



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 12:57 PM JST

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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

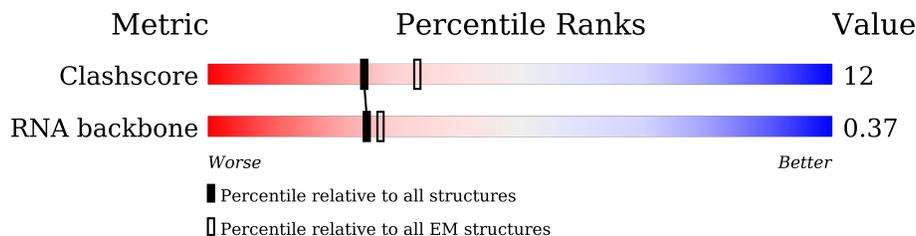
1 Overall quality at a glance

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.

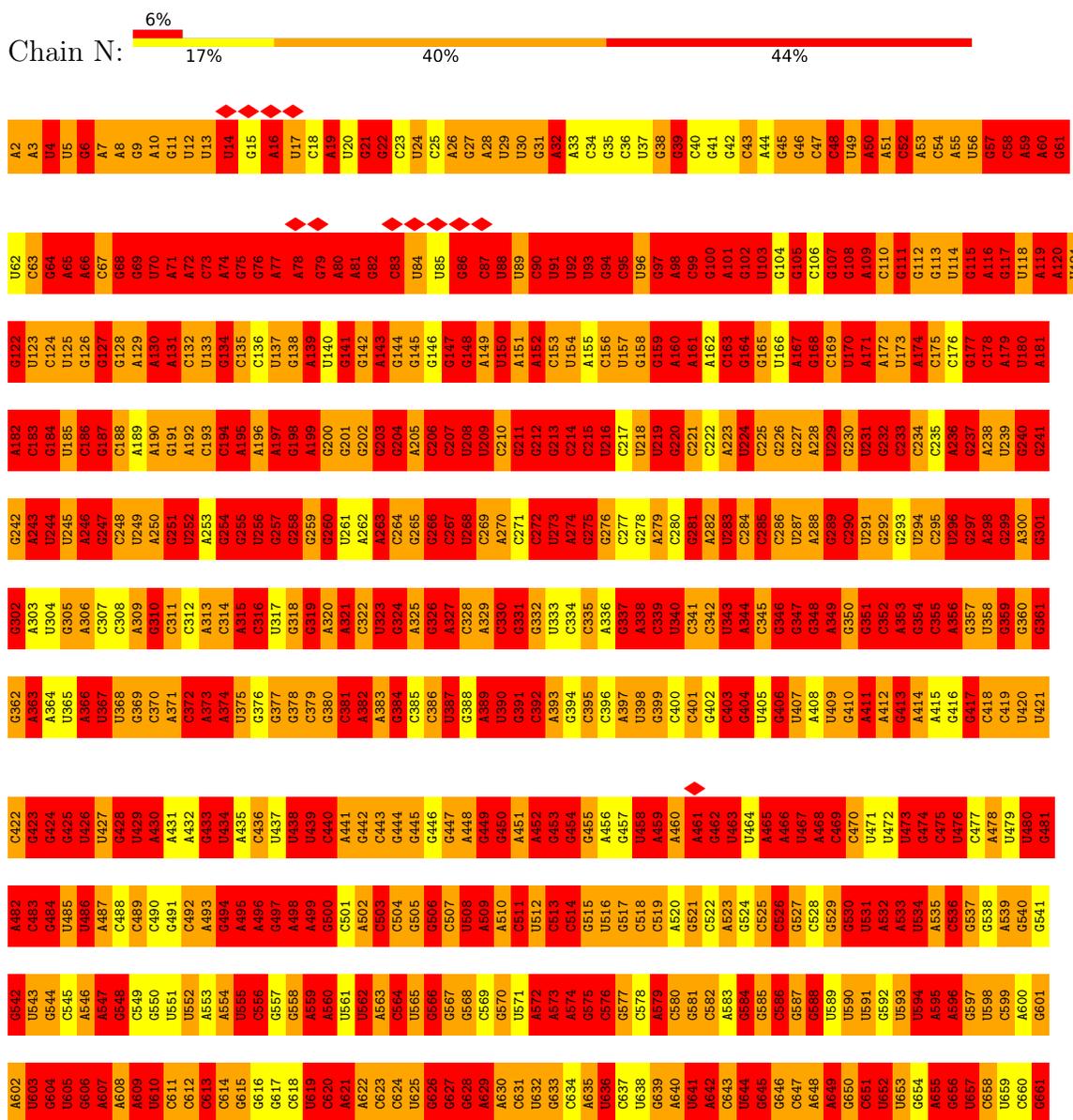
- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	N	1533	49446	14671	16554	6036	10653	1532	0	0

3 Residue-property plots i

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



U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033	U1034	U1035	U1036	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093	U1094	U1095	U1096	U1097	U1098	U1099	U1100	U1101	U1102	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	C1501
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A1502	A1503	G1504	G1505	U1506	A1507	A1508	C1509	C1510	G1511	G1512	A1513	G1514	G1515	G1516	G1517	A1518	A1519	C1520	C1521	U1522	G1523	C1524	G1525	G1526	U1527	U1528	G1529	G1530	A1531	U1532	C1533	A1534
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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	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 (\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	3.48	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 [i](#)

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 [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.

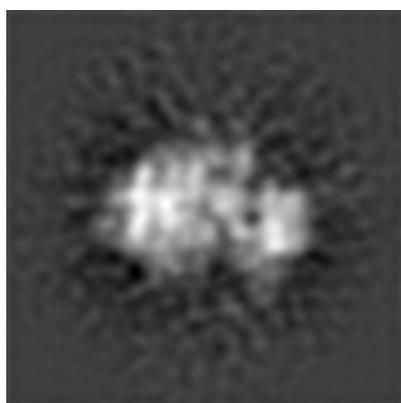
6 Map visualisation [i](#)

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

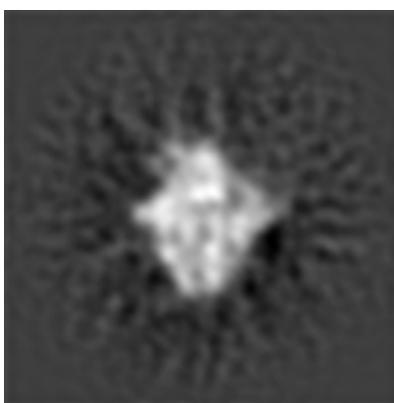
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

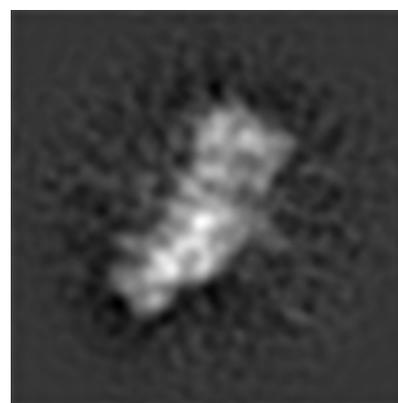
6.1.1 Primary map



X



Y

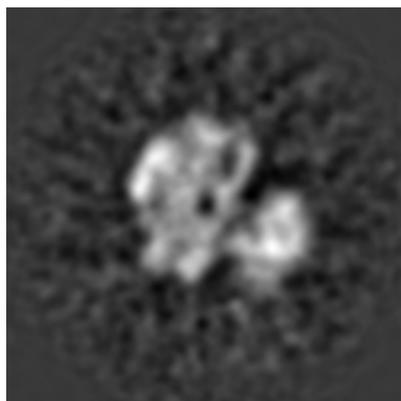


Z

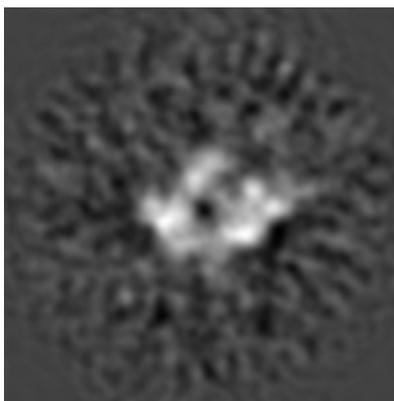
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

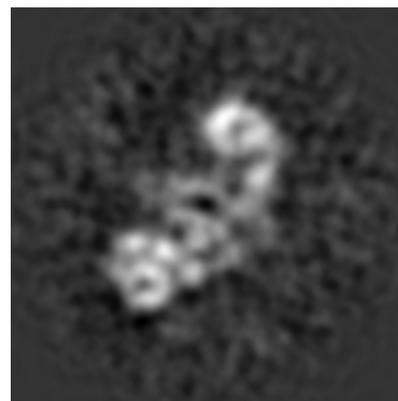
6.2.1 Primary map



X Index: 62



Y Index: 62

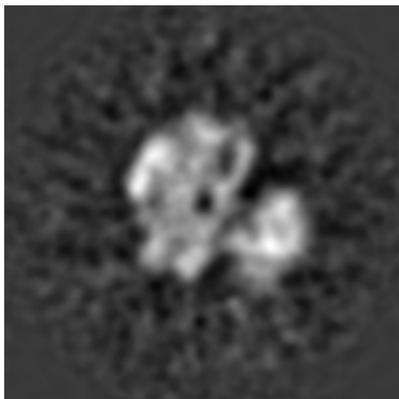


Z Index: 62

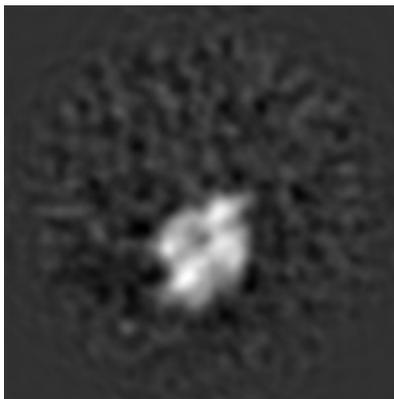
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

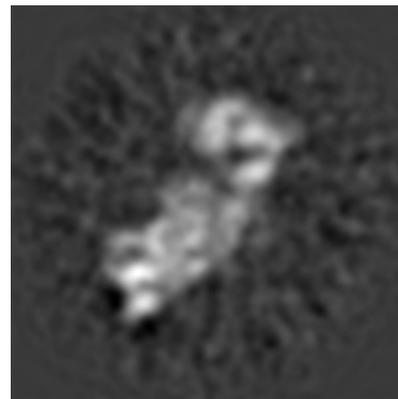
6.3.1 Primary map



X Index: 62



Y Index: 41

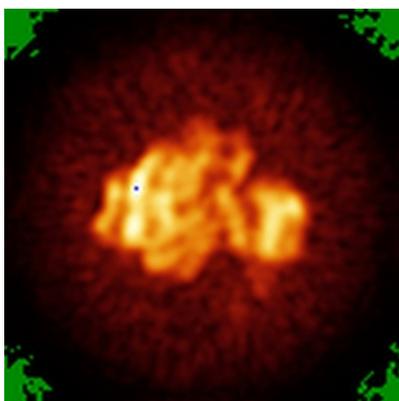


Z Index: 58

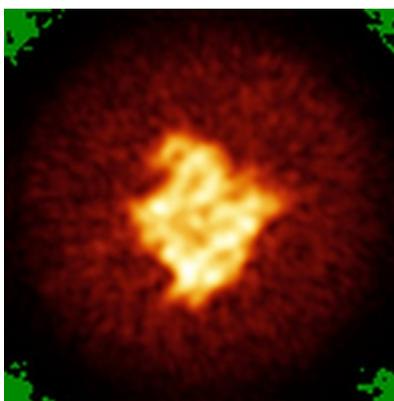
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

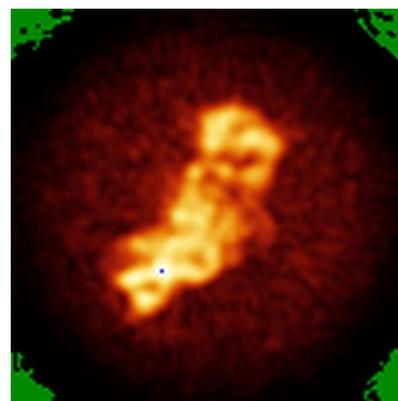
6.4.1 Primary map



X



Y

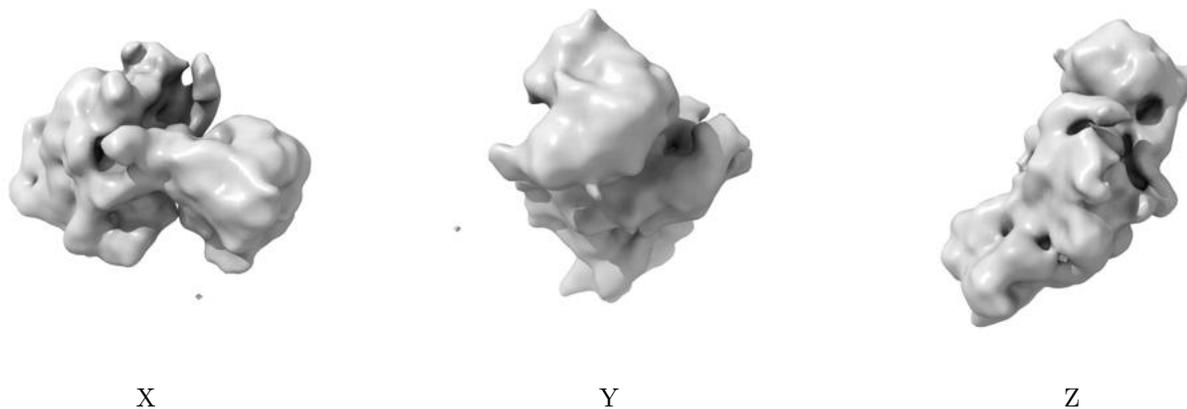


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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.

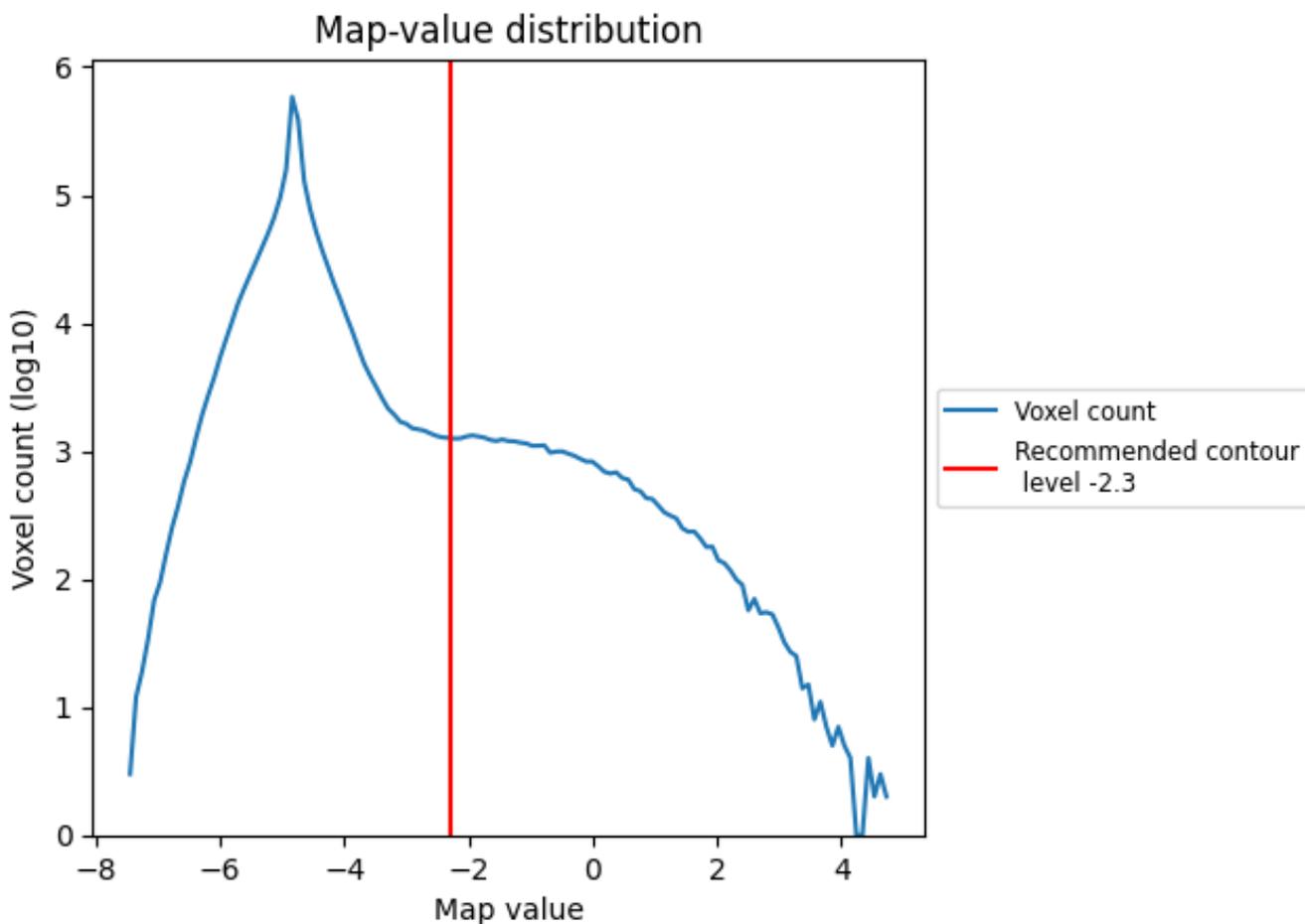
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

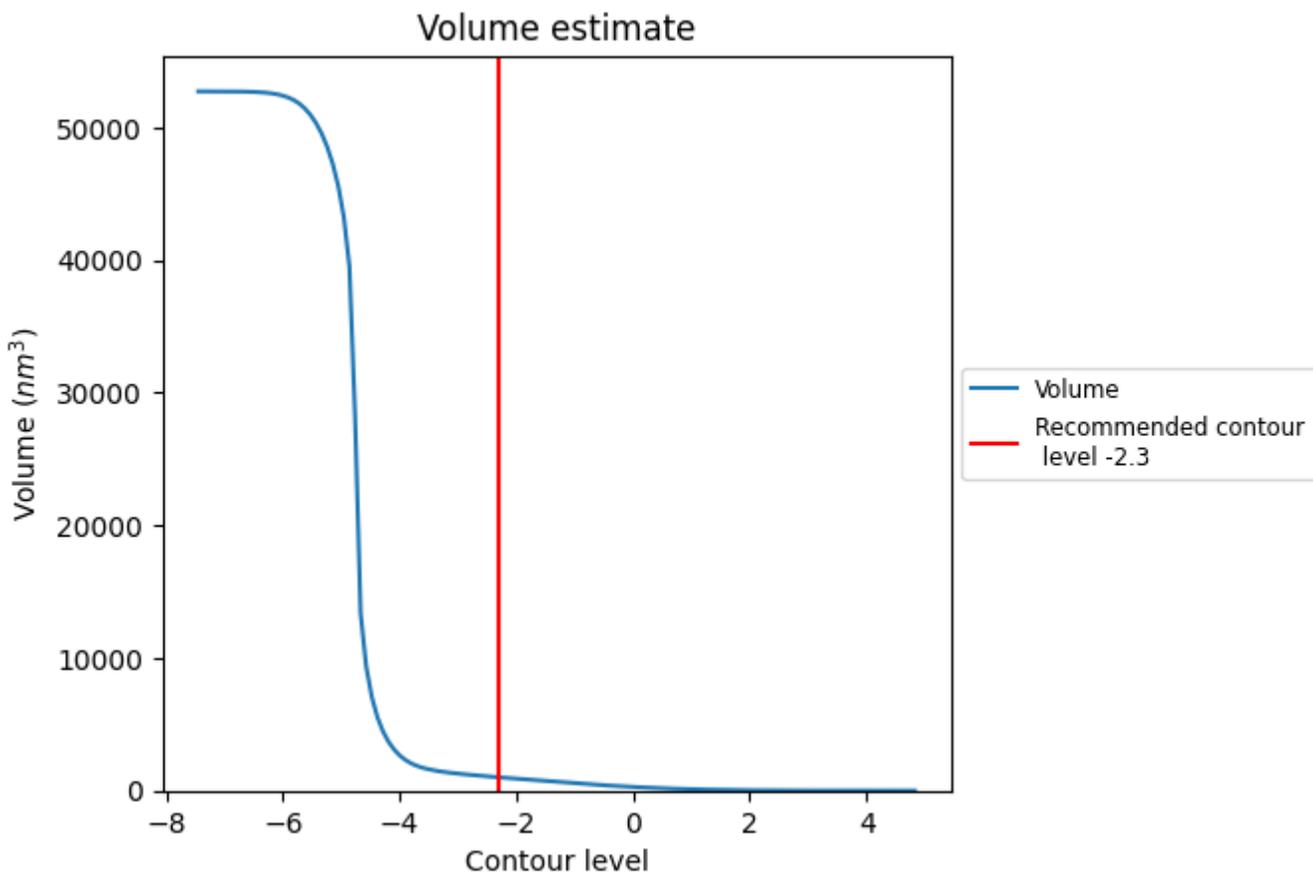
This section contains the results of statistical analysis of the map.

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.

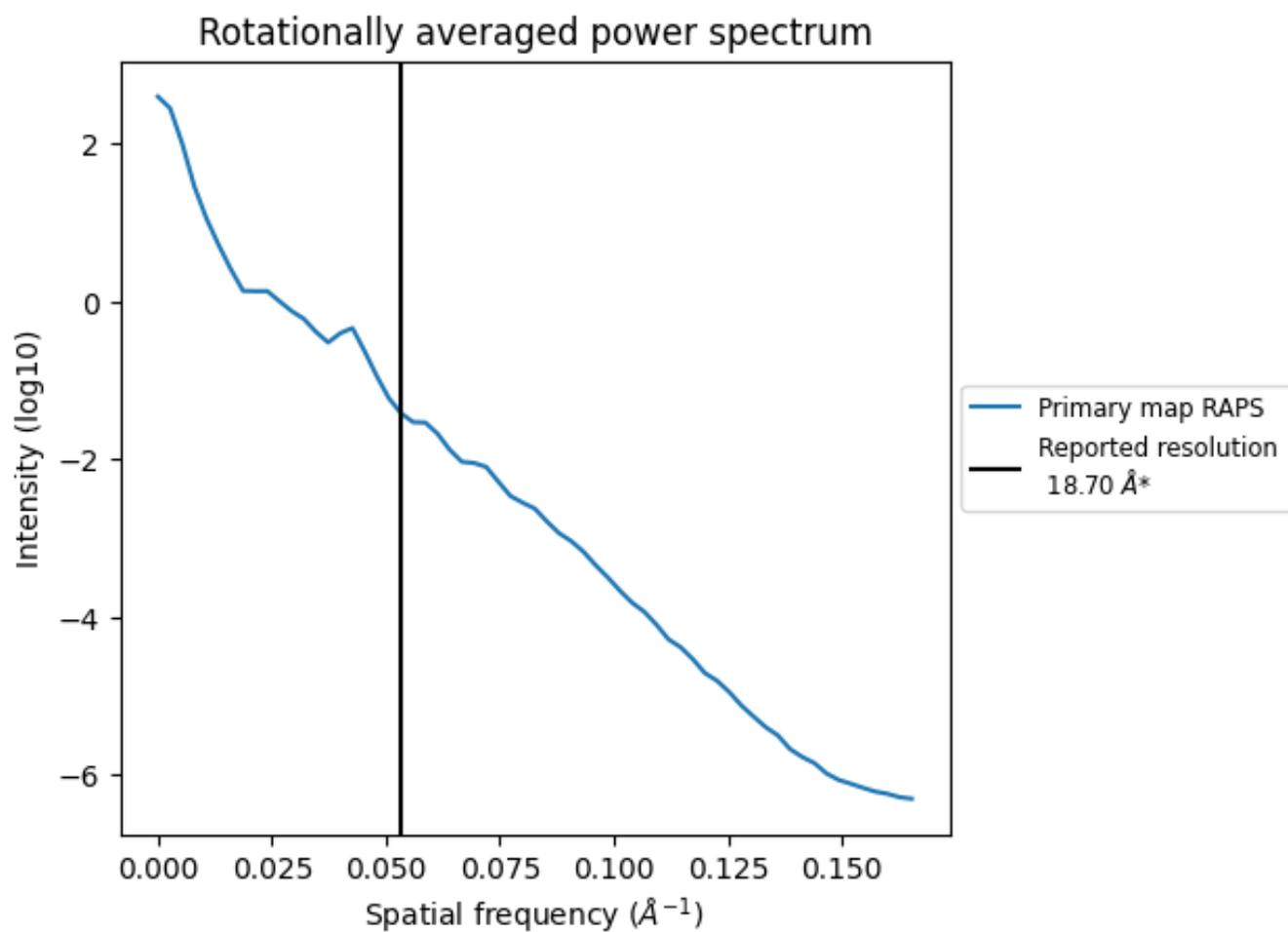
7.2 Volume estimate [i](#)



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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.053 Å⁻¹

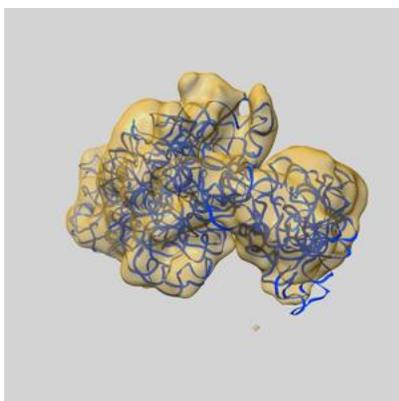
8 Fourier-Shell correlation

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

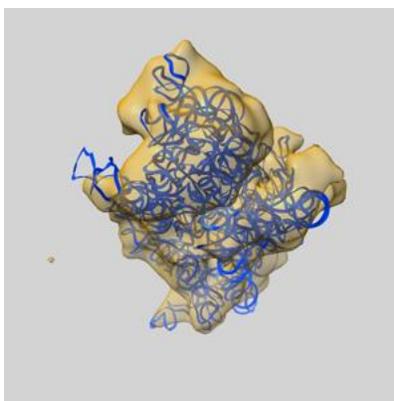
9 Map-model fit [i](#)

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](#).

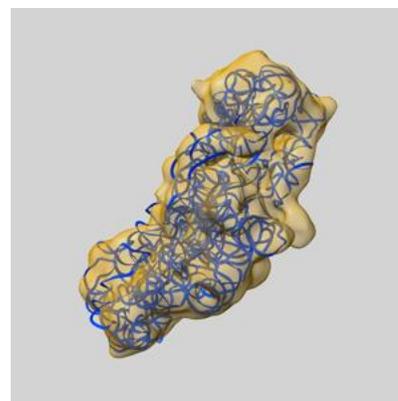
9.1 Map-model overlay [i](#)



X



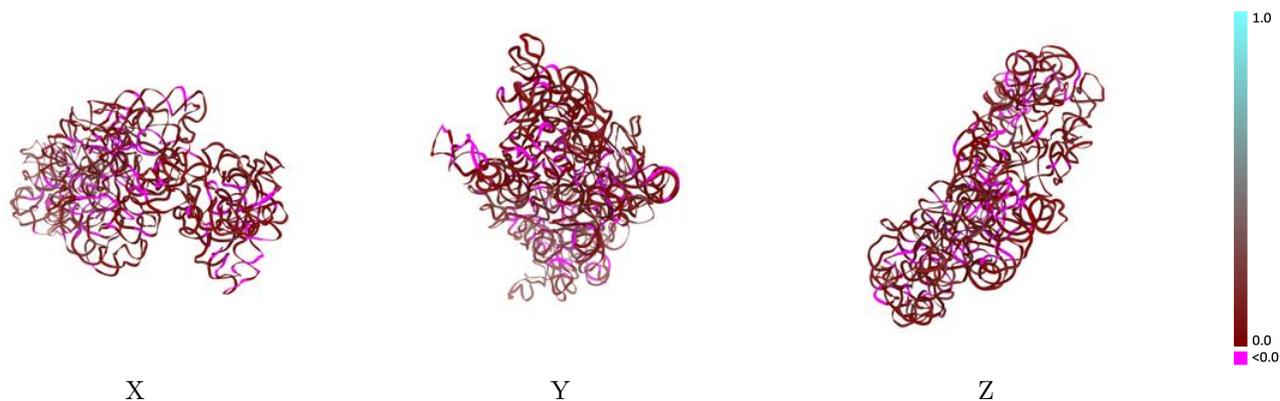
Y



Z

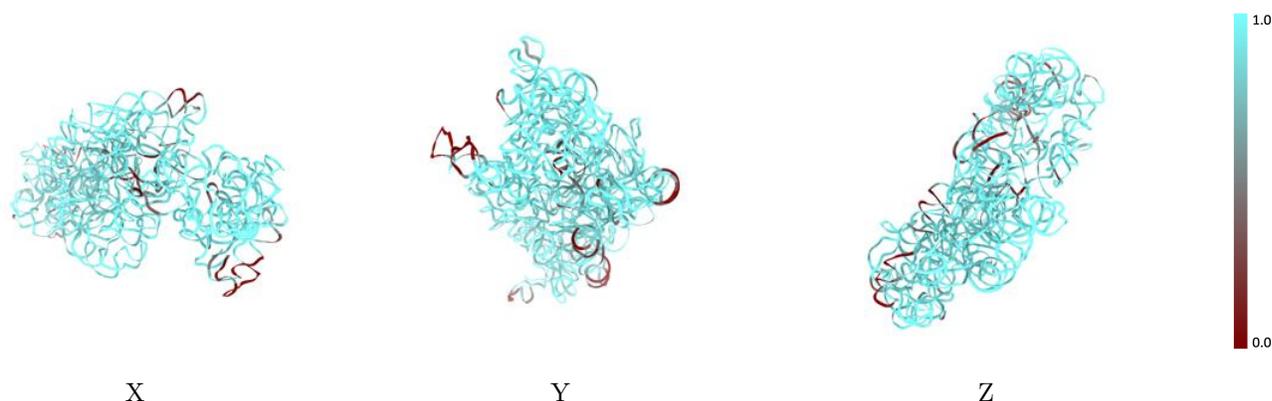
The images above show the 3D surface view of the map at the recommended contour level -2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



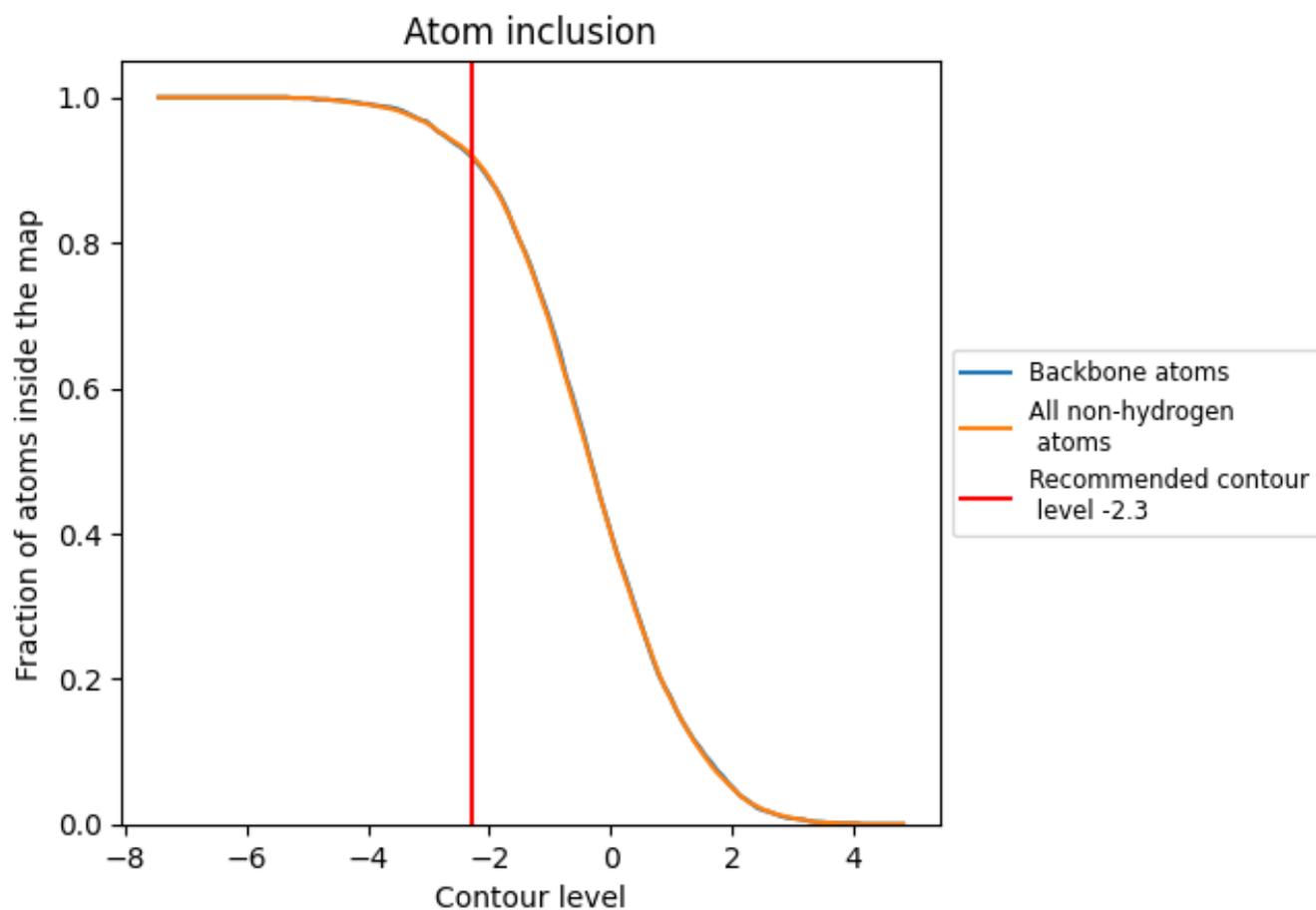
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9210	 0.0670
N	 0.9210	 0.0670

