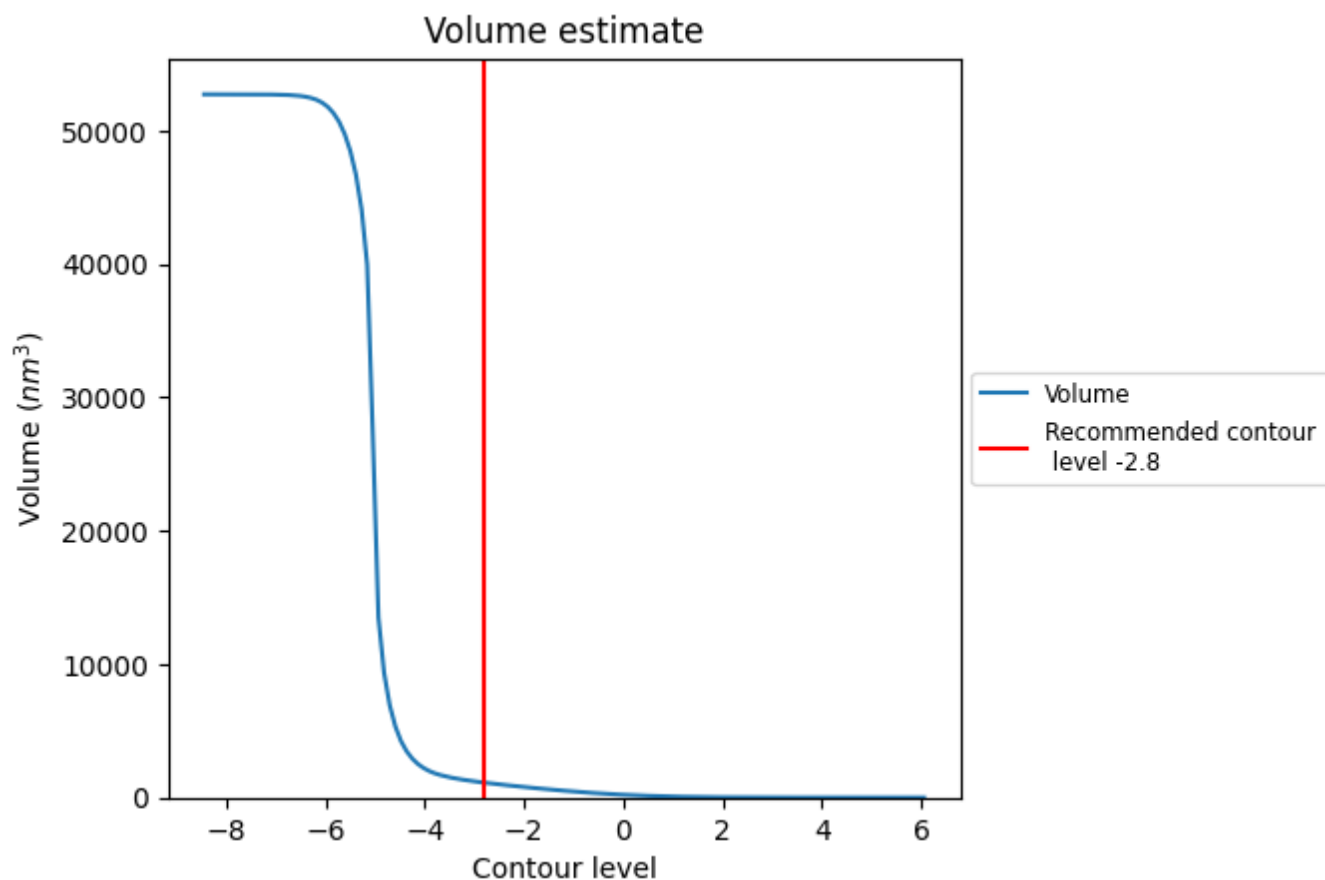
This section contains the results of statistical analysis of the map.

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.

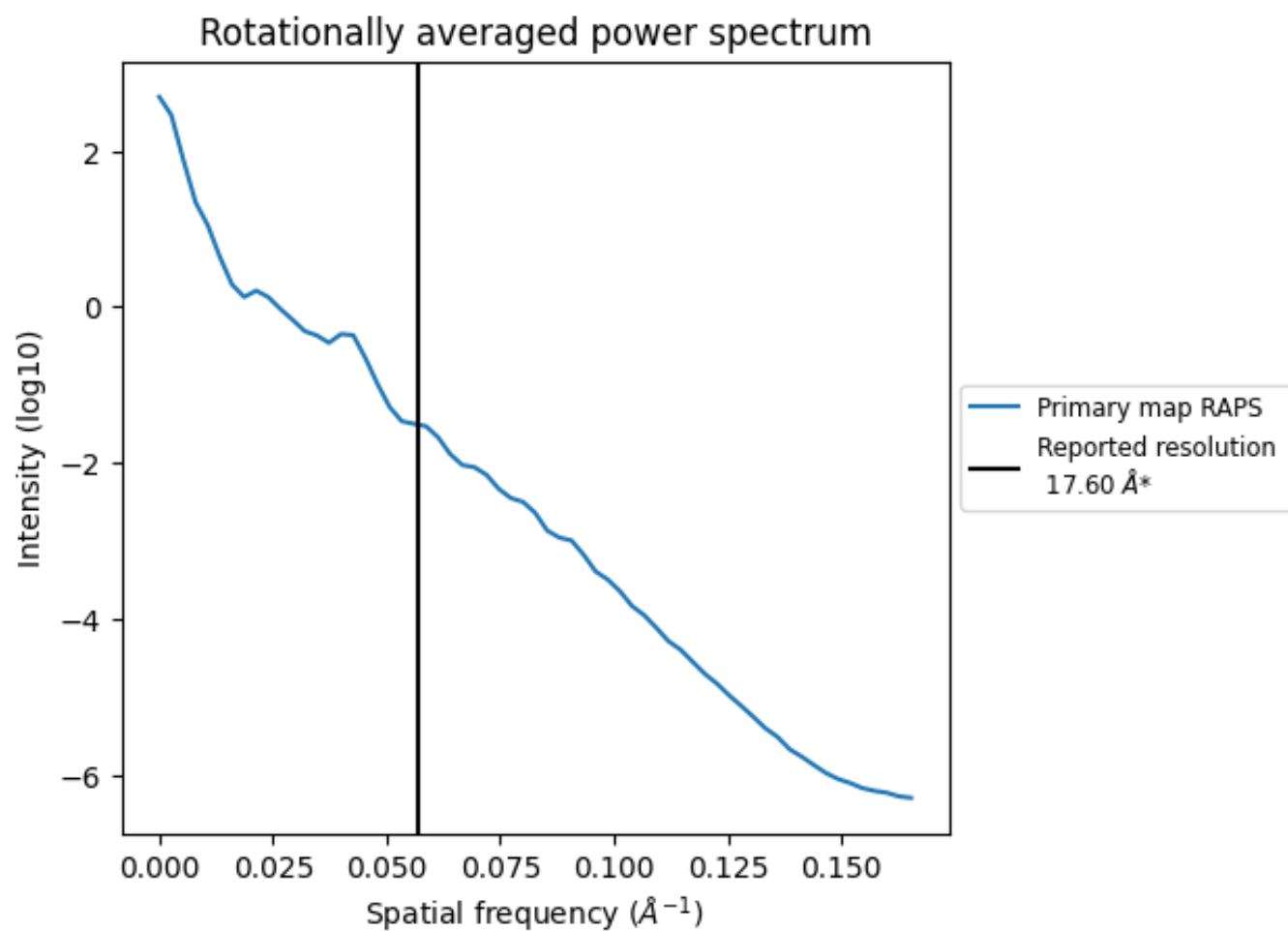
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1116 nm³; this corresponds to an approximate mass of 1009 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 0.057 Å⁻¹

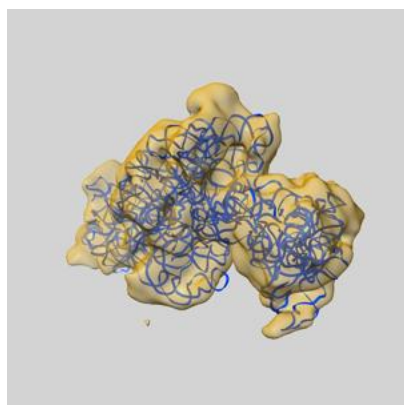
8 Fourier-Shell correlation

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

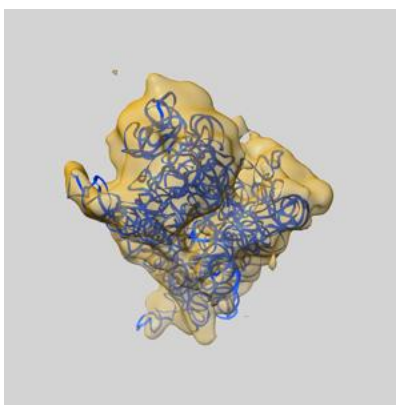
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5508 and PDB model 3J2F. Per-residue inclusion information can be found in section 3 on page 4.

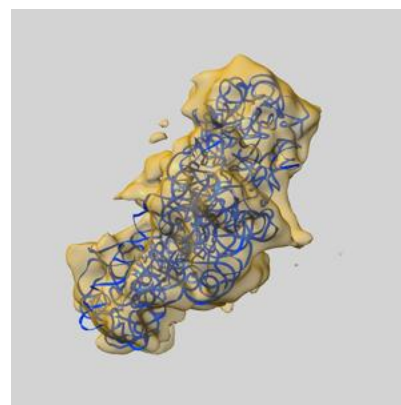
9.1 Map-model overlay [i](#)



X



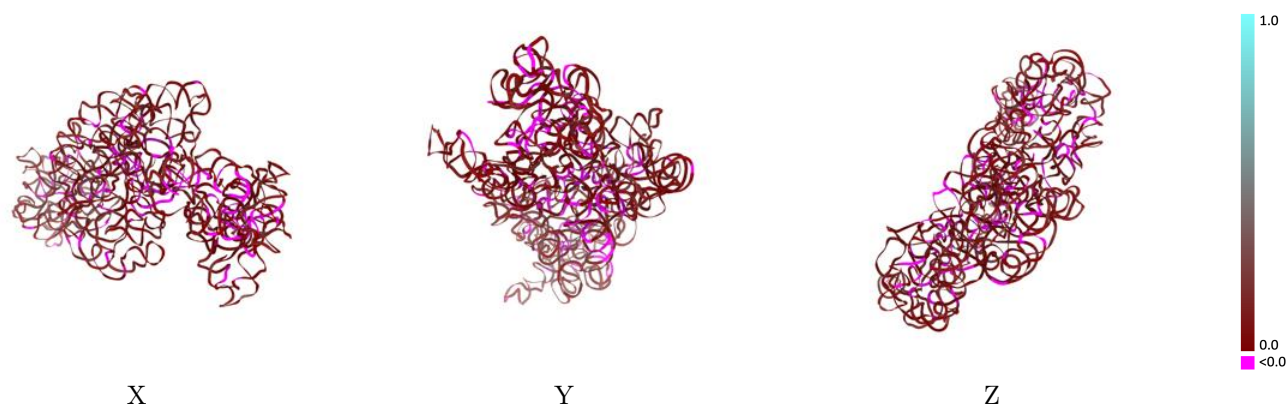
Y



Z

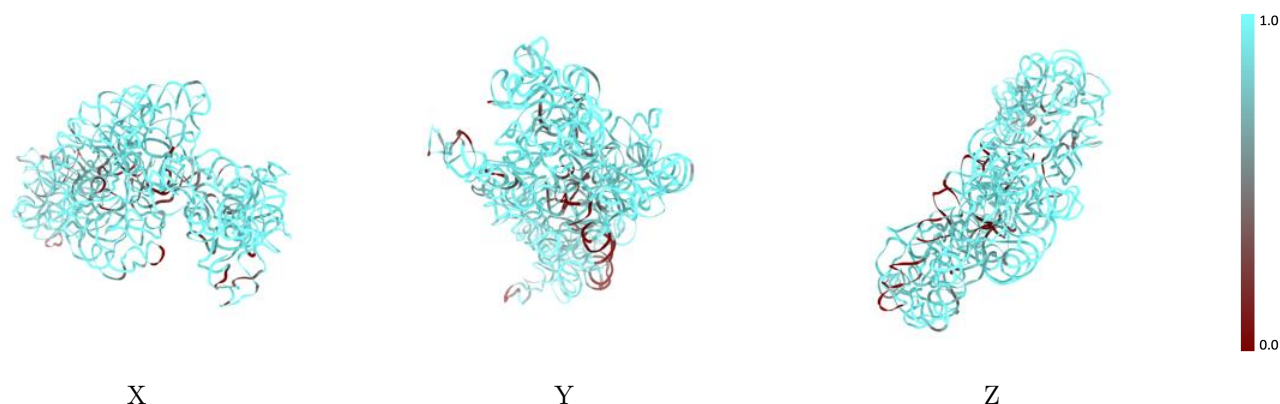
The images above show the 3D surface view of the map at the recommended contour level -2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



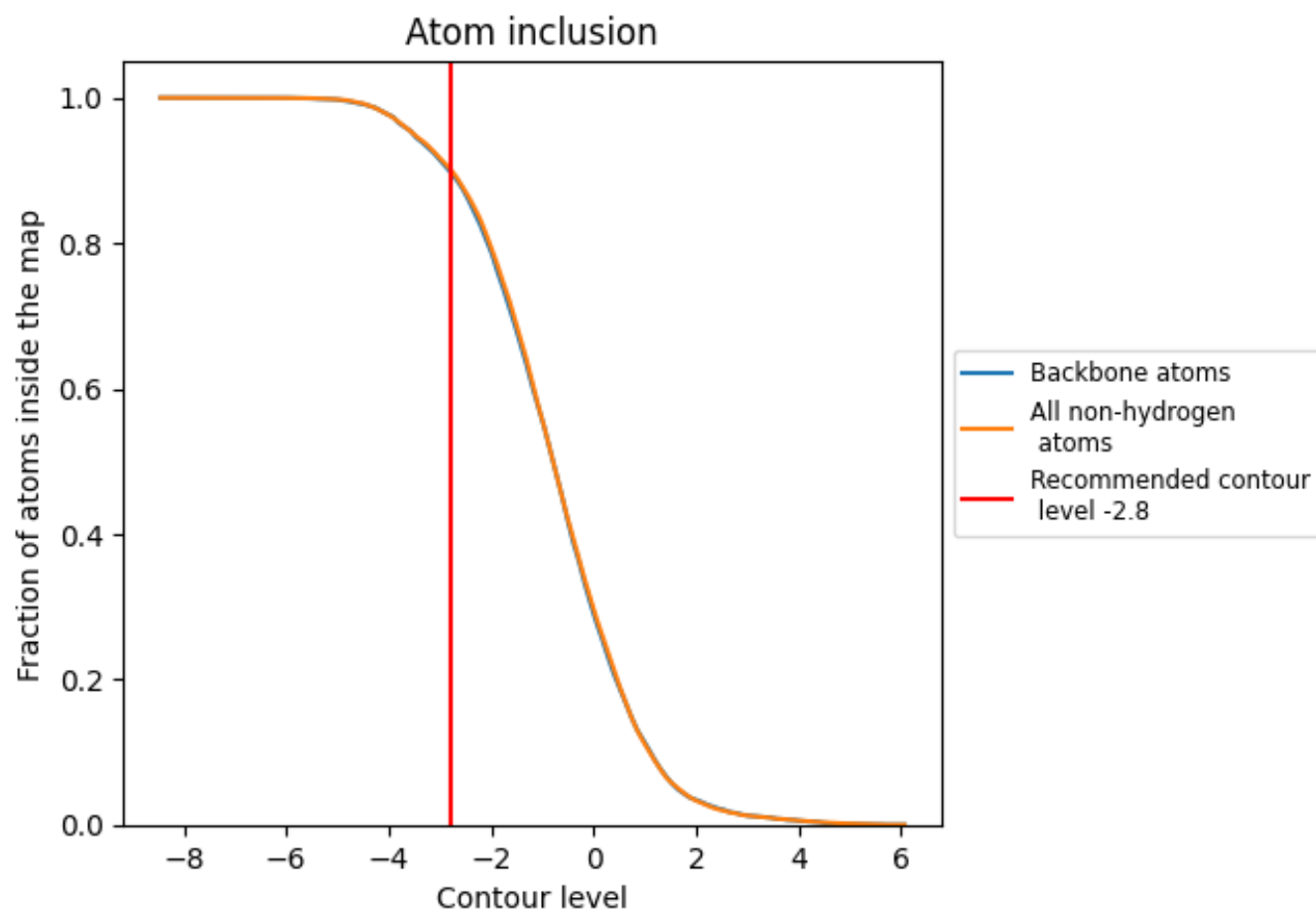
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 90% of all backbone atoms, 90% 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> 0.9016	<div></div> 0.0710
N	<div></div> 0.9023	<div></div> 0.0710

