



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 12:50 PM EST

PDB ID : 3J2B
EMDB ID : EMD-5503
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 : 13.60 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

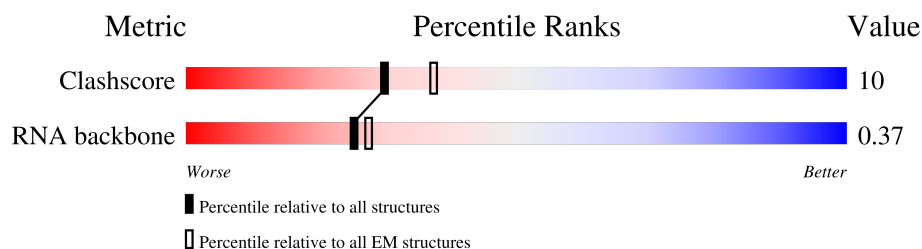
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.60 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.

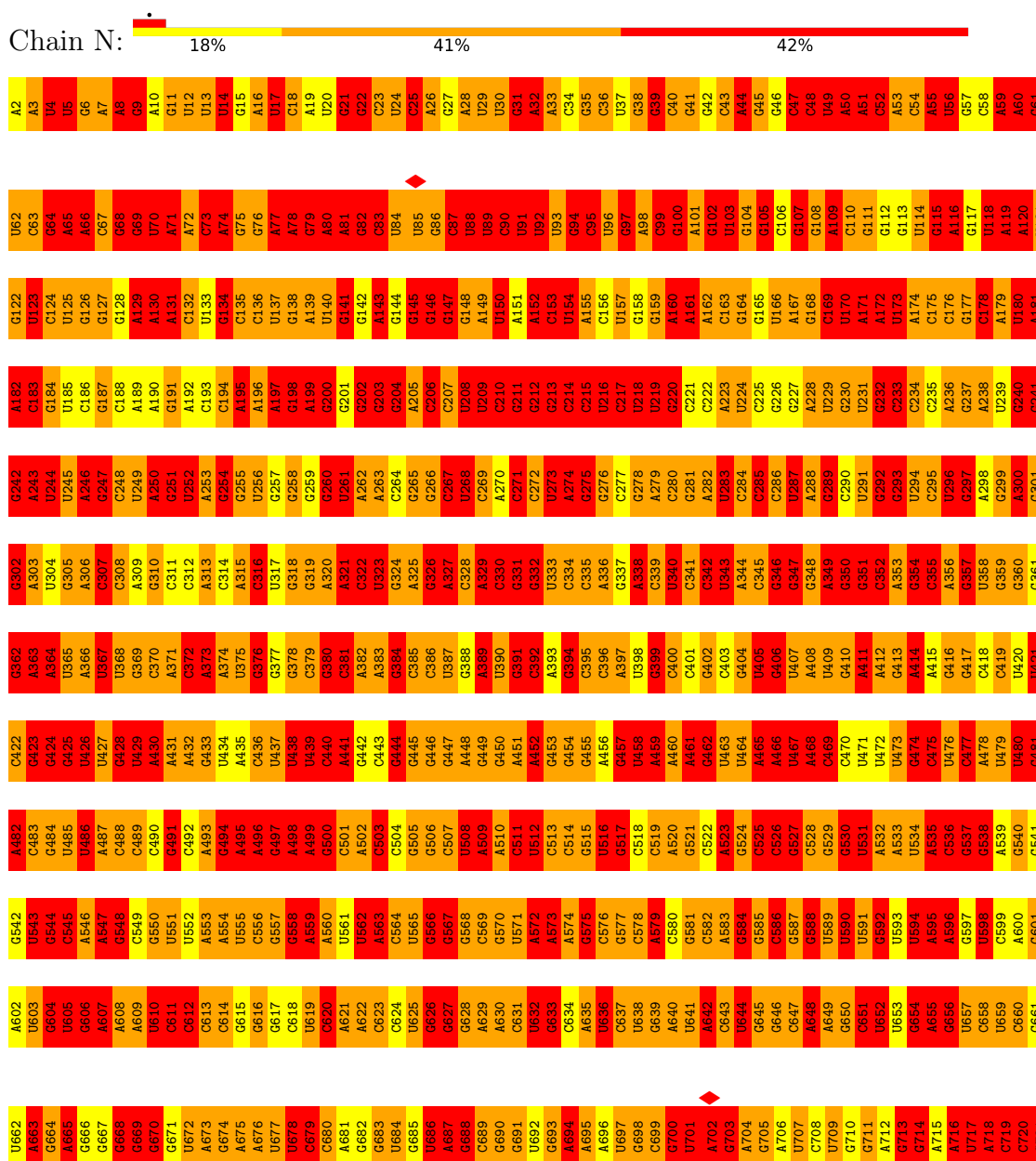
- Molecule 1 is a RNA chain called 16S rRNA.

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



A1502	G1442	C1382	C1262	U1202	G1142	A1082	A1022	C962	G902	U842	A782	G722
A1503	C1443	C1383	C1263	C1203	G1143	U1083	U1023	G963	G903	U843	C783	U723
G1504	U1444	C1384	C1264	A1204	G1144	U1084	G1024	A964	U904	G844	C784	G724
G1505	C1385	C1325	C1265	U1205	A1145	U1085	U1025	U965	U905	A845	G785	G725
U1506	G1386	G1326	G1266	G1206	A1146	U1086	G1026	G966	A906	G846	G786	C726
A1507	G1387	U1327	C1267	G1207	C1147	G1087	C1027	C967	A907	G847	A787	G727
A1508	C1388	C1328	G1268	C1208	U1148	U1088	U1028	A968	A908	C848	U788	A728
C1509	A1389	A1329	A1269	C1209	C1149	G1089	U1029	A969	A909	G849	U789	A729
C1510	U1390	U1330	G1270	C1210	A1150	U1090	U1030	C970	C910	U850	A790	G730
U1511	G1391	G1331	A1271	U1211	A1151	U1091	C1031	G971	U911	G851	G791	G731
U1512	G1392	A1332	G1272	U1212	A1152	A1092	G1032	C972	C912	G852	A792	C732
U1451	U1393	A1333	C1273	A1213	G1153	A1093	G1033	G973	A913	C853	U793	G733
C1452	G1394	G1334	A1274	C1214	G1154	G1094	G1034	A974	A914	U854	A794	G734
G1453	U1395	U1335	A1275	G1215	A1155	U1095	A1035	A975	A915	U855	C785	C735
G1454	A1396	C1396	G1276	A1216	G1156	C1096	A1036	G976	U916	C856	C796	C736
G1455	C1397	G1337	C1277	C1217	A1157	C1097	G1037	G977	U917	C857	C797	C737
A1456	A1398	G1338	G1278	C1218	U1158	C1098	C1038	A978	A918	G858	U798	C738
A1518	C1399	A1339	G1279	A1219	U1159	G1099	G1039	C979	A919	G859	G799	C739
G1457	U1400	A1340	A1280	G1220	G1160	C1100	U1040	C980	U920	G860	G800	U740
G1458	C1401	C1281	C1281	G1221	C1161	A1101	G1041	U981	U921	C861	U801	G741
U1459	G1402	C1342	C1282	G1222	C1162	A1102	A1042	U982	G922	C862	A802	G742
C1460	C1403	G1343	U1283	C1223	A1163	C1103	G1043	A983	C923	U863	G803	A743
G1461	C1404	C1344	C1284	U1224	G1164	G1104	A1044	C984	C924	A864	U804	C744
G1462	G1405	U1345	A1285	A1225	U1165	A1105	G1045	C985	G925	A865	C805	G745
A1346	U1406	A1346	G1286	C1226	G1166	G1106	A1046	U986	G926	C866	C806	A746
G1347	C1407	G1347	U1287	A1227	A1167	C1107	G1047	C987	G927	C867	A807	A747
A1464	A1408	U1348	A1288	C1228	U1168	G1108	G1048	C988	G928	C868	C808	G748
A1465	C1409	A1349	A1289	A1229	A1169	C1109	U1049	U989	G929	C869	G809	A749
C1466	A1410	U1350	G1290	C1230	A1170	A1110	G1050	C990	C930	U870	C810	G750
C1467	C1411	U1351	U1291	G1231	A1171	A1111	C1051	U991	C931	U871	C811	U751
A1468	C1412	G1352	C1292	U1232	U1172	C1112	U1052	U992	G932	A872	G812	G752
C1469	A1413	U1353	C1293	G1233	G1173	C1113	G1053	G993	C933	C873	U813	A753
U1470	U1414	G1354	G1294	C1234	G1174	C1114	C1054	A994	G934	A874	A814	C754
U1471	G1415	G1355	U1295	U1235	G1175	U1115	A1055	C995	A935	C875	A815	C755
G1416	G1416	G1356	C1296	A1236	A1176	U1116	U1056	A996	G936	C876	C816	G756
G1417	A1417	U1357	G1297	C1237	G1177	A1117	G1057	U997	A937	G877	C817	U757
A1418	C1358	U1358	U1298	A1238	A1178	U1118	C1058	C998	G938	A878	G818	C758
U1474	A1418	C1359	A1299	A1239	A1179	C1119	C1059	C999	G939	C879	A819	A759
G1475	G1419	G1360	G1300	U1240	G1180	C1120	U1060	A1000	C940	C880	U820	G760
A1476	U1420	A1361	U1301	G1241	G1181	U1121	G1061	C1001	G941	C881	G821	G761
U1477	G1421	A1362	C1302	G1242	U1182	U1122	U1062	G1002	G942	C882	U822	U762
U1478	G1422	A1363	C1303	C1243	U1183	U1123	C1063	G1003	U943	C883	C823	G763
C1479	G1423	U1364	G1304	G1244	G1184	G1124	G1064	U1004	G944	U884	G824	C764
A1480	U1424	G1365	A1305	C1245	G1185	U1125	U1065	A1005	G945	C885	A825	G765
U1481	U1425	C1366	A1306	A1246	G1186	U1126	C1066	G1006	A946	C886	C826	A766
G1482	G1426	C1367	U1307	U1247	G1187	G1127	A1067	U1007	G947	C887	U827	A767
A1483	U1427	C1368	U1308	A1248	A1188	C1128	G1068	G888	C948	C888	U828	A768
C1484	C1427	G1370	G1309	C1249	U1189	C1129	C1069	A889	A949	A889	G829	G774
U1485	A1428	A1371	A1310	A1250	G1190	A1130	U1070	G890	U950	G890	G830	C770
G1486	A1429	U1372	U1311	A1251	A1191	G1131	C1071	U891	G951	U891	A831	G771
C1487	A1430	G1373	U1312	A1252	C1192	C1132	G1072	A892	U952	A892	G832	U772
G1488	A1431	A1374	U1313	G1253	G1193	G1133	U1073	C893	G953	C893	G833	G773
G1489	G1432	A1375	C1314	A1254	U1194	G1134	G1074	G894	G954	G894	U834	G774
U1490	A1433	U1376	U1315	G1255	C1195	U1135	U1075	G895	U955	G895	U835	G775
G1491	A1434	U1377	G1316	A1256	A1196	C1136	U1076	G896	U956	C896	G836	G776
A1492	A1435	A1378	C1317	A1257	A1197	C1137	G1077	U897	U957	C897	U837	A777
A1493	G1436	A1379	U1318	A1258	G1198	G1138	U1078	G898	A958	C898	G838	G778
C1494	U1437	C1380	A1319	G1259	U1199	G1139	G1079	C899	A959	C899	C839	C779
U1495	A1438	U1381	C1320	G1260	C1200	C1140	A1080	A900	U960	C840	U780	A781
C1496	G1439	U1382	A1261	A1261	A1201	C1141	A1081	A901	U961	C841	C841	
G1497	U1439	U1383										
U1498	A1493											
A1499	C1500											
C1501	C1501											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30892	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	5.345	Depositor
Minimum map value	-7.752	Depositor
Average map value	-4.176	Depositor
Map value standard deviation	0.605	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	3.50	5275/36831 (14.3%)	3.96	9425/57458 (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	935

The worst 5 of 5275 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	205	A	N7-C5	-20.49	1.26	1.39
1	N	499	A	N7-C5	-19.93	1.27	1.39
1	N	923	A	N7-C5	-19.93	1.27	1.39
1	N	3	A	N3-C4	-18.54	1.23	1.34
1	N	549	C	N3-C4	17.73	1.46	1.33

The worst 5 of 9425 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1519	A	N1-C6-N6	26.47	134.48	118.60
1	N	376	G	N1-C6-O6	26.45	135.77	119.90
1	N	832	G	C5-C6-O6	-25.79	113.13	128.60
1	N	722	G	N1-C6-O6	25.48	135.19	119.90
1	N	1261	A	N1-C6-N6	24.80	133.48	118.60

There are no chirality outliers.

5 of 935 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	11	G	Sidechain
1	N	4	U	Sidechain
1	N	5	U	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	16532	493	0
All	All	32892	16554	16532	493	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 493 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:1123:U:H3	1:N:1150:A:H61	1.28	0.81
1:N:688:G:C8	1:N:688:G:H5''	2.18	0.78
1:N:1255:G:H2'	1:N:1279:G:H1	1.54	0.72
1:N:1240:U:C6	1:N:1241:G:H5'	2.24	0.71
1:N:50:A:H1'	1:N:52:C:C6	2.27	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%)	441 (28%)	162 (10%)

5 of 441 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 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1064	G
1	N	1331	G
1	N	1129	C
1	N	1197	A
1	N	1364	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.

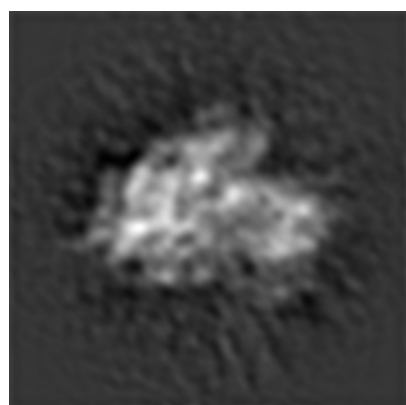
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5503. These allow visual inspection of the internal detail of the map and identification of artifacts.

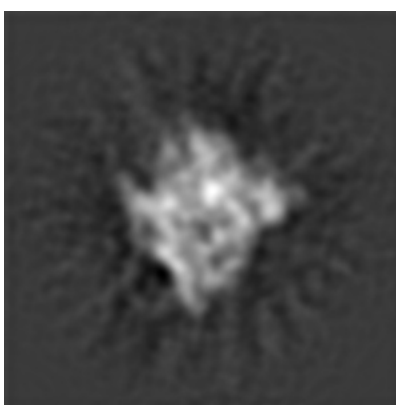
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

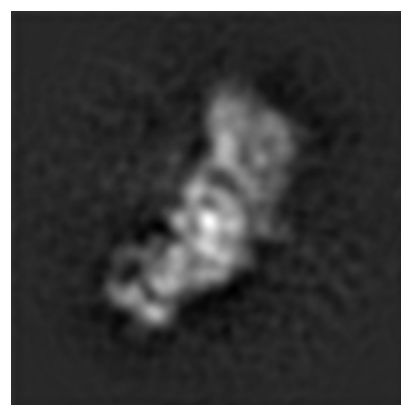
6.1.1 Primary map



X



Y

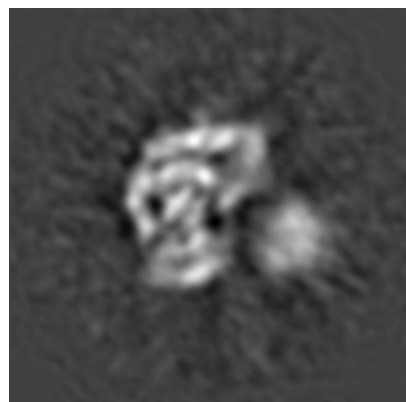


Z

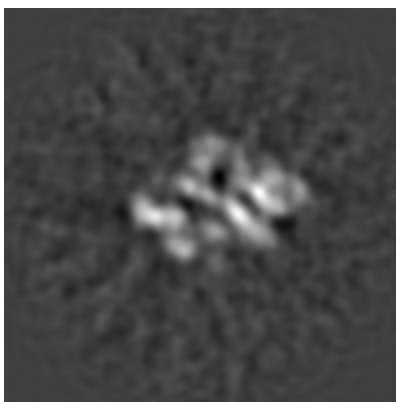
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

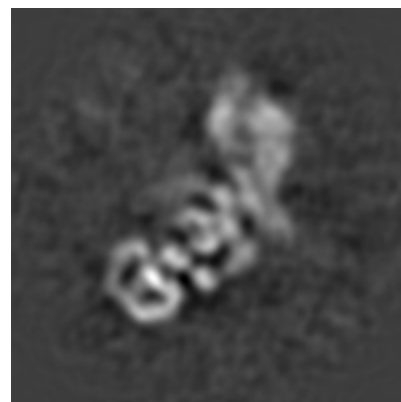
6.2.1 Primary map



X Index: 62



Y Index: 62

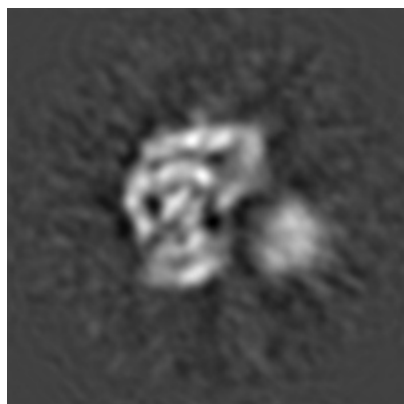


Z Index: 62

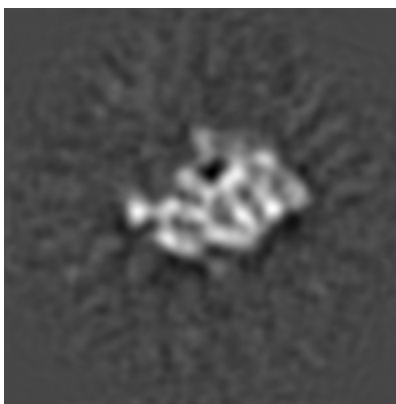
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

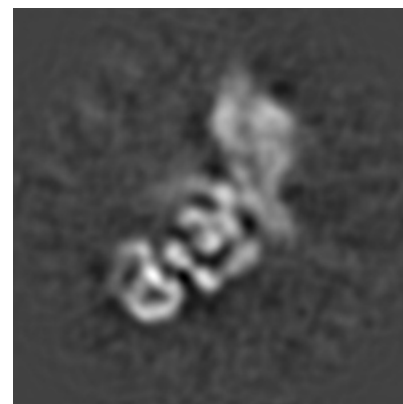
6.3.1 Primary map



X Index: 62



Y Index: 58

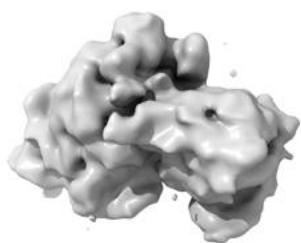


Z Index: 63

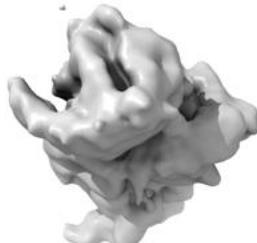
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

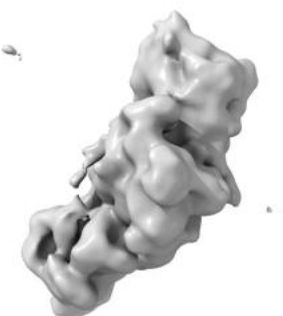
6.4.1 Primary map



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.

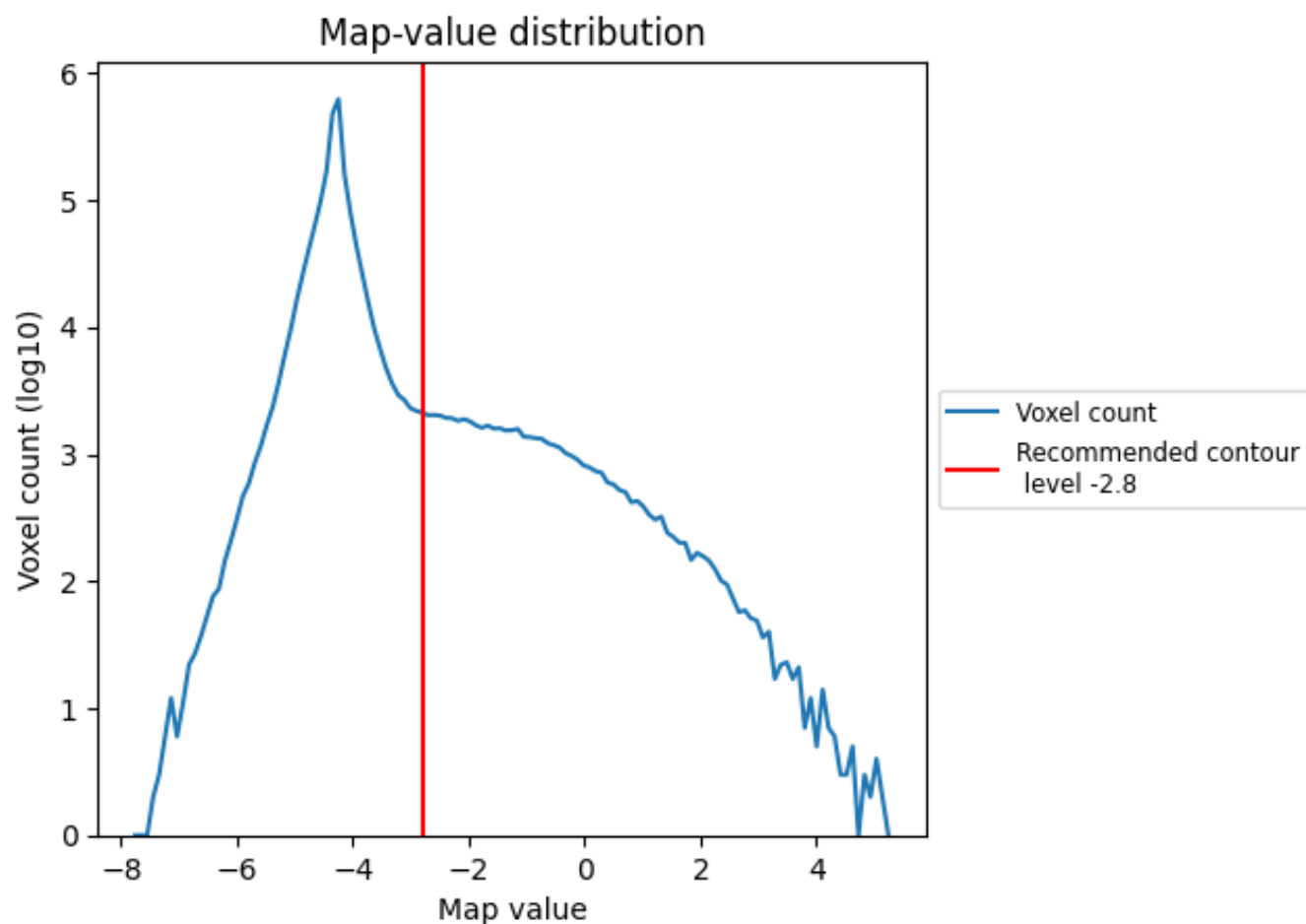
6.5 Mask visualisation

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

7 Map analysis [i](#)

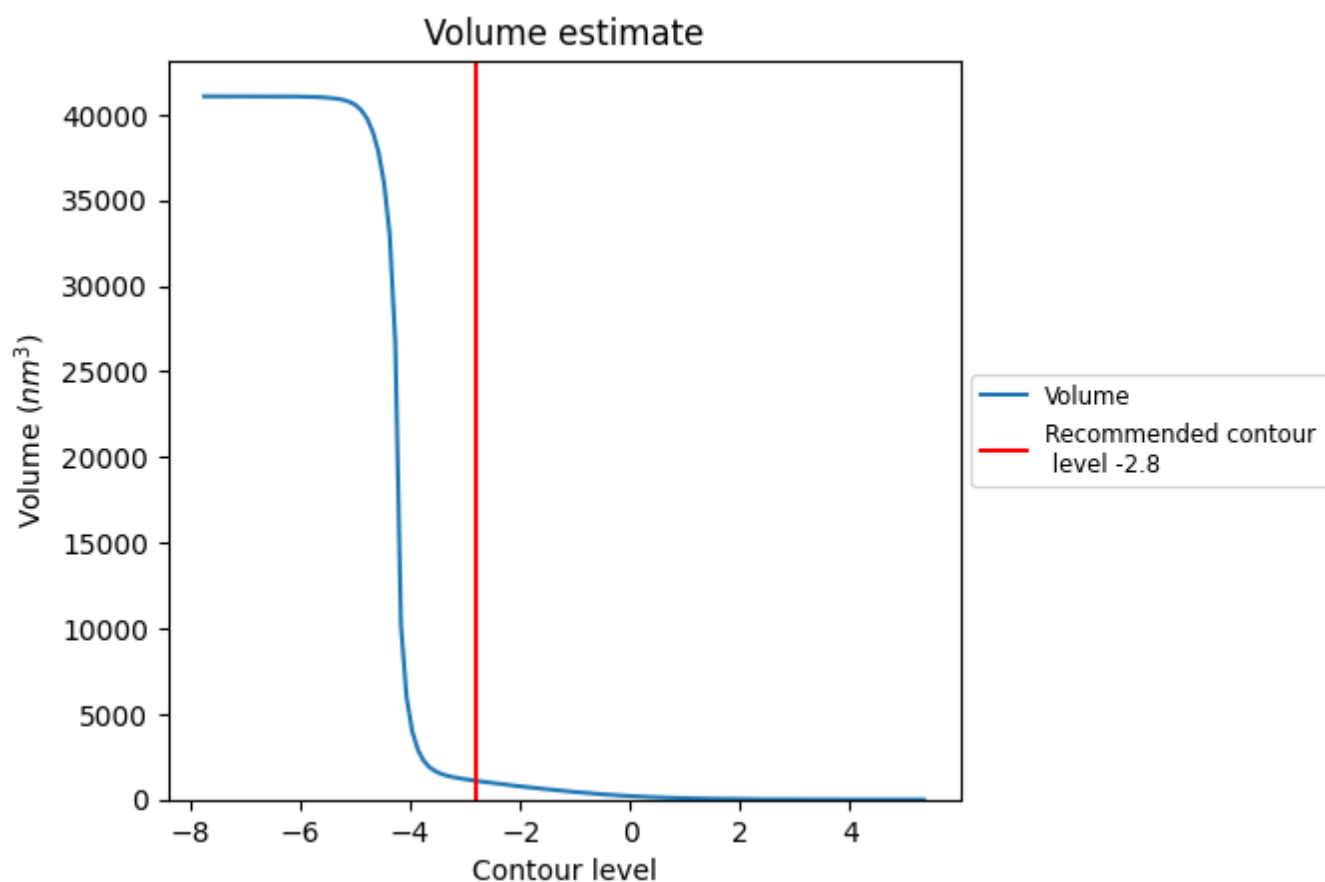
This section contains the results of statistical analysis of the map.

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.

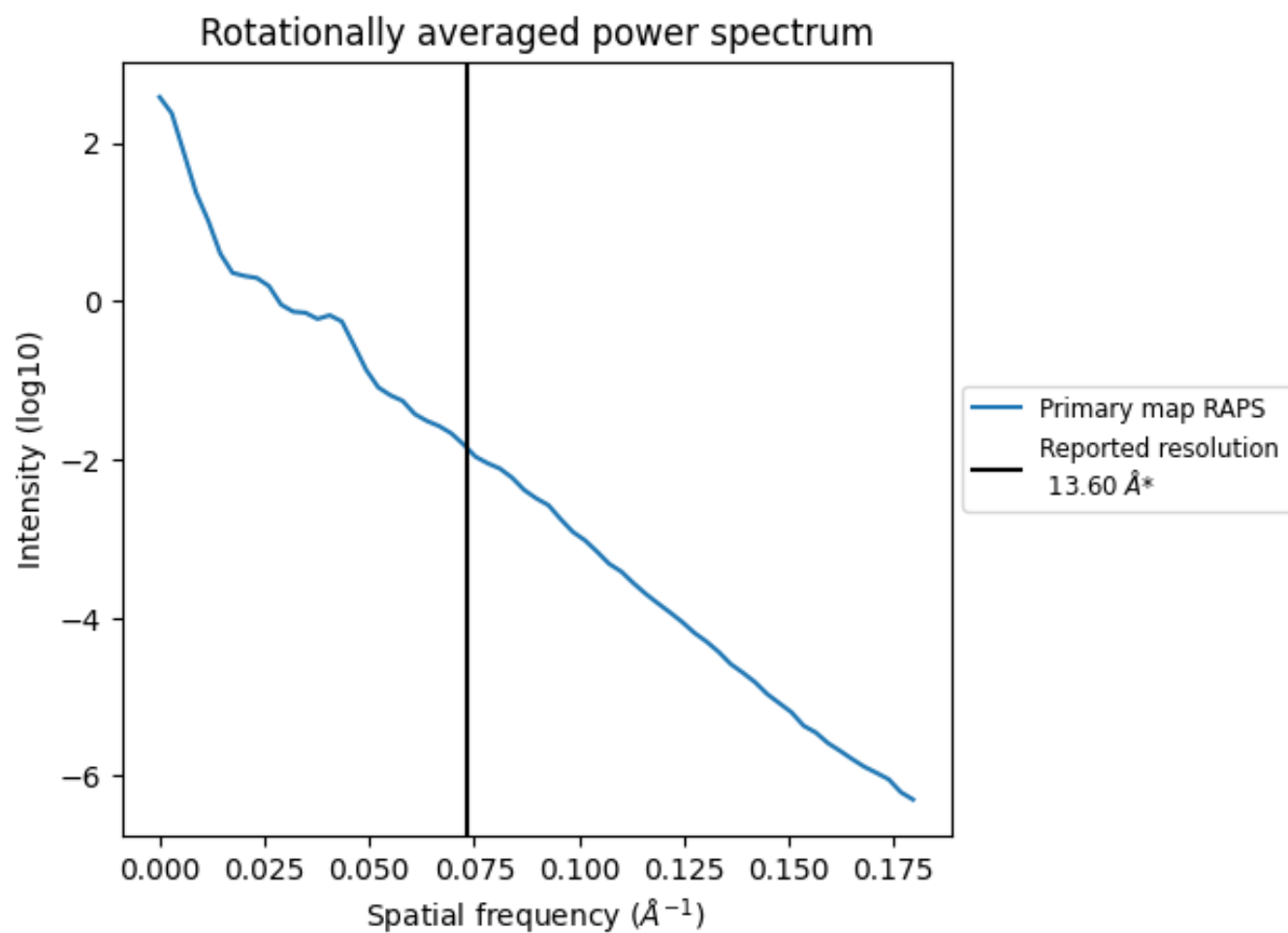
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1092 nm^3 ; this corresponds to an approximate mass of 986 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 0.074 Å⁻¹

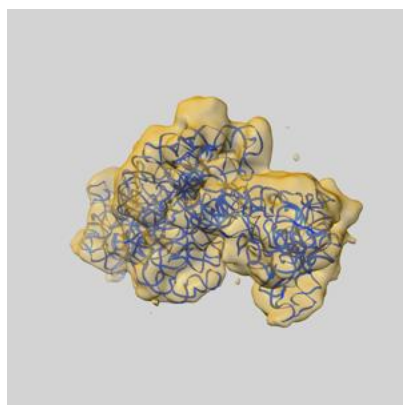
8 Fourier-Shell correlation

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

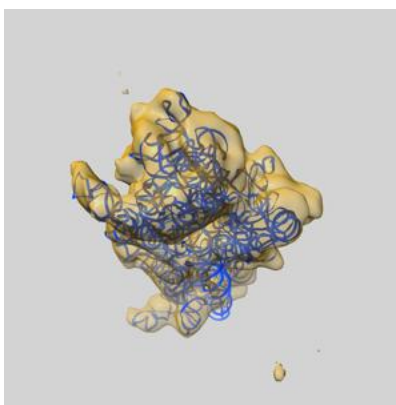
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5503 and PDB model 3J2B. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

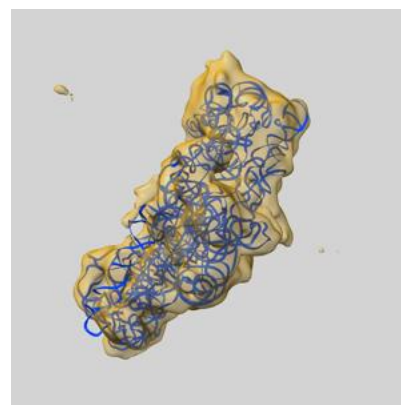
9.1 Map-model overlay [i](#)



X



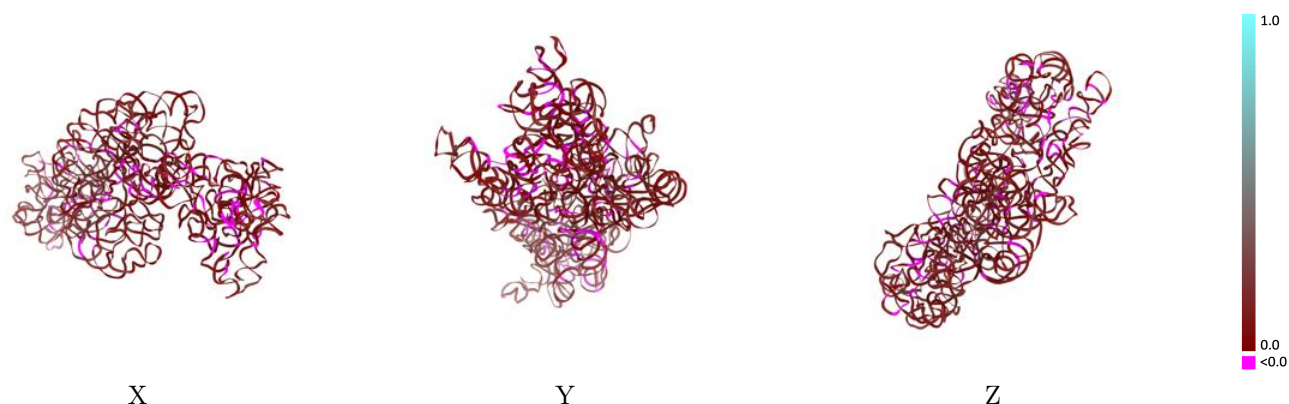
Y



Z

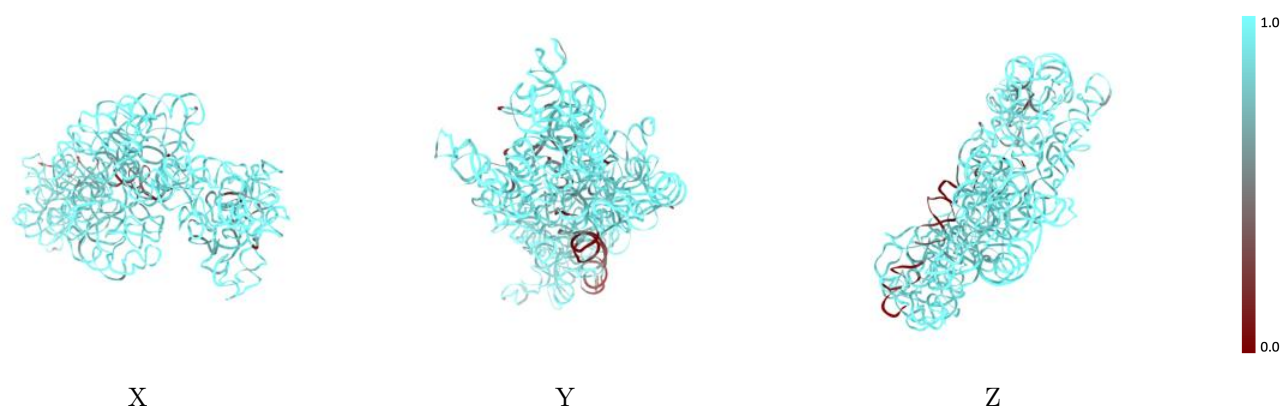
The images above show the 3D surface view of the map at the recommended contour level -2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



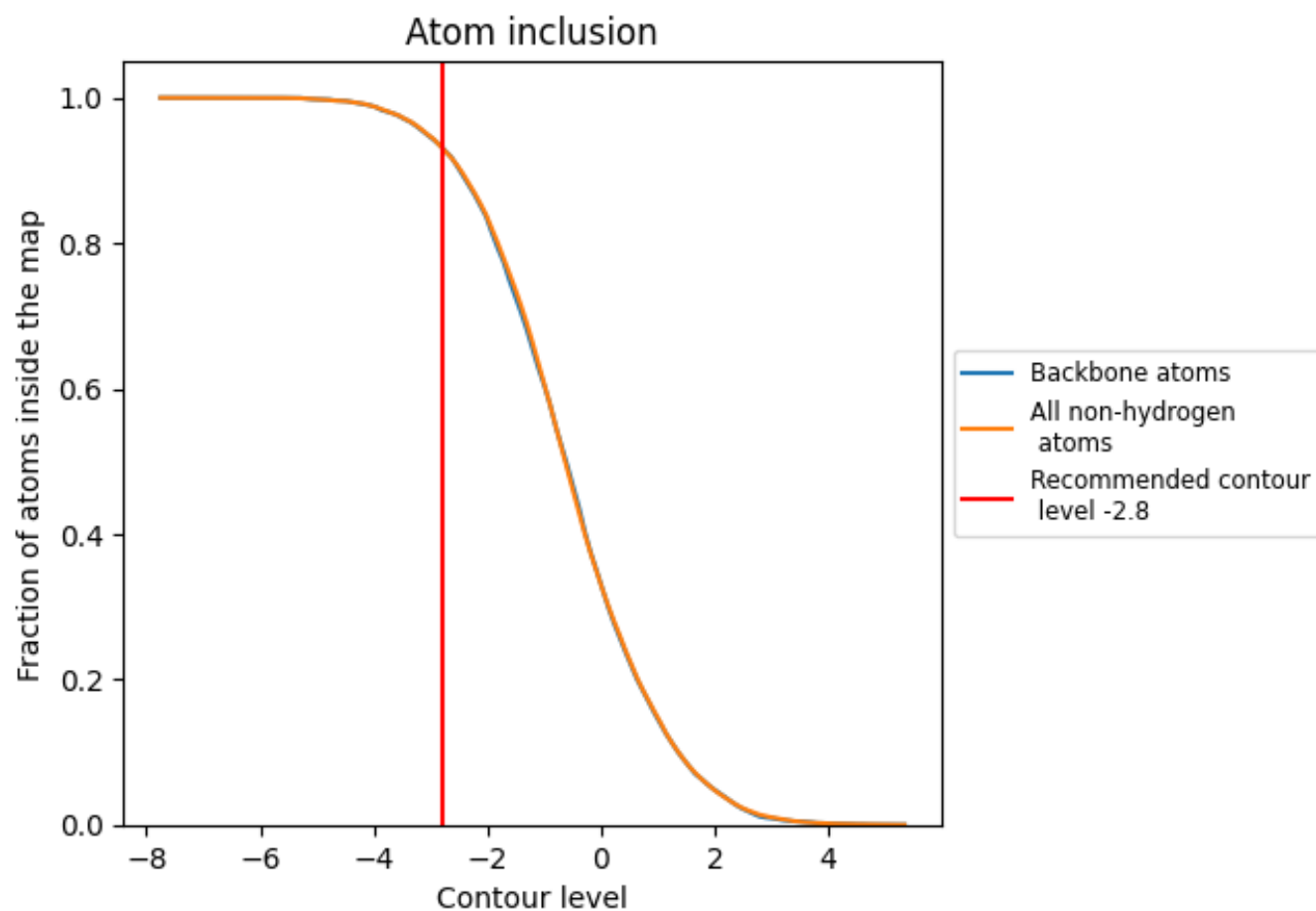
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 93% of all backbone atoms, 93% 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> 0.9312	<div><div></div></div> 0.0880
N	<div><div></div></div> 0.9315	<div><div></div></div> 0.0880

