



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 12:04 PM EST

PDB ID : 3J28
EMDB ID : EMD-5500
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 : 12.90 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

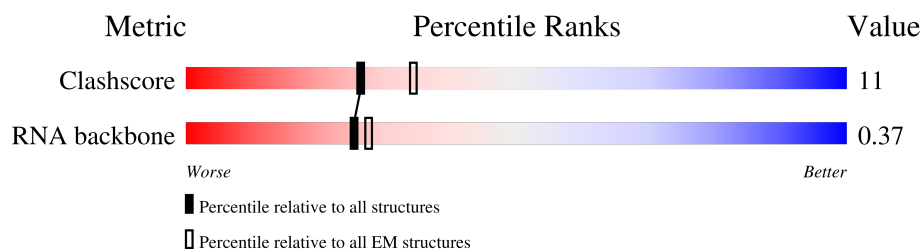
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is 12.90 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.

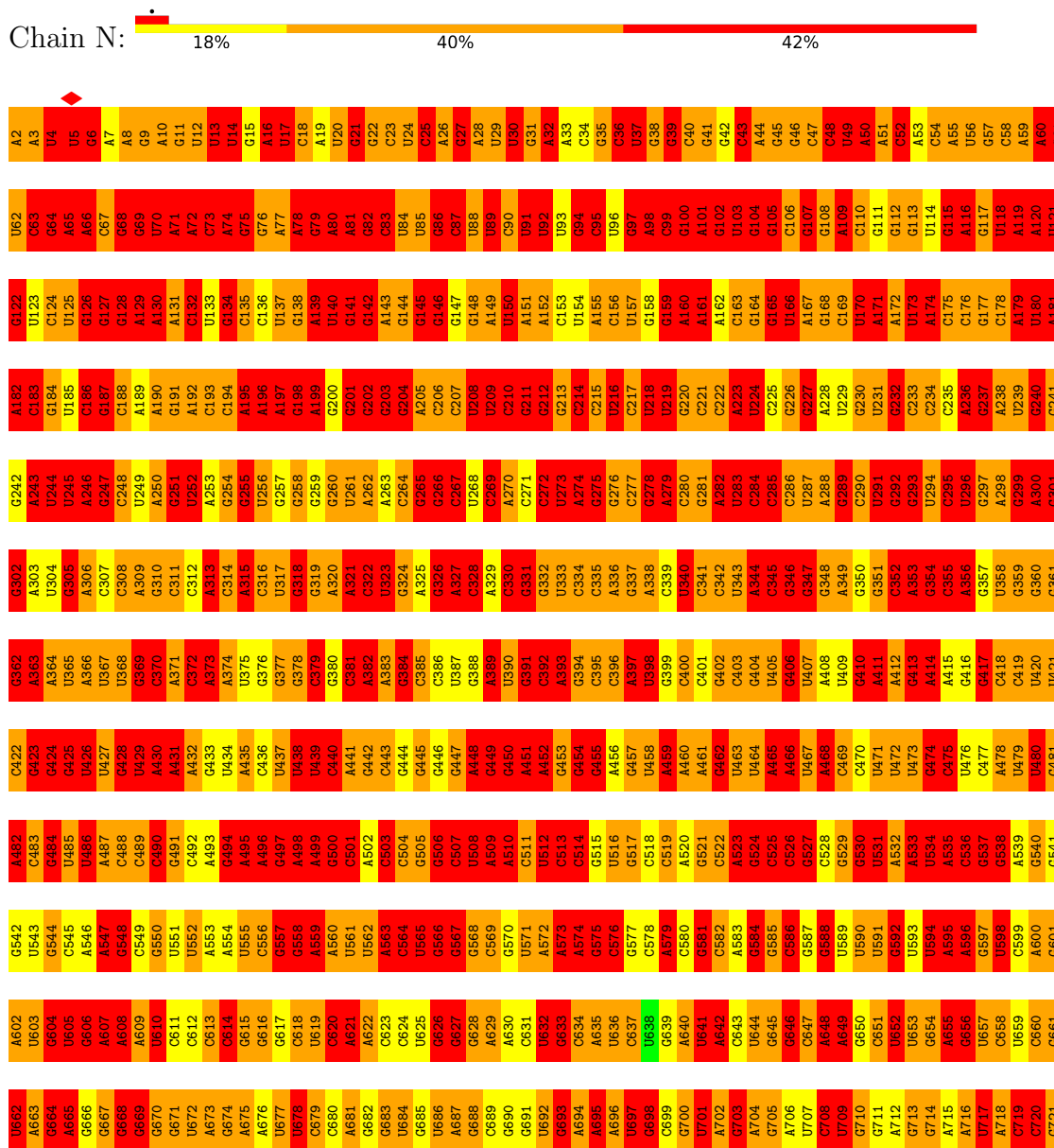
- Molecule 1 is a RNA chain called 16S rRNA.

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	C1322	C1262	U1202	G1142	A1082	U1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	G1323	C1263	C1203	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	C1384	A1324	A1264	A1204	U1144	G1084	G1024	A964	U904	A784	A764	G724
G1505	U1445	C1385	C1325	C1265	U1205	A1145	U1085	U1025	U965	U905	A845	G785	G725
U1506	A1446	G1386	U1326	G1266	G1206	A1146	G1086	G1026	G966	A906	G846	G786	G726
U1507	A1447	G1387	C1327	G1267	G1207	C1147	G1087	U1027	C967	A907	G847	A787	G727
A1508	C1448	C1388	C1328	G1268	C1208	U1148	G1088	C1027	C968	A908	C848	U788	A728
A1509	C1449	C1389	A1329	A1269	C1209	A1149	G1089	C1028	A969	A909	C849	U789	A729
C1510	U1450	U1390	U1330	G1270	C1210	A1150	U1090	U1029	U969	C910	U850	U790	G730
U1512	U1451	G1391	G1331	A1271	U1211	A1151	U1091	C970	G971	G911	G851	G791	G731
A1513	U1452	C1392	A1332	G1272	U1212	A1152	A1092	C972	G973	C912	G852	A792	G732
G1514	C1453	U1393	C1333	C1273	C1213	G1153	A1093	G1031	G974	A913	C853	U793	G733
C1515	C1454	C1394	G1334	A1274	C1214	G1154	G1094	G1032	C975	A914	U854	A794	G734
G1516	G1455	C1395	U1335	A1275	G1215	A1155	U1095	G1033	G976	A915	U855	C796	G735
G1517	G1456	C1396	C1336	G1276	C1216	G1156	C1096	A1035	A977	U916	C856	C797	G736
A1518	C1457	C1397	G1337	C1277	C1217	A1157	C1097	G1034	G978	A918	C857	C798	G737
U1519	A1458	A1398	G1338	G1278	C1218	C1158	C1098	A1036	A979	A919	U858	U798	C738
C1520	G1459	C1399	A1339	A1279	A1219	U1159	G1099	C1037	A977	A919	G859	G799	C739
C1521	G1460	G1401	U1341	A1280	G1220	G1160	C1100	G1038	C979	U920	G800	U740	U740
U1522	G1461	C1402	C1342	C1281	G1221	C1161	A1101	G1039	U981	U921	C861	U801	G741
C1523	C1462	C1403	G1343	C1282	U1223	A1163	C1103	G1041	U982	C923	U863	G803	A743
C1524	C1463	C1404	C1344	C1284	C1224	G1164	G1104	A1042	A984	C924	A864	U804	C744
G1525	U1463	G1405	A1345	A1285	A1225	U1165	A1105	G1043	C984	G925	A865	C805	G745
U1526	U1464	U1406	U1346	U1286	C1226	G1166	G1106	A1044	C985	G926	C866	C806	A746
U1527	A1465	C1407	G1347	A1287	A1227	A1167	C1107	A1045	U986	C927	C867	A807	A747
U1528	A1466	A1408	A1348	A1288	C1228	U1168	G1108	A1046	U987	G928	C868	C808	G748
G1529	C1467	C1409	U1349	A1289	A1229	U1169	C1109	G1047	G988	G929	G869	G809	A749
U1530	A1468	A1410	A1350	C1290	C1230	A1170	A1110	G1048	U989	C930	U870	C810	C750
A1531	C1469	C1411	U1351	U1291	G1231	A1171	A1111	U1049	C990	C931	U871	C811	U751
U1532	U1470	C1412	C1352	G1292	U1232	C1172	C1112	G1050	C991	G932	A872	G812	G752
C1533	U1471	A1413	G1353	C1293	G1233	U1173	C1113	C1051	U992	C933	A873	U813	A753
A1534	G1472	U1414	U1354	G1294	C1234	G1174	C1114	U1052	G993	C934	G874	A814	C754
	G1473	G1415	G1355	U1295	U1235	U1175	U1115	G1053	A994	A935	U875	A815	G755
	U1474	G1416	G1356	C1296	U1236	A1176	G1116	C1054	C995	C936	C876	A816	C756
	G1475	G1417	A1357	G1297	A1237	G1177	A1117	A1055	A996	A937	G877	C817	U757
	A1476	A1418	U1358	U1298	C1238	U1178	C1118	U1056	U997	G938	A878	G818	G758
	U1477	G1419	C1359	A1299	A1239	A1179	C1119	G1057	C998	G939	C879	A819	A759
	U1478	U1420	A1360	G1300	U1240	A1180	C1120	G1058	C999	C940	C880	U820	G760
	C1479	G1421	G1361	U1301	G1241	G1181	U1121	C1059	A1000	G941	G881	G821	G761
	A1480	G1422	A1362	C1302	G1242	U1182	U1122	U1060	C1001	G942	C882	U822	U762
	U1481	U1424	U1363	C1303	C1243	U1183	U1123	G1061	C1002	U943	C883	C823	G763
	G1482	G1425	U1364	G1304	G1244	G1184	G1124	U1062	G1003	G944	U884	G824	C764
	A1483	C1427	G1365	G1305	C1245	G1185	U1125	C1063	G1004	G945	A825	A765	G765
	C1484	A1428	C1366	A1306	A1246	G1186	U1126	G1064	A1005	A946	G886	C826	A766
	U1485	U1429	C1367	U1307	U1247	G1187	G1127	U1065	G947	G947	G887	U827	A767
	G1486	A1430	A1368	U1308	A1248	U1188	C1128	C1066	G1006	C948	G888	U828	A768
	U1487	A1431	G1373	C1313	G1253	G1193	C129	G1067	A889	G949	G889	G829	G769
	G1488	G1432	A1374	C1314	A1254	U1194	A1130	C1069	U1007	U950	G890	G830	C770
	U1489	A1433	U1375	U1315	G1255	C1195	C1136	U1070	U1008	G951	U891	A831	G771
	A1490	A1434	U1376	G1316	A1256	C1196	C1137	G1071	U1009	U952	A892	G832	U772
	G1491	G1435	A1377	C1317	G1257	U1197	G1138	G1072	U1010	G953	C893	G833	G773
	A1492	A1436	C1378	A1318	A1258	A1198	U1139	G1073	G954	G954	G894	U834	G774
	C1493	U1437	G1379	A1319	C1259	U1199	C1140	U1074	U1009	U955	G895	U835	G775
	U1494	G1438	U1380	C1320	G1260	C1200	C1141	G1075	U1009	U956	C896	G836	G776
	G1495	U1439	U1381	U1321	A1261	A1201	C1142	U1076	U1015	U957	C897	U837	A777
	C1496	U1440					U1194	G1077	A1016	A958	C898	G838	G778
	U1498	A1441					C1195	U1078	U1017	A959	C899	C839	C779
	A1499						U1196	G1079	G1018	U960	A900	C840	A780
	A1500						C1200	A1080	A1019	U961	A901	C841	A781
	C1501						A1201	A1081	G1020				
									A1021				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32152	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	4.191	Depositor
Minimum map value	-6.676	Depositor
Average map value	-4.024	Depositor
Map value standard deviation	0.567	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	3.47	5260/36831 (14.3%)	3.94	9443/57458 (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	948

The worst 5 of 5260 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	16	A	N7-C5	-19.48	1.27	1.39
1	N	563	A	N7-C5	-18.95	1.27	1.39
1	N	1396	A	N3-C4	-18.85	1.23	1.34
1	N	28	A	N7-C5	-18.07	1.28	1.39
1	N	1243	C	N1-C6	17.88	1.47	1.37

The worst 5 of 9443 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1362	A	P-O3'-C3'	29.77	155.43	119.70
1	N	1004	A	N1-C6-N6	26.64	134.59	118.60
1	N	766	A	N1-C6-N6	26.51	134.50	118.60
1	N	191	G	C5-C6-O6	-25.76	113.14	128.60
1	N	94	G	P-O3'-C3'	24.94	149.63	119.70

There are no chirality outliers.

5 of 948 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	10	A	Sidechain
1	N	2	A	Sidechain
1	N	4	U	Sidechain
1	N	5	U	Sidechain
1	N	6	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	16511	547	0
All	All	32892	16554	16511	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:664:G:H22	1:N:741:G:H1	1.31	0.76
1:N:596:A:H61	1:N:644:U:H3	1.37	0.73
1:N:116:A:H61	1:N:313:A:H1'	1.56	0.70
1:N:67:C:H2'	1:N:68:G:C8	2.26	0.70
1:N:381:C:C5	1:N:382:A:C5	2.81	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%)	451 (29%)	150 (9%)

5 of 451 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	8	A

5 of 150 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1190	G
1	N	1440	U
1	N	1201	A
1	N	1319	A
1	N	428	G

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.

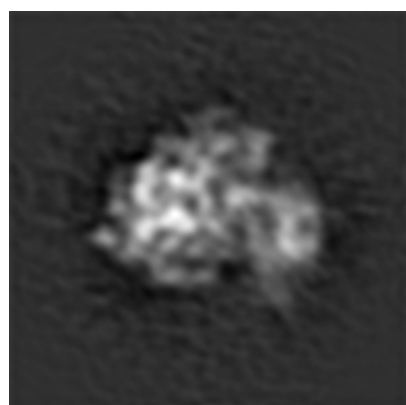
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5500. These allow visual inspection of the internal detail of the map and identification of artifacts.

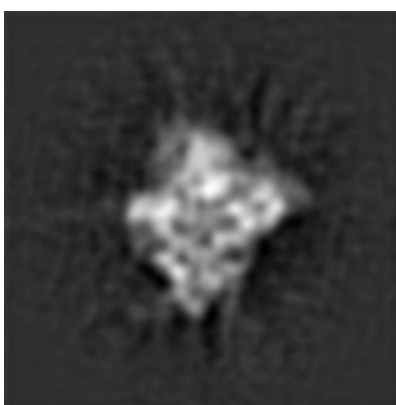
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

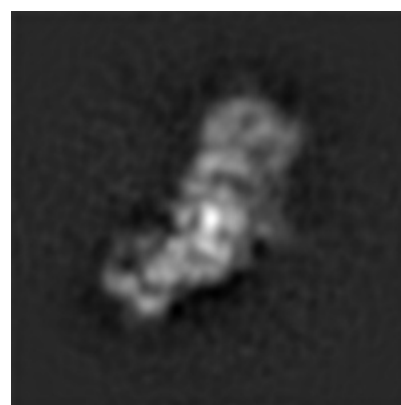
6.1.1 Primary map



X



Y

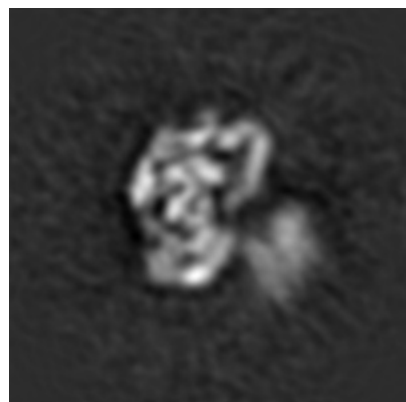


Z

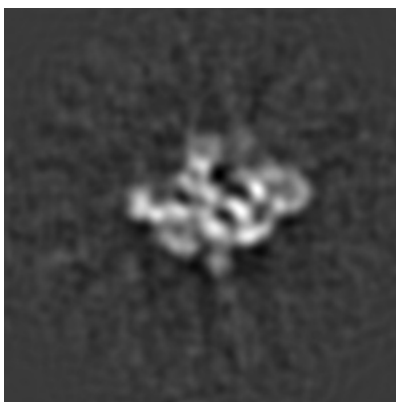
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

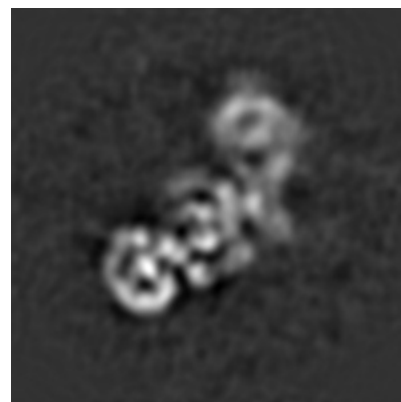
6.2.1 Primary map



X Index: 62



Y Index: 62

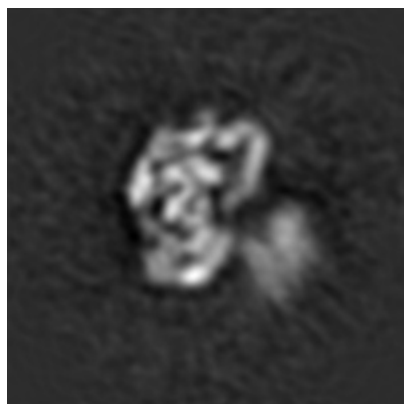


Z Index: 62

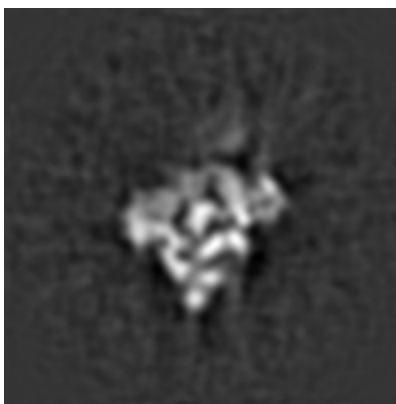
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

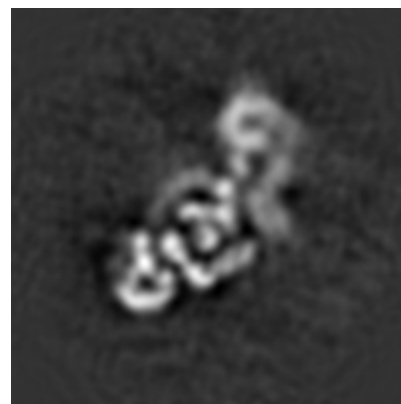
6.3.1 Primary map



X Index: 62



Y Index: 51

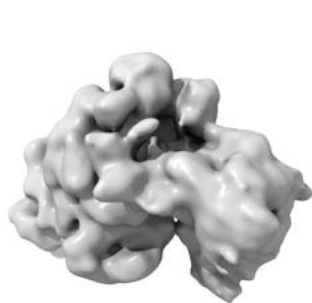


Z Index: 64

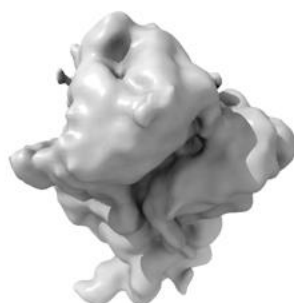
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

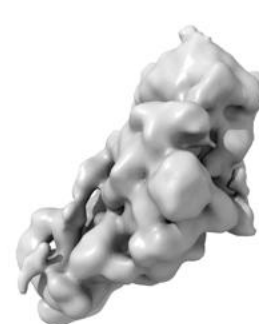
6.4.1 Primary map



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.

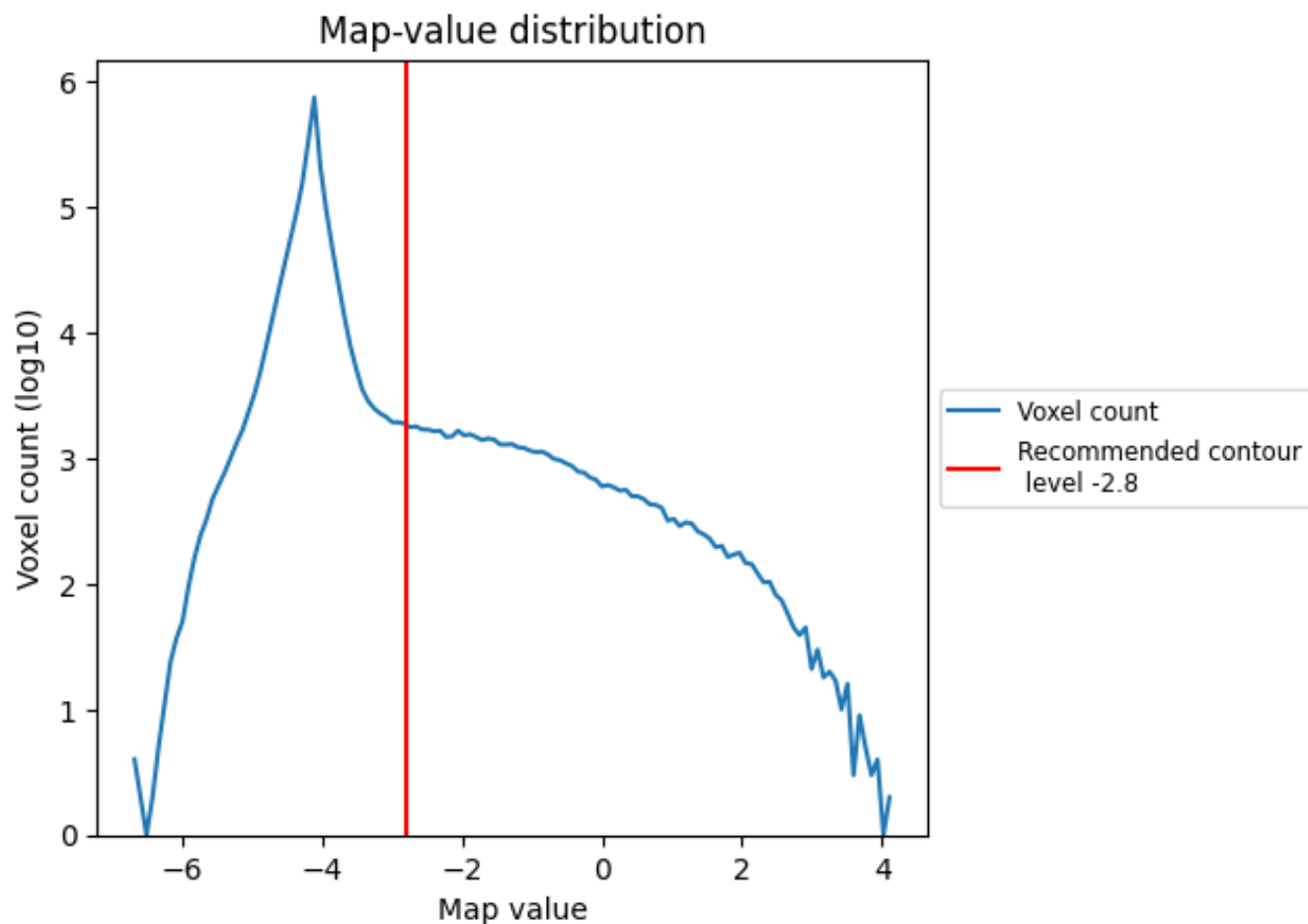
6.5 Mask visualisation

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

7 Map analysis [i](#)

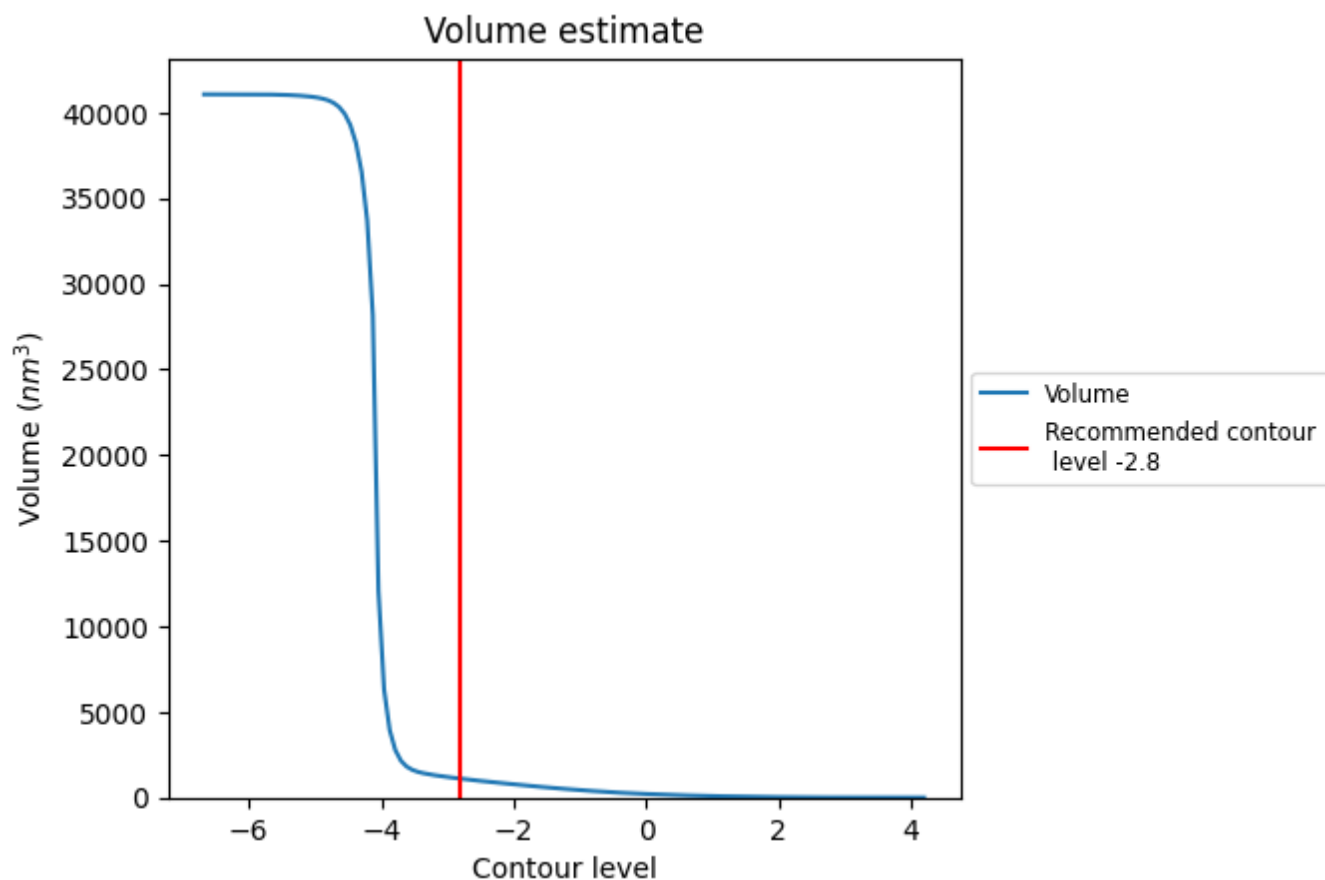
This section contains the results of statistical analysis of the map.

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.

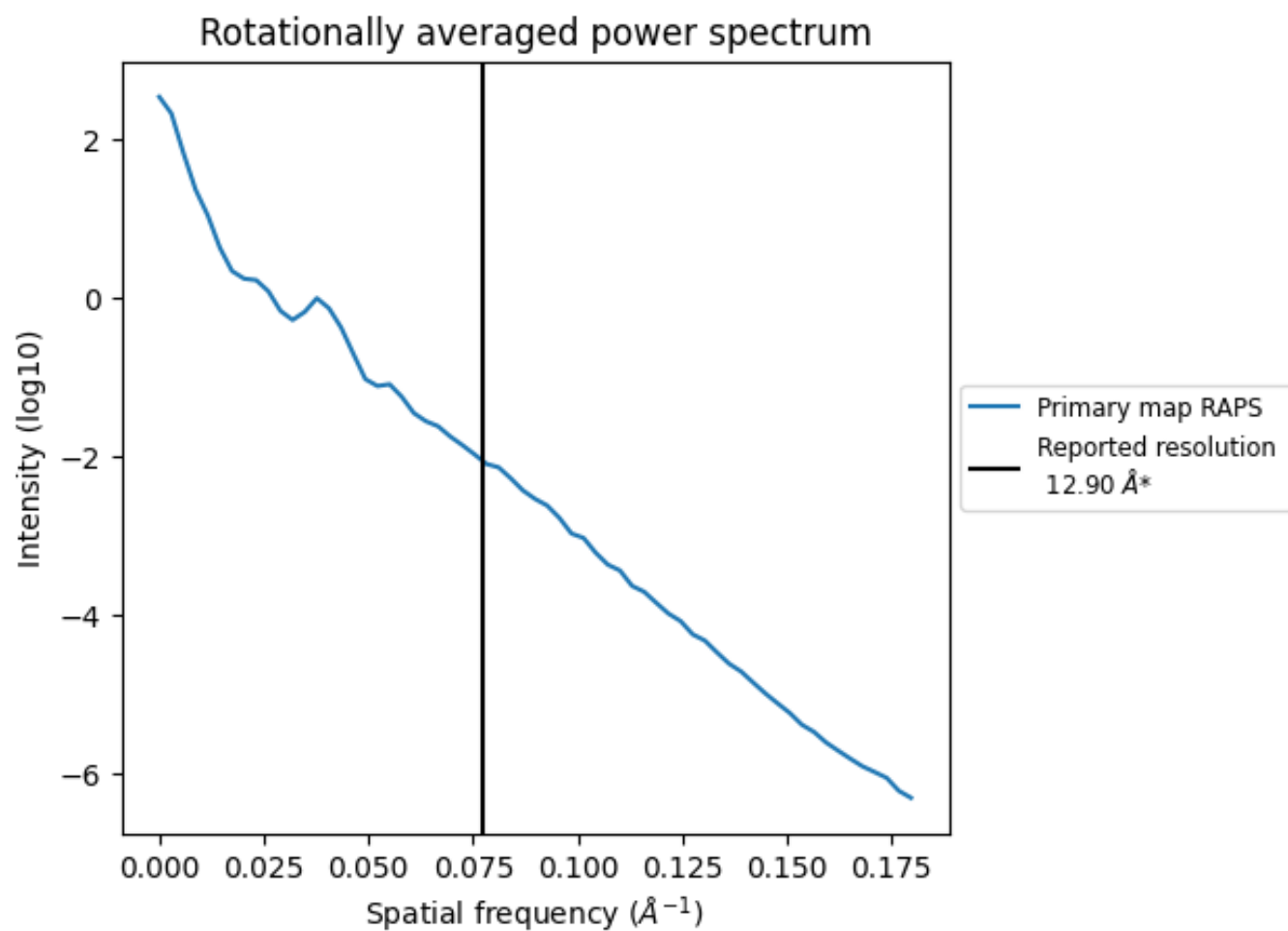
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1102 nm³; this corresponds to an approximate mass of 995 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 0.078 Å⁻¹

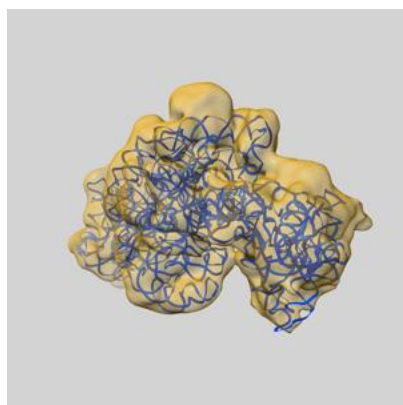
8 Fourier-Shell correlation

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

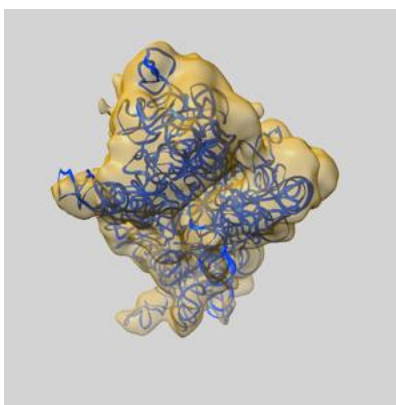
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5500 and PDB model 3J28. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

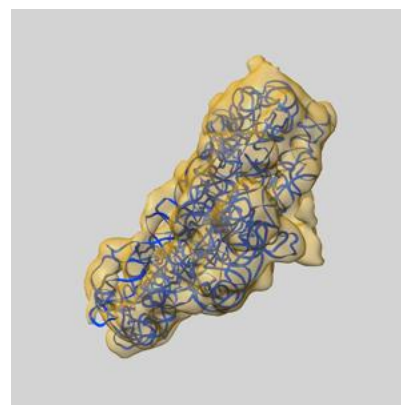
9.1 Map-model overlay [i](#)



X



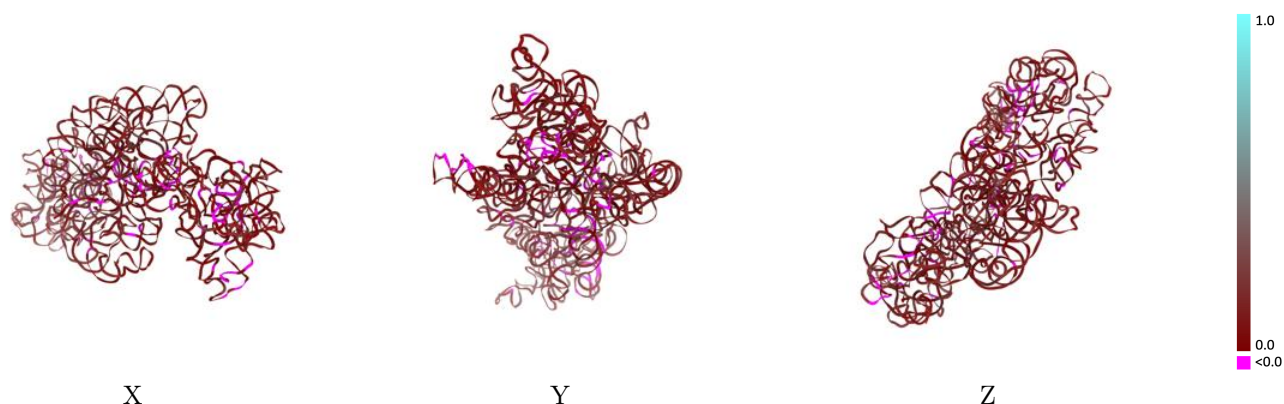
Y



Z

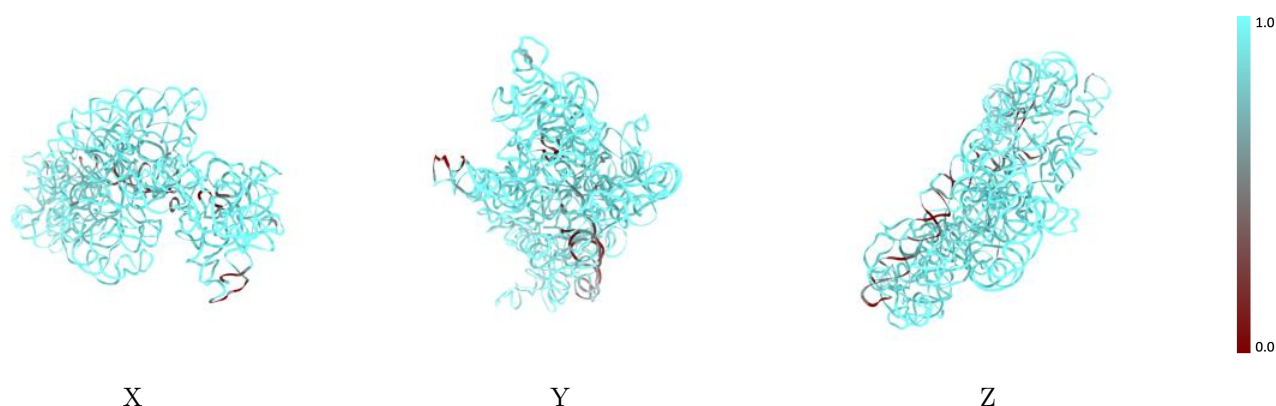
The images above show the 3D surface view of the map at the recommended contour level -2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



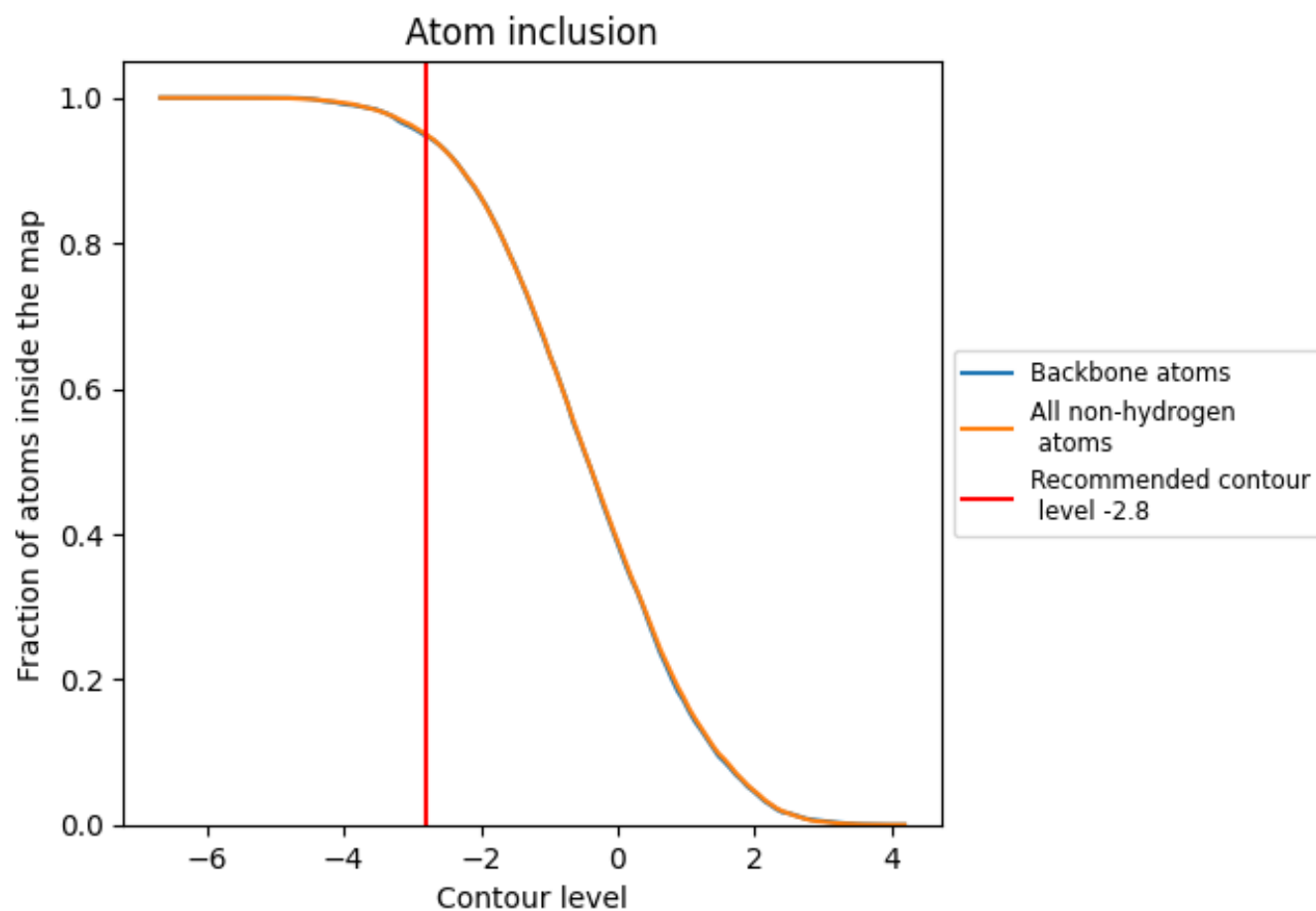
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 95% 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> 0.9497	<div></div> 0.1010
N	<div></div> 0.9500	<div></div> 0.1010

