



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 01:13 PM EST

PDB ID : 3J2D
EMDB ID : EMD-5506
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 : 18.70 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

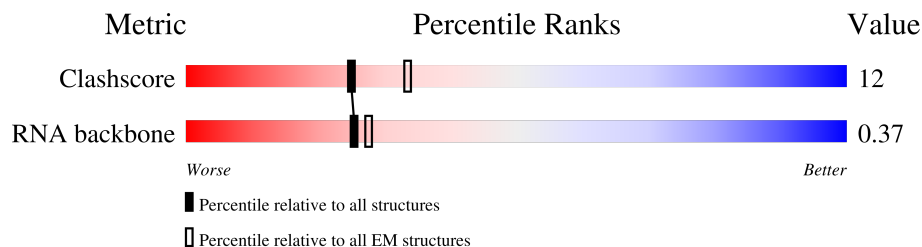
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 18.70 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.

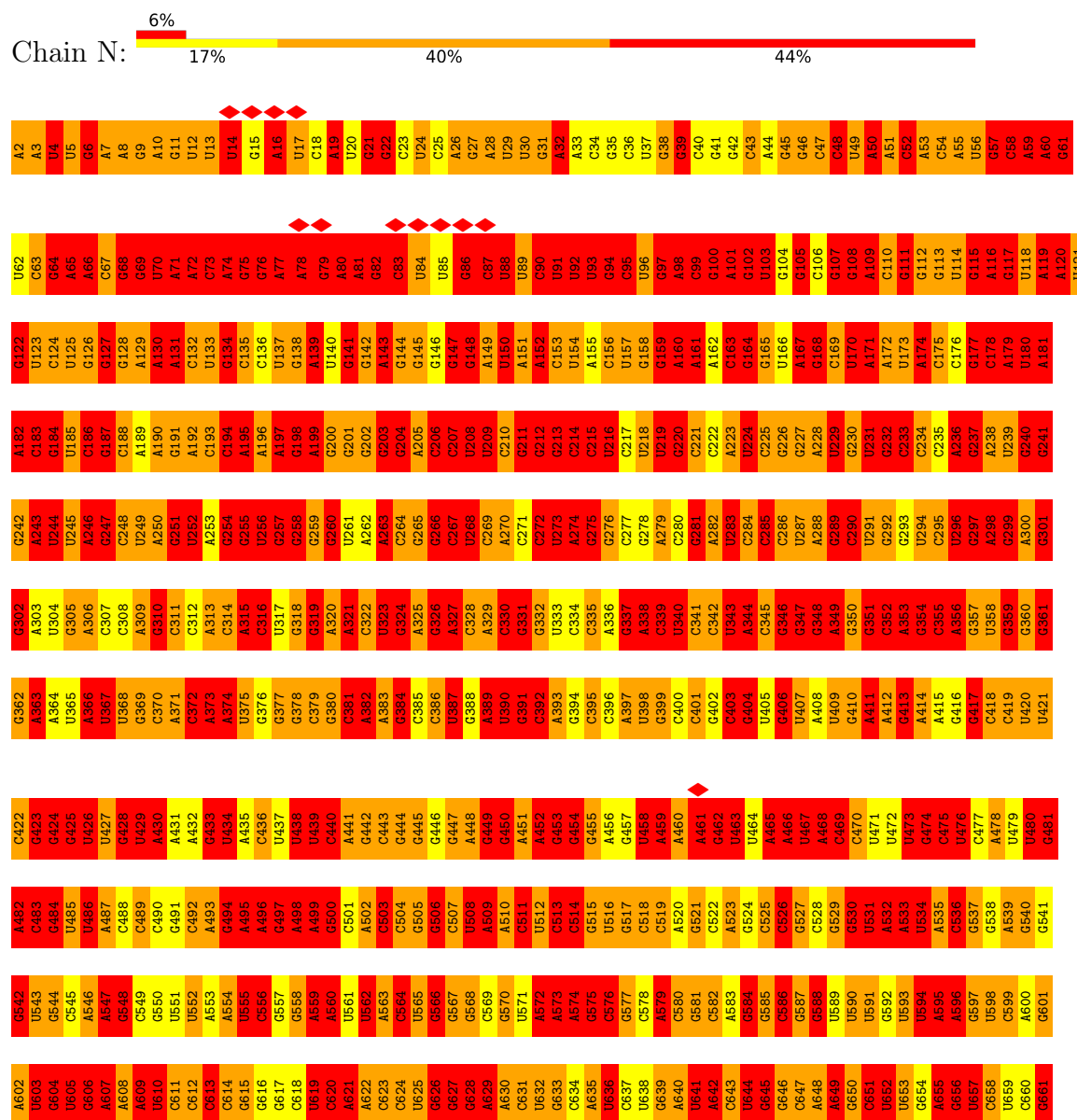
- Molecule 1 is a RNA chain called 16S rRNA.

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



G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	C1501
C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1440	C1441
G1322	G1323	G1324	G1325	G1326	G1327	G1328	G1329	G1330	G1331	G1332	G1333	G1334	G1335	G1336	G1337	G1338	G1339	G1340	G1341	G1342	G1343	G1344	G1345	G1346	G1347	G1348	G1349	G1350	G1351	G1352	G1353	G1354	G1355	G1356	G1357	G1358	G1359	G1360	G1361	G1362	G1363	G1364	G1365	G1366	G1367	G1368	G1369	G1370	G1371	G1372	G1373	G1374	G1375	G1376	G1377	G1378	G1379	G1380	G1381
C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	C1270	C1271	C1272	C1273	C1274	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287	C1288	C1289	C1290	C1291	C1292	C1293	C1294	C1295	C1296	C1297	C1298	C1299	C1300	C1301	C1302	C1303	C1304	C1305	C1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	C1318	C1319	C1320	C1321
G1142	G1143	G1144	G1145	G1146	G1147	G1148	G1149	G1150	G1151	G1152	G1153	G1154	G1155	G1156	G1157	G1158	G1159	G1160	G1161	G1162	G1163	G1164	G1165	G1166	G1167	G1168	G1169	G1170	G1171	G1172	G1173	G1174	G1175	G1176	G1177	G1178	G1179	G1180	G1181	G1182	G1183	G1184	G1185	G1186	G1187	G1188	G1189	G1190	G1191	G1192	G1193	G1194	G1195	G1196	G1197	G1198	G1199	G1200	G1201
A1082	U1083	G1084	U1085	G1086	G1087	G1088	G1089	U1090	U1091	A1092	A1093	G1094	U1095	G1096	G1097	G1098	G1099	G1100	A1101	A1102	G1103	G1104	A1105	G1106	G1107	G1108	G1109	A1110	A1111	C1112	C1113	C1114	U1115	U1116	U1117	U1118	C1119	G1120	U1121	U1122	U1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130	G1131	C1132	C1133	G1134	U1135	G1136	C1137	G1138	G1139	C1140	C1141
A1022	U1023	G1024	U1025	G1026	G1027	C1028	G1029	U1030	A1031	G1032	G1033	A1034	G1035	A1036	C1037	G1038	G1039	U1040	A1041	A1042	G1043	A1044	G1045	A1046	G1047	G1048	U1049	G1050	C1051	U1052	G1053	G1054	A1055	U1056	G1057	C1058	C1059	U1060	G1061	U1062	C1063	U1064	U1065	C1066	A1067	G1068	C1069	U1070	G1071	U1072	G1073	U1074	G1075	U1076	G1077	U1078	A1079	A1080	A1081
C962	G963	U964	U965	G966	C967	A968	A969	G970	G971	A972	G973	A974	A975	G976	A977	A978	C979	C980	U981	G982	A983	C984	C985	U986	G987	G988	C989	U990	C991	U992	G993	A994	C995	A996	U997	C998	C999	A1000	C1001	G1002	G1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	G1011	A1012	U1013	A1014	G1015	A1016	U1017	G1018	A1019	G1020	A1021
G902	G903	U904	U905	A906	A907	A908	A909	C910	U911	G912	A913	A914	A915	U916	A917	A918	A919	U920	G921	A922	A923	C924	G925	G926	G927	G928	C929	U930	C931	C932	G933	A934	A935	C936	A937	A938	C939	C940	G941	G942	U943	G944	G945	A946	G947	C948	A949	U950	G951	U952	G953	G954	U955	U956	U957	A958	A959	U960	U961
U842	U843	G844	A845	G846	G847	C848	C849	U850	G851	G852	C853	U854	U855	C856	G857	G858	G859	A860	G861	C862	U863	A864	A865	C866	G867	C868	G869	U870	U871	C872	A873	U874	C875	A876	A877	C878	C879	C880	G881	C882	C883	U884	G885	G886	G887	G888	A889	G890	U891	A892	C893	G894	G895	C896	U897	G898	C899	A900	A901
A782	C783	A784	G785	G786	G787	U788	U789	U790	G791	G792	C793	U794	C795	C796	G797	U798	G799	U800	U801	A802	G803	U804	C805	C806	G807	C808	G809	C810	C811	G812	U813	A814	C815	A816	C817	G818	A819	U820	G821	U822	G823	C824	A825	C826	U827	U828	G829	U830	A831	C832	G833	U834	G835	U836	U837	G838	C839	A840	C841
G722	U723	G724	G725	G726	G727	A728	U729	G730	C731	G732	C733	U734	C735	C736	C737	C738	U739	U740	G741	A742	C743	C744	G745	A746	G747	G748	A749	U750	C751	G752	A753	C754	G755	C756	U757	C758	A759	G760	G761	U762	G763	C764	G765	A766	A767	U768	G769	U770	C771	U772	G773	G774	U775	G776	U777	G778	C779	A780	U781
U662	A663	G664	A665	G666	G667	A668	G669	G670	G671	U672	A673	G674	A675	A676	U677	U678	U679	U680	A681	G682	C683	U684	G685	G686	U687	G688	A689	G690	C691	G692	G693	A694	A695	A696	U697	G698	C699	G700	U701	A702	G703	A704	G705	A706	U707	C708	U709	G710	G711	A712	U713	G714	A715	U716	U717	A718	C719	G720	G721

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	18809	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	4.826	Depositor
Minimum map value	-7.449	Depositor
Average map value	-4.686	Depositor
Map value standard deviation	0.703	Depositor
Recommended contour level	-2.3	Depositor
Map size (Å)	375.0, 375.0, 375.0	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	3.48	5387/36831 (14.6%)	4.00	9573/57458 (16.7%)

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	971

The worst 5 of 5387 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	778	G	N7-C5	-23.11	1.25	1.39
1	N	243	A	N7-C5	-20.09	1.27	1.39
1	N	382	A	N7-C5	-18.91	1.27	1.39
1	N	696	A	N7-C5	-18.62	1.28	1.39
1	N	809	G	C6-N1	18.30	1.52	1.39

The worst 5 of 9573 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	28	A	N1-C6-N6	28.37	135.62	118.60
1	N	94	G	P-O3'-C3'	27.41	152.59	119.70
1	N	1362	A	P-O3'-C3'	27.37	152.54	119.70
1	N	559	A	N1-C6-N6	26.79	134.68	118.60
1	N	468	A	N1-C6-N6	25.93	134.16	118.60

There are no chirality outliers.

5 of 971 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	10	A	Sidechain
1	N	11	G	Sidechain
1	N	2	A	Sidechain
1	N	4	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	16519	568	0
All	All	32892	16554	16519	568	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 568 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:1084:G:H5''	1:N:1099:G:H22	1.46	0.80
1:N:858:G:H1	1:N:869:G:H2'	1.51	0.75
1:N:1004:A:H5'	1:N:1024:G:H22	1.55	0.71
1:N:67:C:H2'	1:N:68:G:C8	2.25	0.71
1:N:1316:G:C2	1:N:1319:A:C8	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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	N	1532/1533 (99%)	454 (29%)	154 (10%)

5 of 454 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 154 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1191	A
1	N	1396	A
1	N	1224	U
1	N	1331	G
1	N	1506	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.

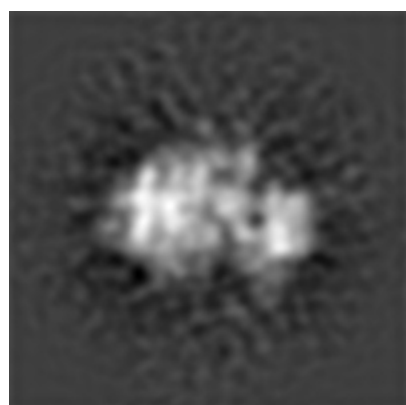
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5506. These allow visual inspection of the internal detail of the map and identification of artifacts.

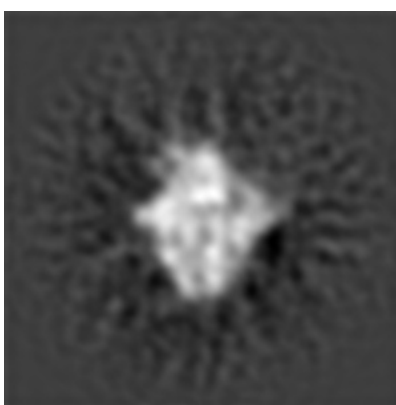
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

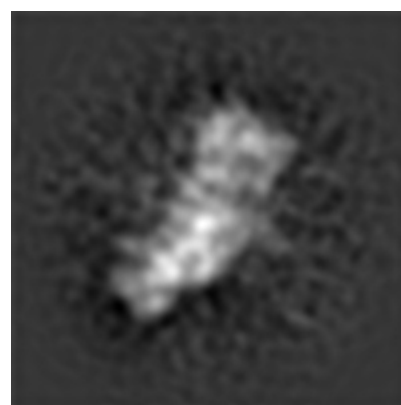
6.1.1 Primary map



X



Y

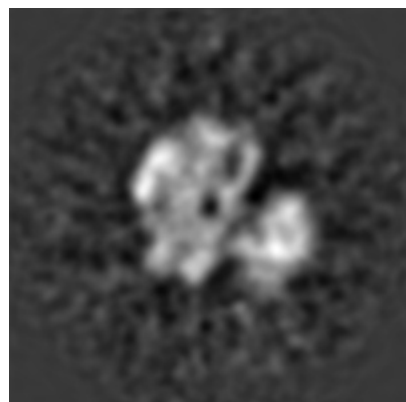


Z

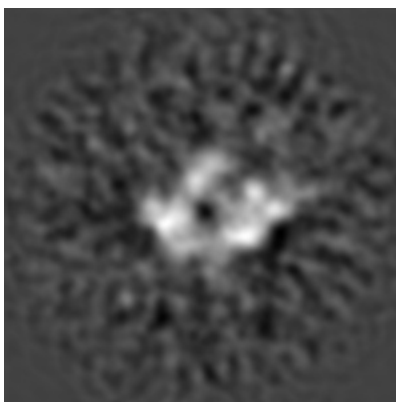
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

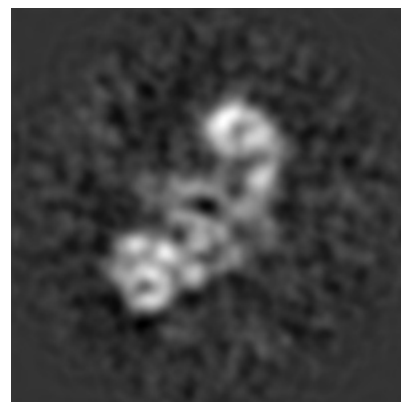
6.2.1 Primary map



X Index: 62



Y Index: 62

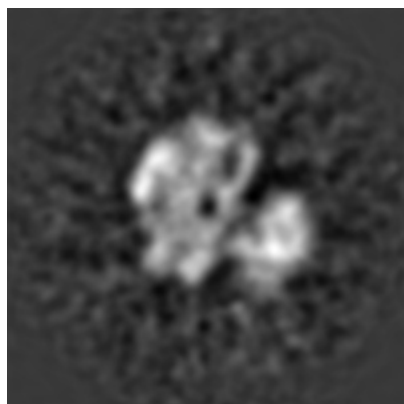


Z Index: 62

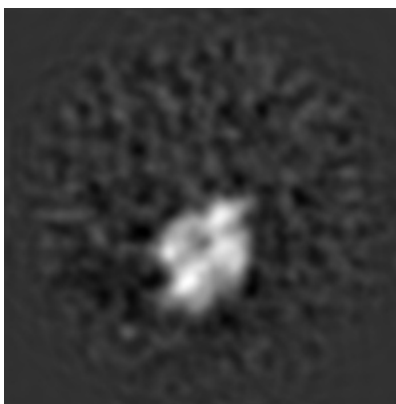
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

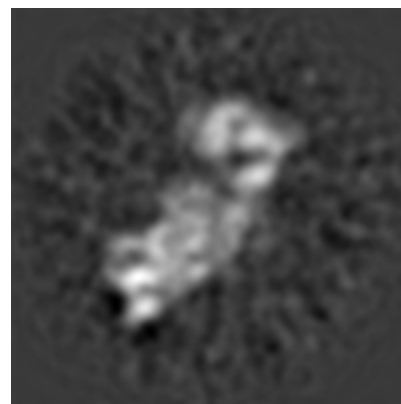
6.3.1 Primary map



X Index: 62



Y Index: 41

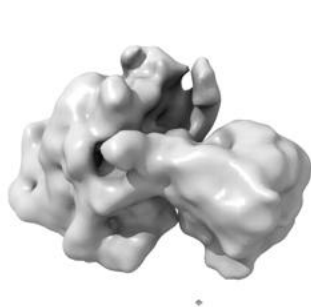


Z Index: 58

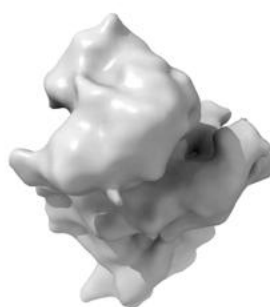
The images above show the largest variance slices of the map in three orthogonal directions.

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.

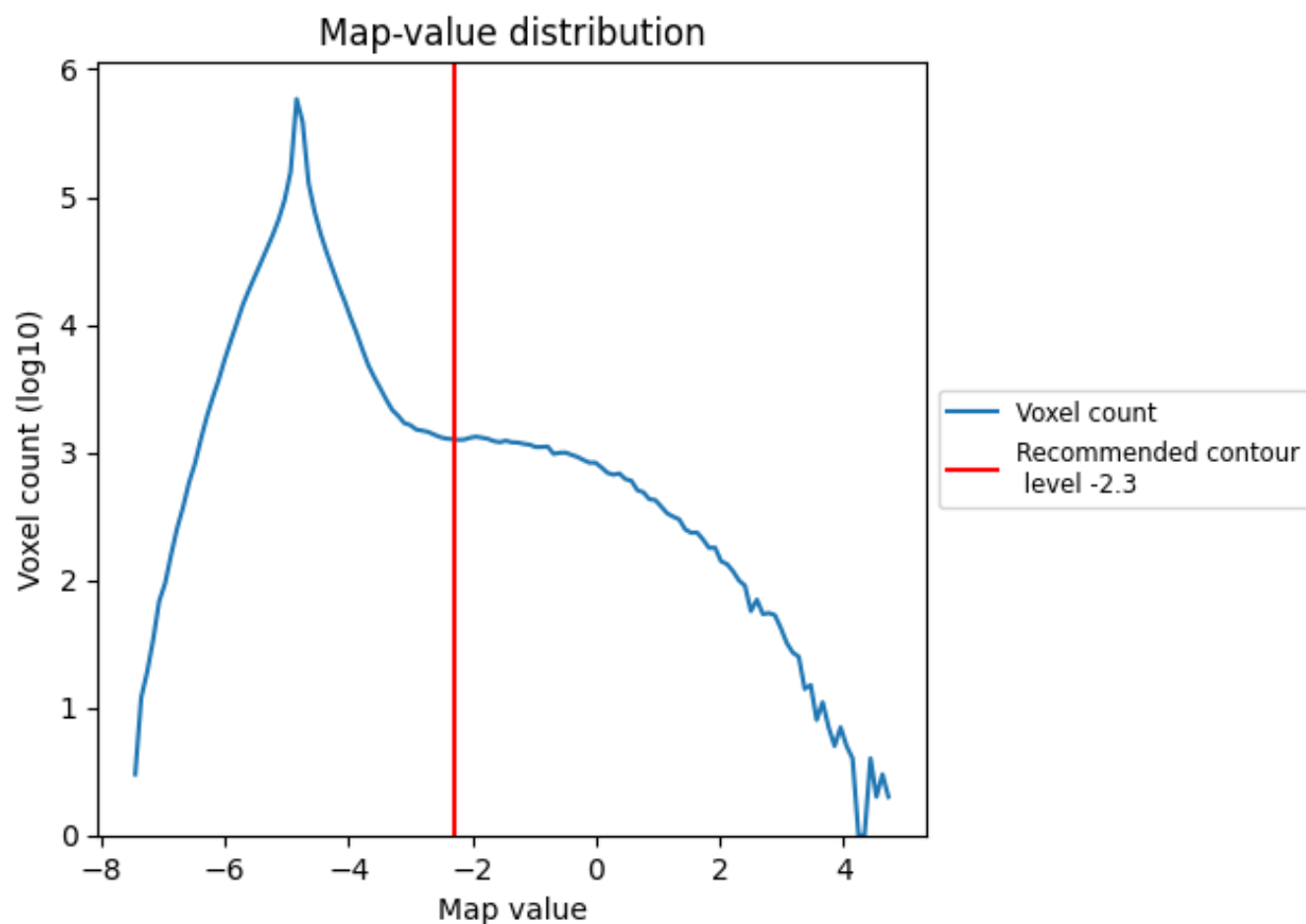
6.5 Mask visualisation

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

7 Map analysis [i](#)

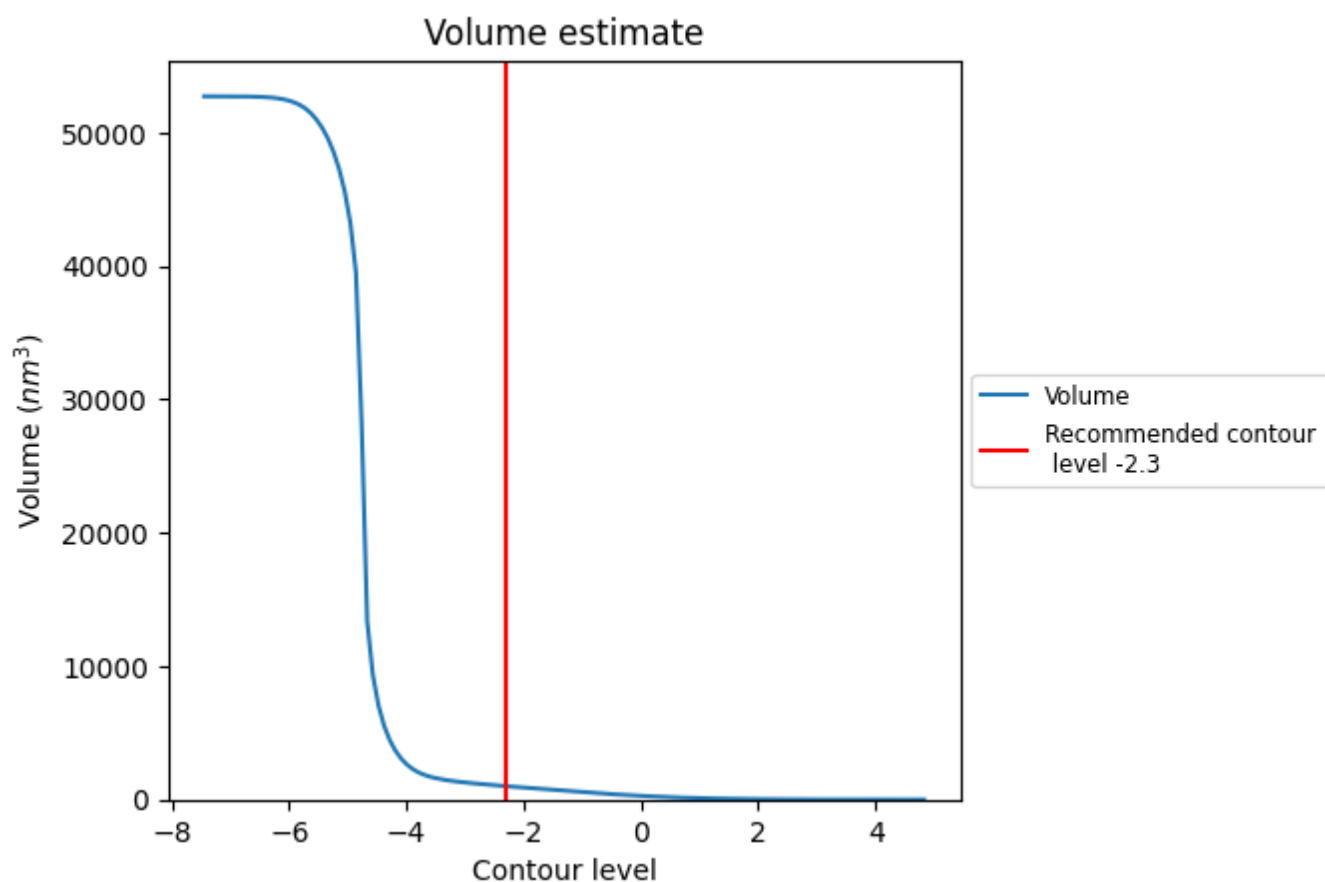
This section contains the results of statistical analysis of the map.

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.

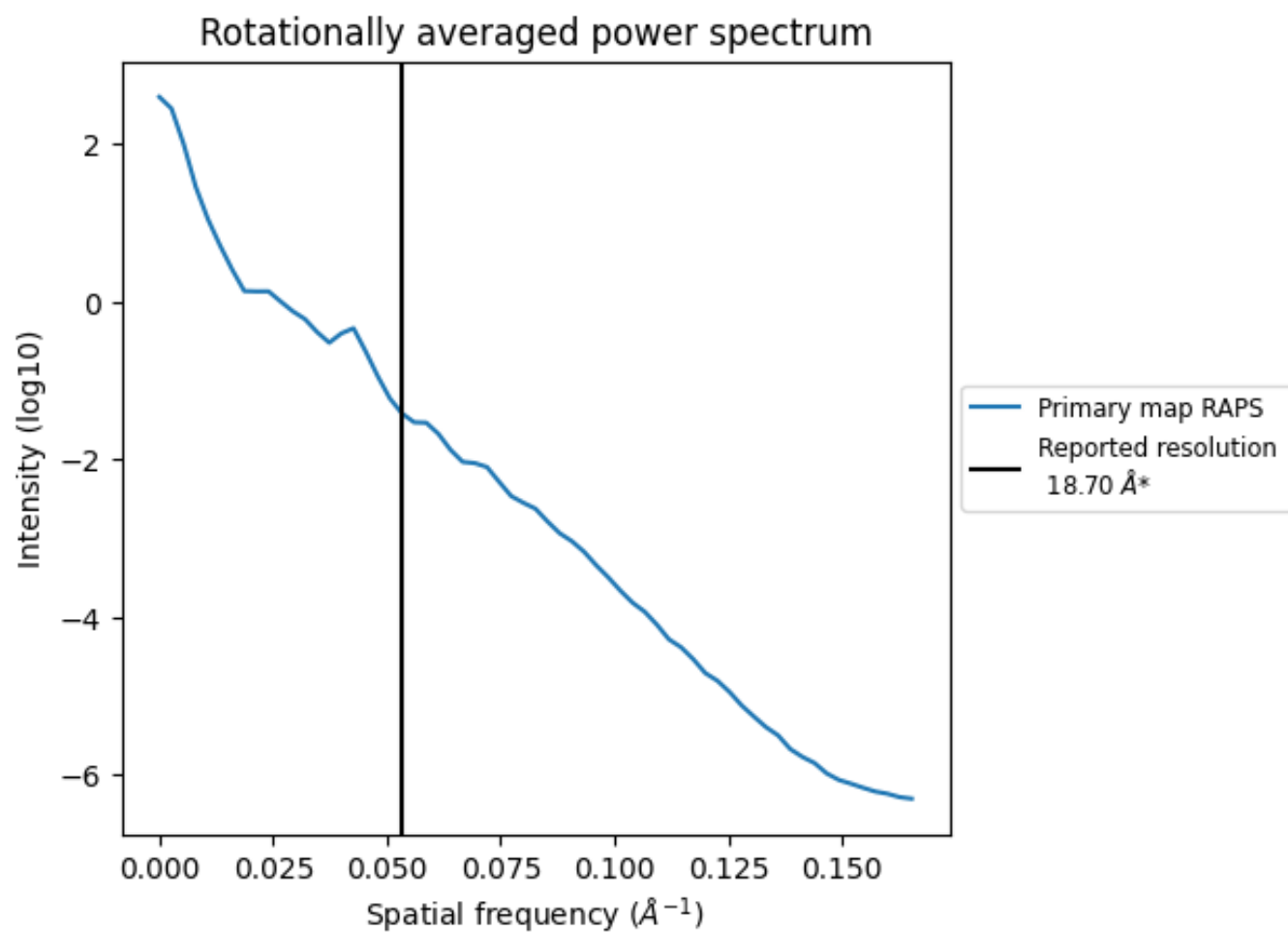
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1003 nm³; this corresponds to an approximate mass of 906 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

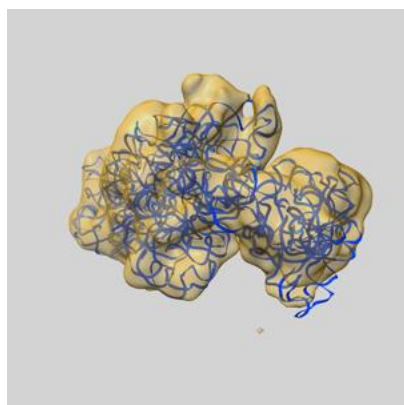
8 Fourier-Shell correlation

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

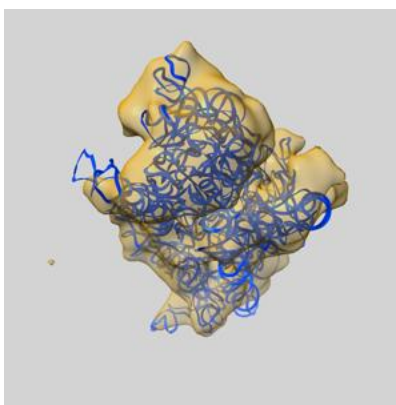
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5506 and PDB model 3J2D. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

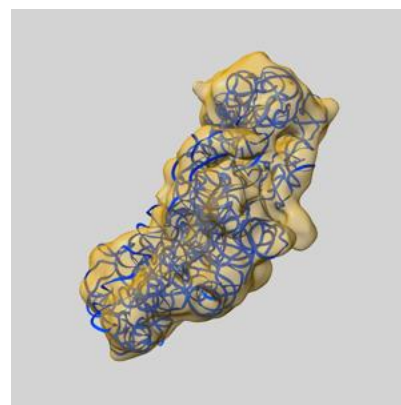
9.1 Map-model overlay [i](#)



X



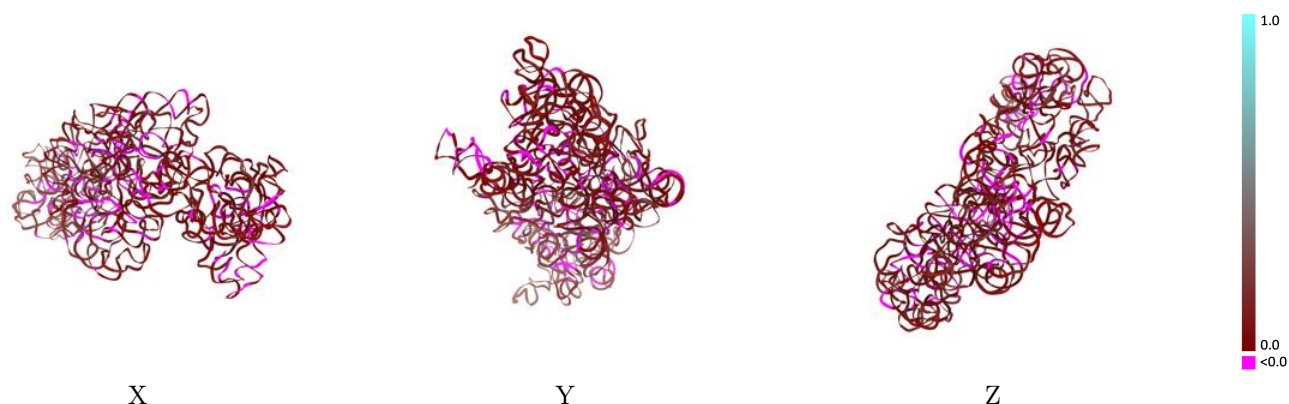
Y



Z

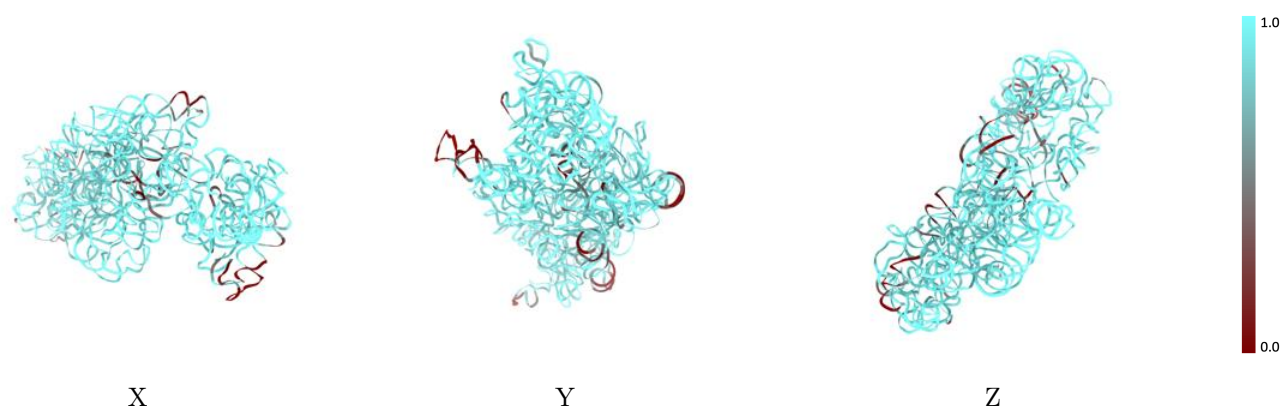
The images above show the 3D surface view of the map at the recommended contour level -2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



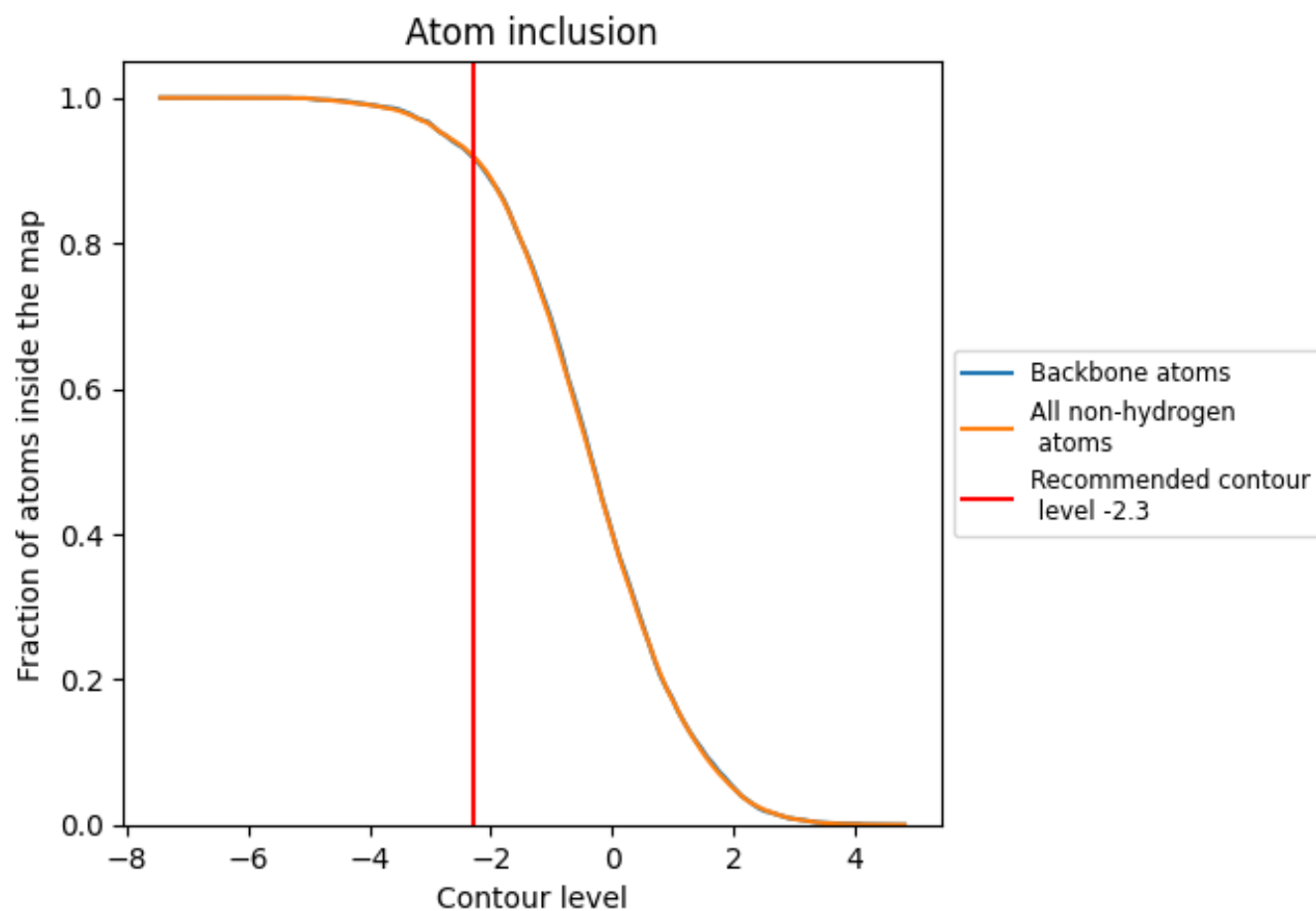
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (-2.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9206	<div></div> 0.0670
N	<div></div> 0.9207	<div></div> 0.0670

