wwPDB EM Validation Summary Report (i)

Mar 13, 2024 – 12:40 PM JST

PDB ID	:	3J2H
EMDB ID	:	EMD-5510
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	:	18.80 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 (i) 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 (i)) were used in the production of this report:

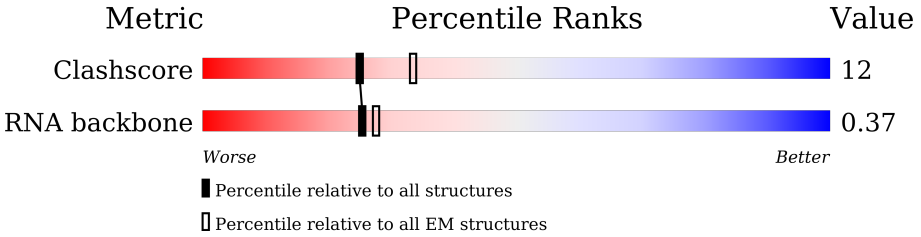
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 18.80 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 <=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 (i)

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.

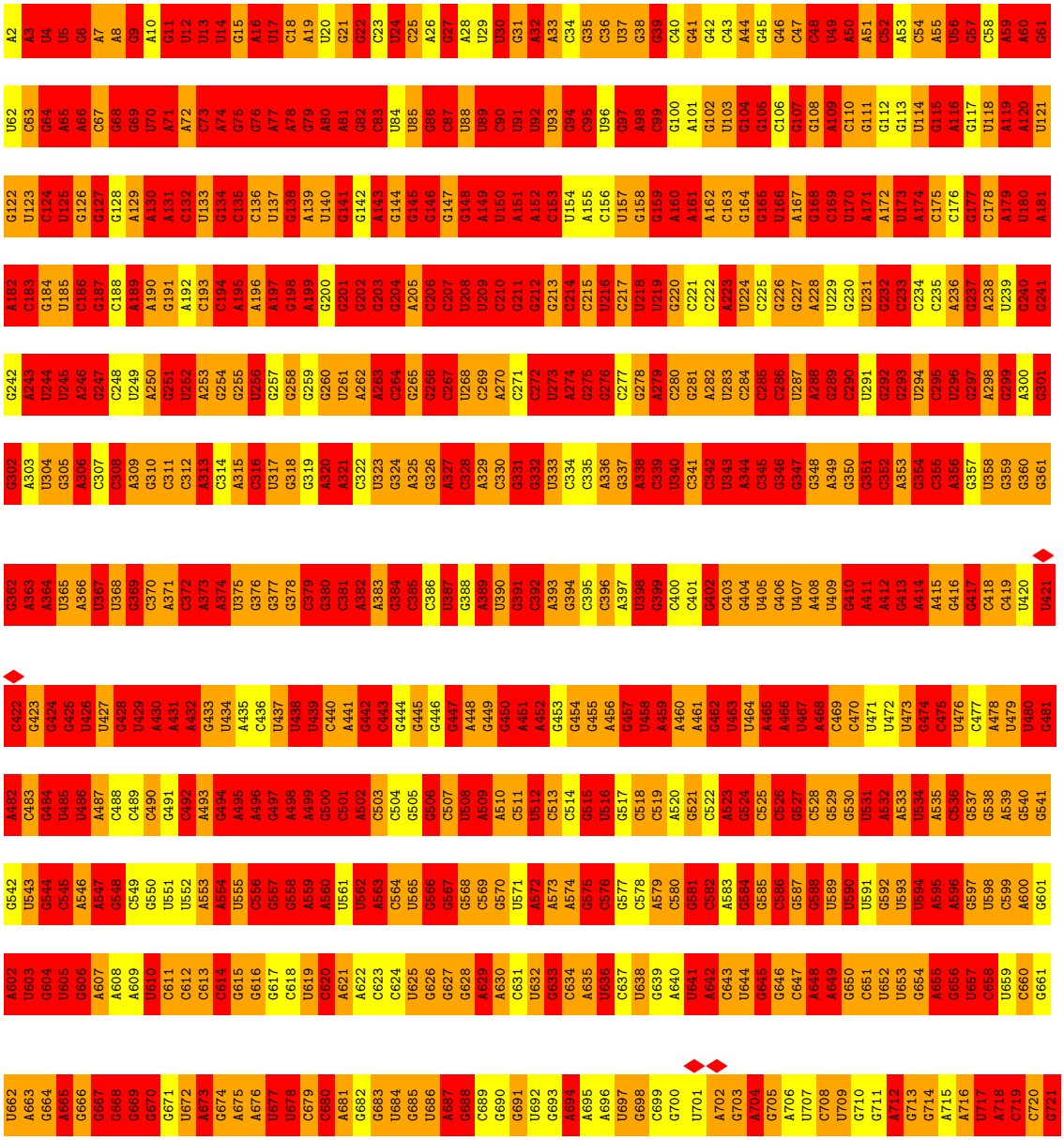
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	N	1533	49446	14671	16554	6036	10653	1532	0	0

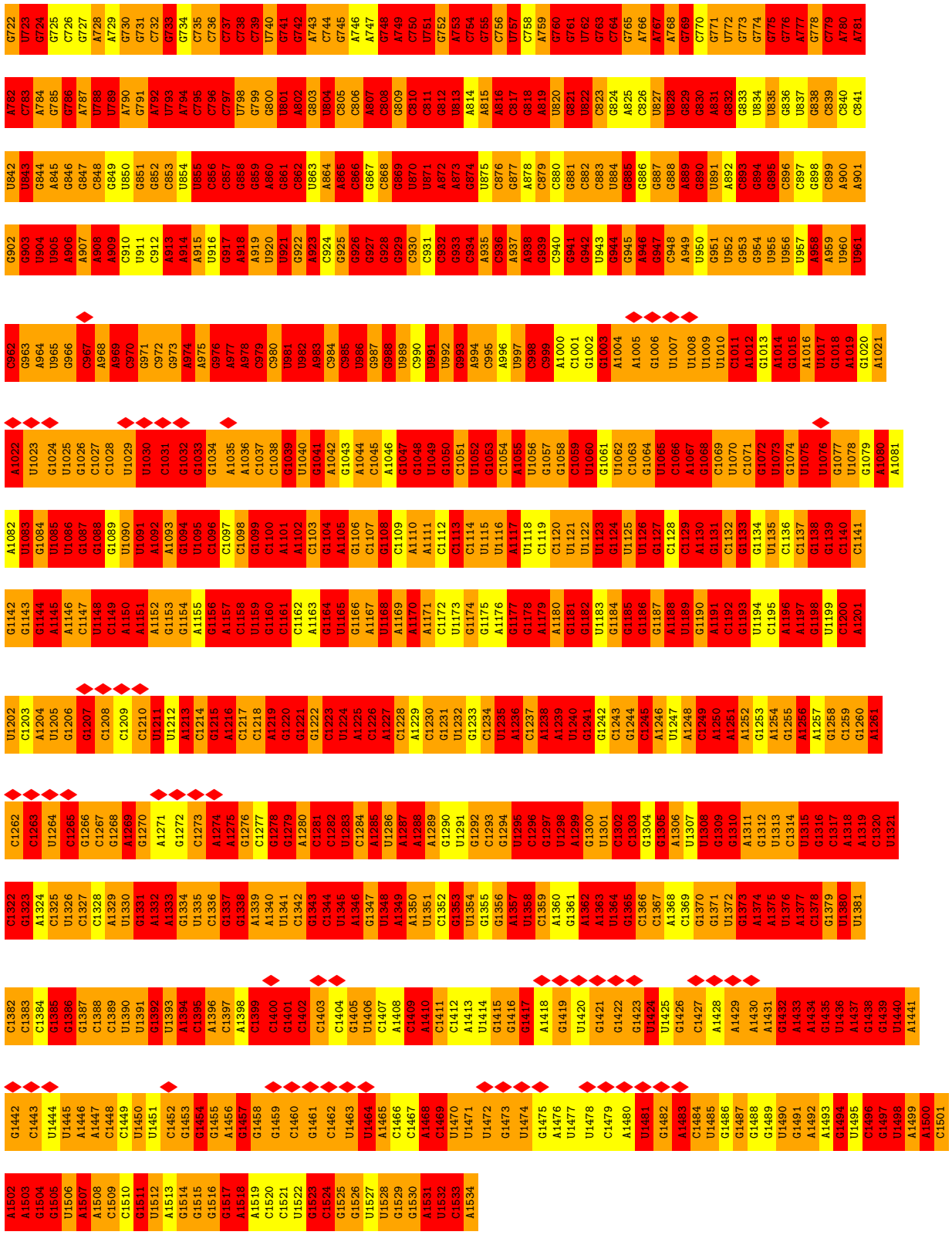
3 Residue-property plots (i)

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

Chain N: 17% 38% 45%




G722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 G733 G734 C735 C736 C737 C738 C739 U740 G741 G742 A743 C744 G745 A746 A747 G748 A749 C750 U751 G752 A753 C754 G755 C756 U757 C758 A759 G760 G761 U762 G763 C764 G765 A766 A767 A768 G769 C770 G771 U772 G773 G774 G775 G776 A777 G778 C779 A780 A781
A782 C783 A784 G785 G786 A787 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 U798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 G812 U813 A814 A815 A816 C817 G818 A819 U820 G821 U822 C823 G824 A825 C826 U827 U828 G829 G830 A831 G832 G833 U834 U835 G836 U837 G838 C839 C840 C841
U842 U843 G844 A845 G846 G847 C848 G849 U850 G851 C852 C853 U854 U855 C856 C857 G858 G859 A860 G861 G862 U863 A864 A865 C866 G867 G868 G869 U870 U871 A872 A873 G874 U875 C876 G877 A878 G879 C880 G881 C882 C883 U884 G885 G886 G887 G888 A889 G890 U891 A892 C893 G894 G895 U896 C897 G898 C899 A900 A901
G902 G903 U904 U905 A906 A907 A908 A909 C910 U911 C912 A913 A914 A915 U916 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 U942 U943 G944 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961
C962 G963 A964 U965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 U986 G987 G988 U989 C990 U991 U992 G993 A994 C995 A996 U997 C998 C999 A1000 C1001 G1002 G1003 A1004 A1005 G1006 U1007 U1008 U1009 U1010 C1011 A1012 G1013 A1014 G1015 A1016 U1017 G1018 A1019 G1020 A1021
A1022 U1023 G1024 U1025 G1026 C1027 C1028 U1029 U1030 A1031 G1032 G1033 G1034 A1035 A1036 C1037 C1038 G1039 U1040 G1041 A1042 G1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 U1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1074 U1075 U1076 G1077 U1078 G1079 A1080 A1081
A1082 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 A1105 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1113 C1114 U1115 U1116 A1117 U1118 C1119 C1120 U1121 U1122 U1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 C1136 C1137 G1138 G1139 C1140 C1141
G1142 G1143 G1144 A1145 A1146 C1147 U1148 C1149 A1150 A1151 A1152 G1153 G1154 A1155 G1156 A1157 C1158 U1159 G1160 C1161 C1162 A1163 G1164 U1165 G1166 A1167 U1168 A1169 A1170 A1171 C1172 U1173 G1174 G1175 A1176 G1177 G1178 A1179 A1180 G1181 G1182 U1183 G1184 G1185 G1186 G1187 A1188 U1189 G1190 A1191 C1192 G1193 U1194 C1195 A1196 A1197 G1198 U1199 C1200 A1201
U1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 A1216 C1217 C1218 A1219 G1220 G1221 G1222 C1223 U1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240 G1241 G1242 C1243 G1244 C1245 A1246 U1247 A1248 C1249 A1250 A1251 A1252 G1253 A1254 G1255 A1256 A1257 G1258 C1259 G1260 A1261
C1262 C1263 U1264 C1265 G1266 C1267 G1268 A1269 G1270 A1271 G1272 C1273 A1274 A1275 G1276 C1277 G1278 G1279 A1280 C1281 C1282 U1283 C1284 A1285 U1286 A1287 A1288 A1289 G1290 U1291 G1292 C1293 G1294 U1295 C1296 G1297 U1298 A1299 G1300 U1301 C1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 A1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 U1321
C1322 G1323 A1324 C1325 U1326 C1327 C1328 A1329 U1330 G1331 A1332 A1333 G1334 U1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 A1346 G1347 U1348 A1349 A1350 U1351 C1352 G1353 U1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 A1362 A1363 U1364 G1365 C1366 C1367 A1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 C1378 G1379 U1380 U1381
C1382 C1383 C1384 G1385 G1386 G1387 C1388 C1389 U1390 U1391 G1392 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 A1408 C1409 A1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 A1418 G1419 U1420 G1421 G1422 G1423 U1424 U1425 G1426 C1427 A1428 A1429 A1430 A1431 G1432 A1433 A1434 G1435 U1436 A1437 G1438 G1439 U1440 A1441
G1442 C1443 U1444 U1445 A1446 A1447 C1448 C1449 U1450 U1451 C1452 G1453 G1454 G1455 A1456 G1457 G1458 G1459 C1460 G1461 C1462 U1463 U1464 A1465 C1466 C1467 A1468 C1469 U1470 U1471 U1472 G1473 G1474 G1475 A1476 U1477 U1478 C1479 A1480 U1481 G1482 A1483 C1484 U1485 G1486 G1487 G1488 G1489 G1490 G1491 A1492 A1493 G1494 U1495 G1496 G1497 U1498 A1499 A1500 C1501
A1502 A1503 G1504 G1505 U1506 A1507 A1508 C1509 C1510 G1511 U1512 A1513 G1514 G1515 G1516 G1517 A1518 A1519 C1520 C1521 U1522 G1523 C1524 G1525 G1526 U1527 U1528 G1529 G1530 A1531 U1532 C1533 A1534

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11474	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 ($e^-/Å^2$)	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	4.629	Depositor
Minimum map value	-7.414	Depositor
Average map value	-4.262	Depositor
Map value standard deviation	0.653	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	3.47	5192/36831 (14.1%)	3.99	9508/57458 (16.5%)

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	978

The worst 5 of 5192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	815	A	N7-C5	-18.92	1.27	1.39
1	N	435	A	N7-C5	-18.59	1.28	1.39
1	N	572	A	N7-C5	-18.24	1.28	1.39
1	N	367	U	C2-N3	17.85	1.50	1.37
1	N	202	G	N7-C5	16.97	1.49	1.39

The worst 5 of 9508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	567	G	C5-C6-O6	-27.97	111.82	128.60
1	N	184	G	N1-C6-O6	26.91	136.04	119.90
1	N	184	G	C5-C6-O6	-26.87	112.48	128.60
1	N	567	G	N1-C6-O6	25.95	135.47	119.90
1	N	713	G	N1-C6-O6	24.64	134.69	119.90

There are no chirality outliers.

5 of 978 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	3	A	Sidechain
1	N	4	U	Sidechain
1	N	5	U	Sidechain
1	N	6	G	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	16521	571	0
All	All	32892	16554	16521	571	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 571 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:32:A:H4'	1:N:48:C:H42	1.50	0.75
1:N:594:U:C4	1:N:595:A:C6	2.74	0.75
1:N:338:A:H61	1:N:351:G:H1	1.36	0.73
1:N:116:A:H61	1:N:313:A:H1'	1.53	0.73
1:N:197:A:H2	1:N:198:G:C4	2.08	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%)	449 (29%)	152 (9%)

5 of 449 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 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	N	1189	U
1	N	1432	G
1	N	1224	U
1	N	1319	A
1	N	1532	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 (i)

There are no chain breaks in this entry.

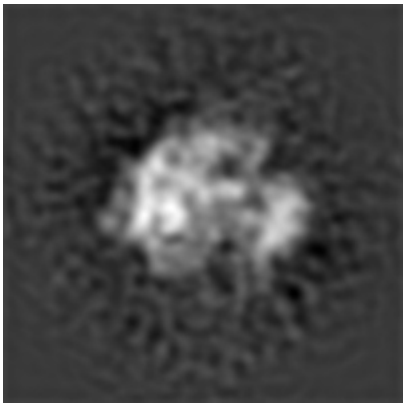
6 Map visualisation (i)

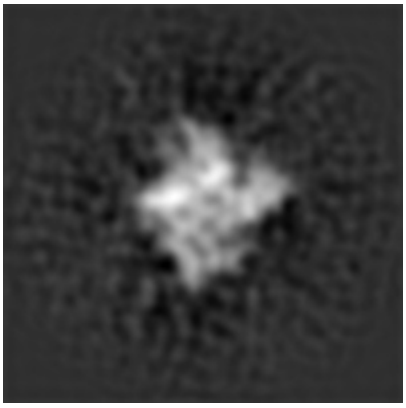
This section contains visualisations of the EMDB entry EMD-5510. These allow visual inspection of the internal detail of the map and identification of artifacts.

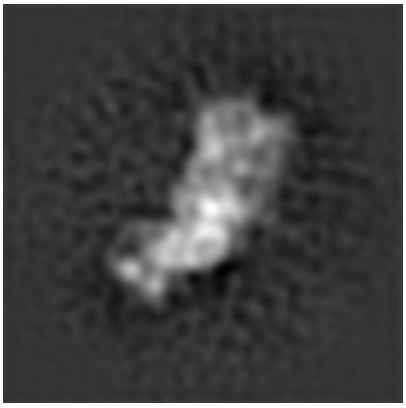
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

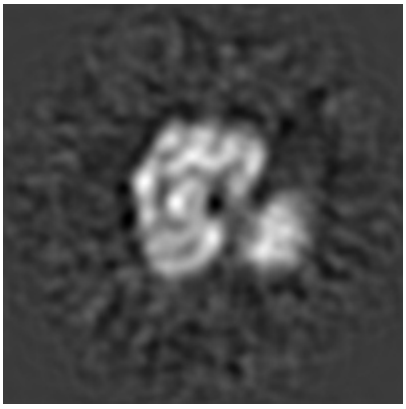

Y

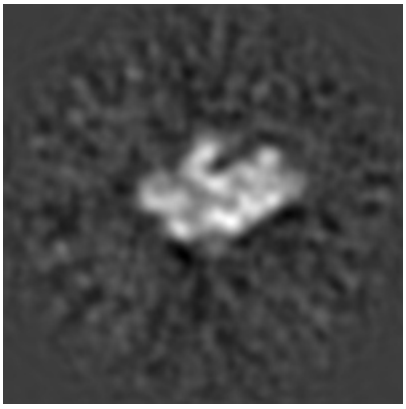

Z

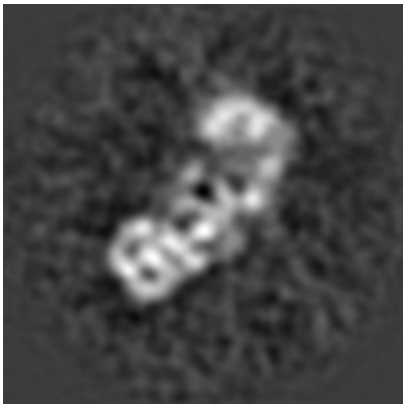
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 62

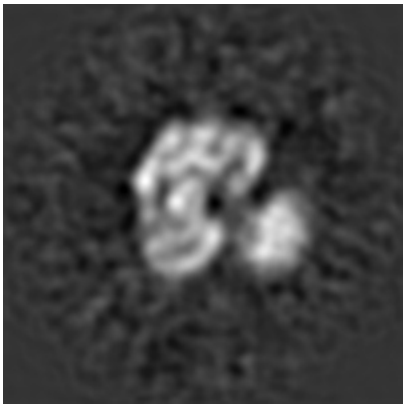

Y Index: 62

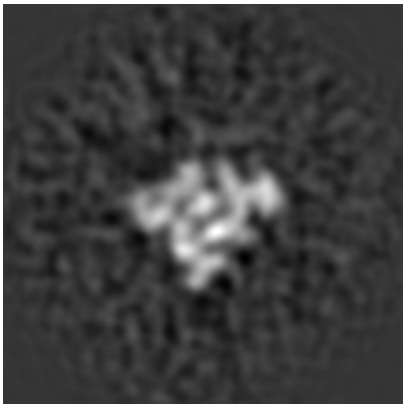

Z Index: 62

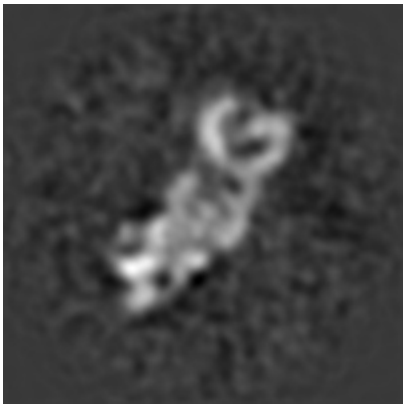
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 63

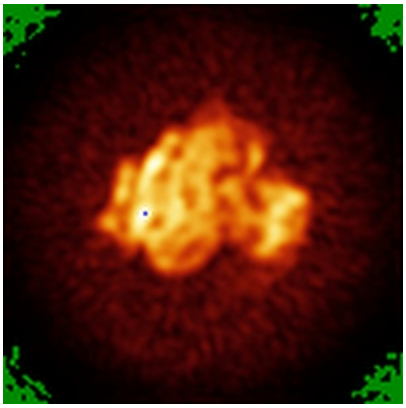

Y Index: 53

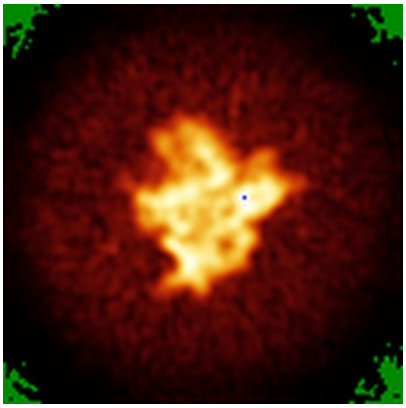

Z Index: 58

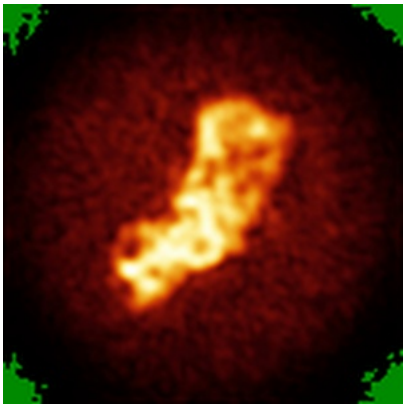
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X

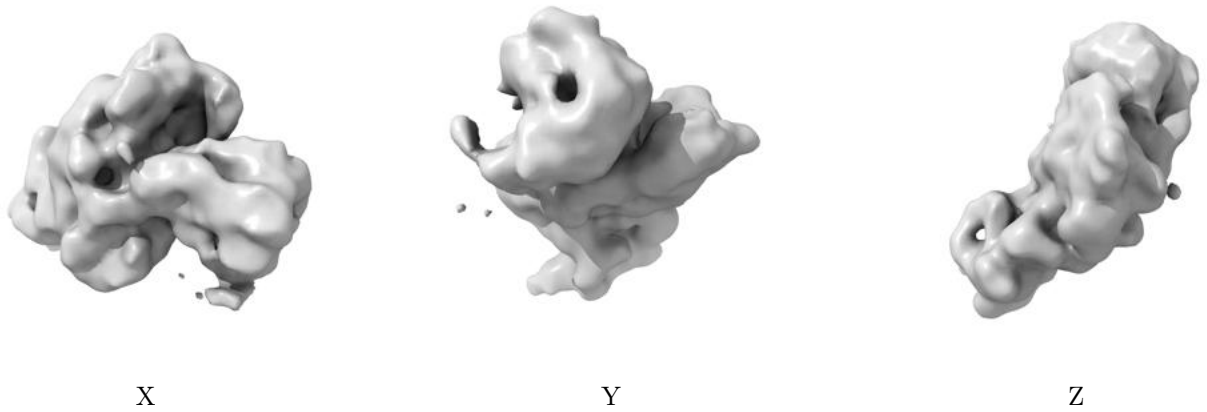

Y


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.

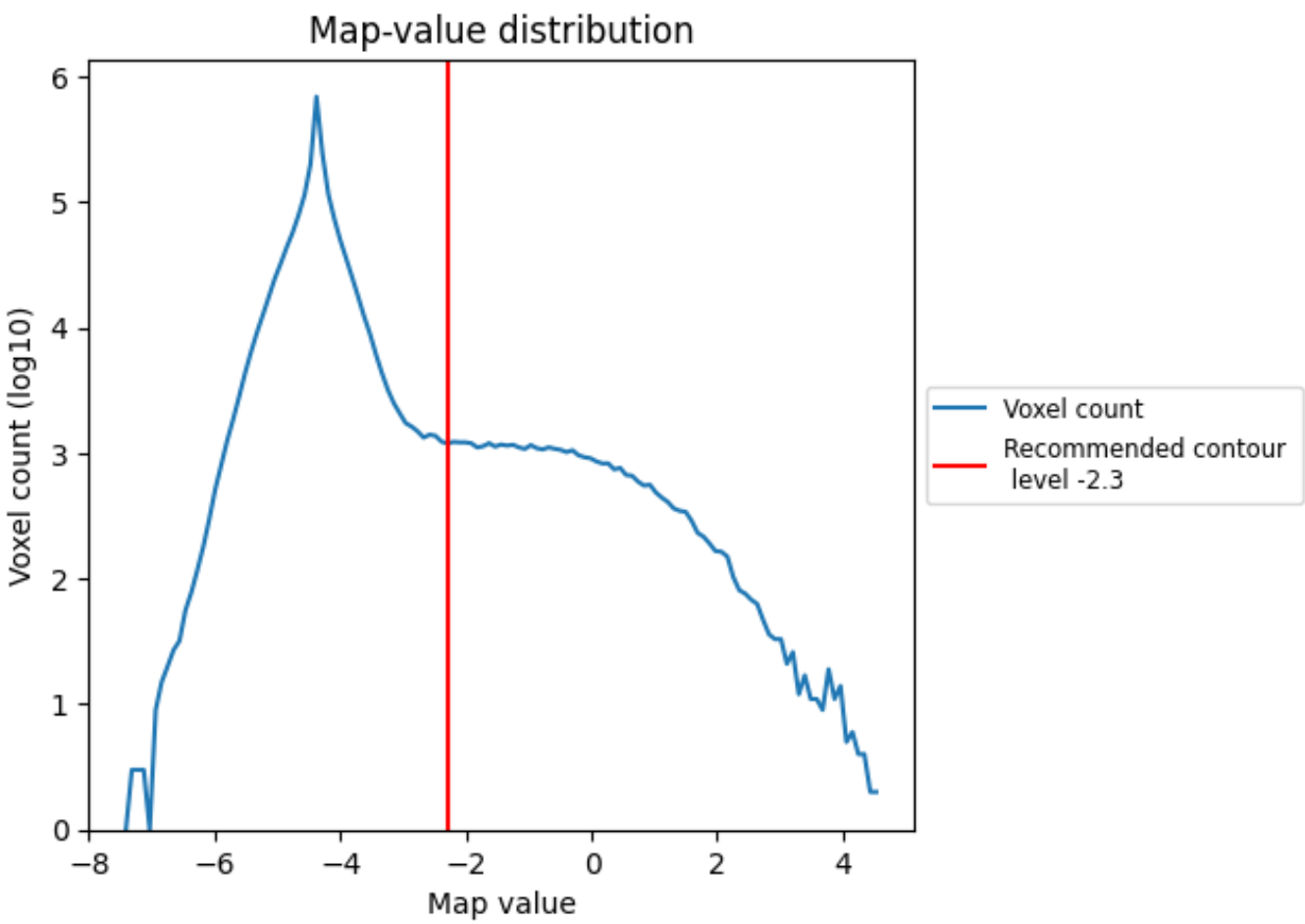
6.6 Mask visualisation (i)

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

7 Map analysis (i)

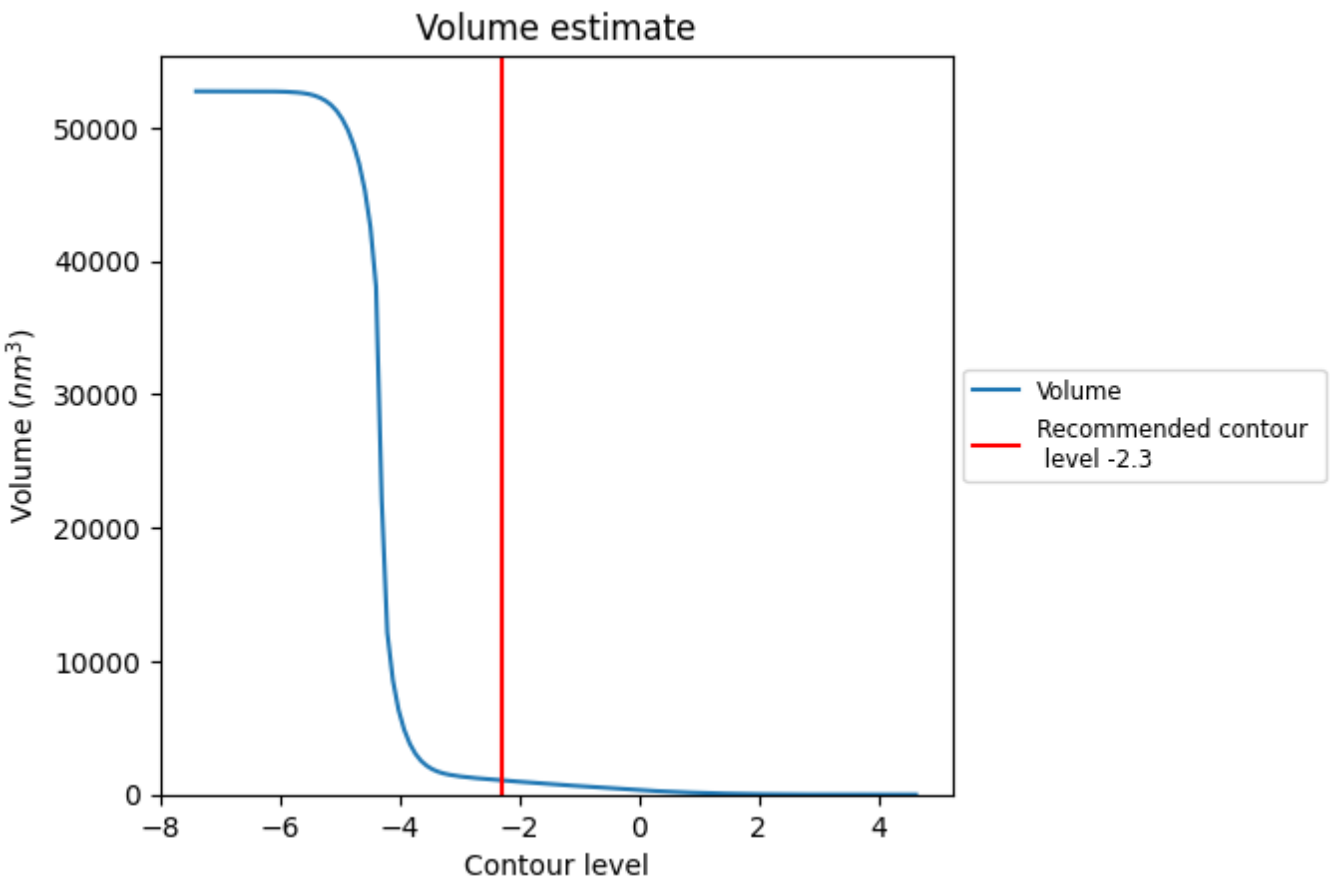
This section contains the results of statistical analysis of the map.

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.

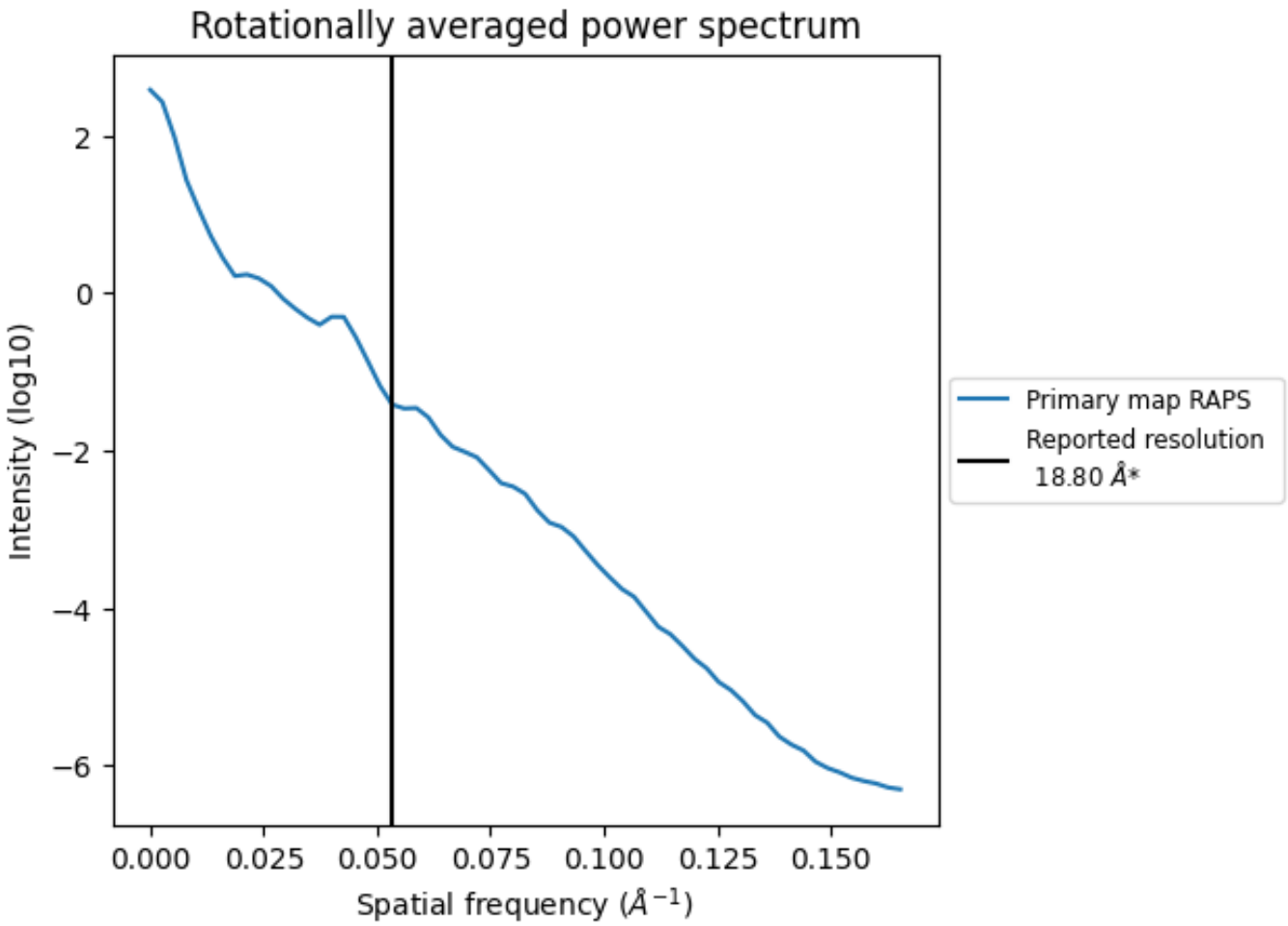
7.2 Volume estimate (i)



The volume at the recommended contour level is 1065 nm^3; this corresponds to an approximate mass of 962 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}

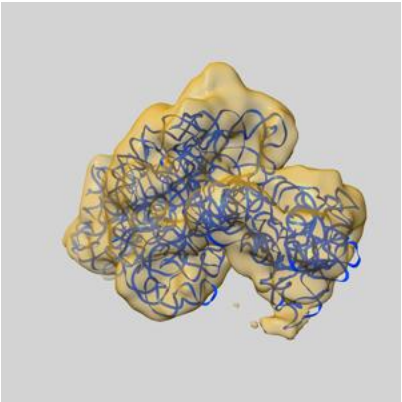
8 Fourier-Shell correlation (i)

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

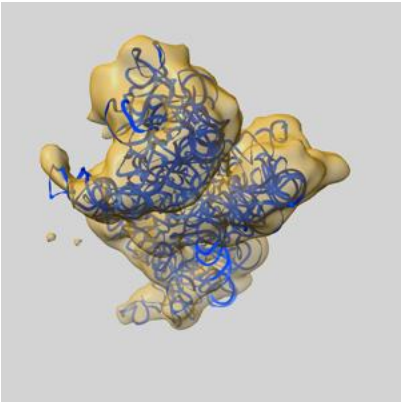
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5510 and PDB model 3J2H. Per-residue inclusion information can be found in section 3 on page 4.

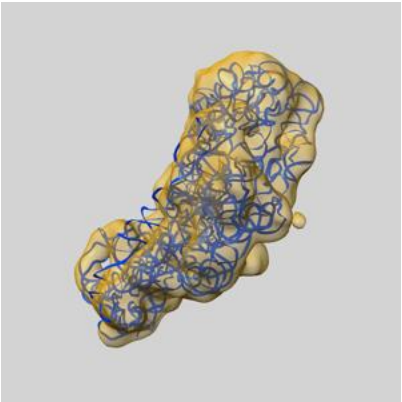
9.1 Map-model overlay (i)



X



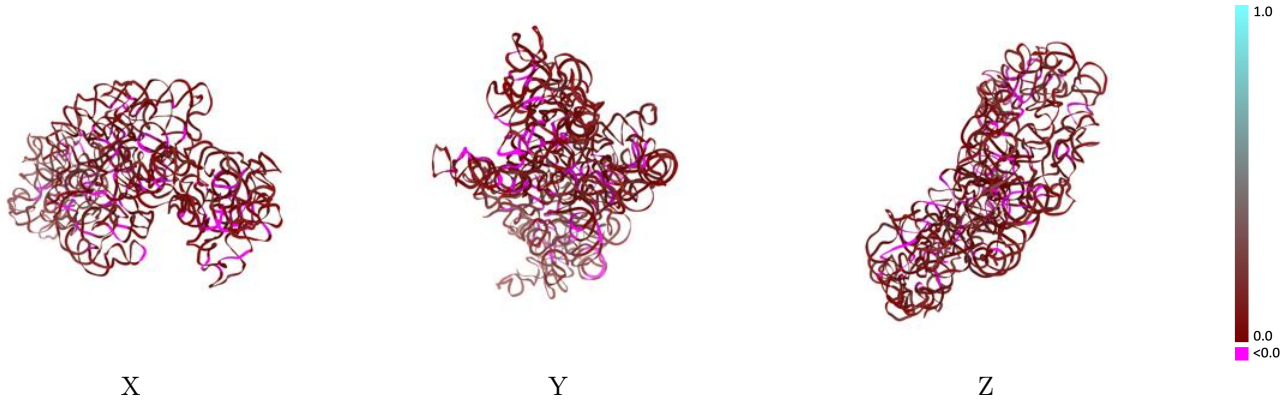
Y



Z

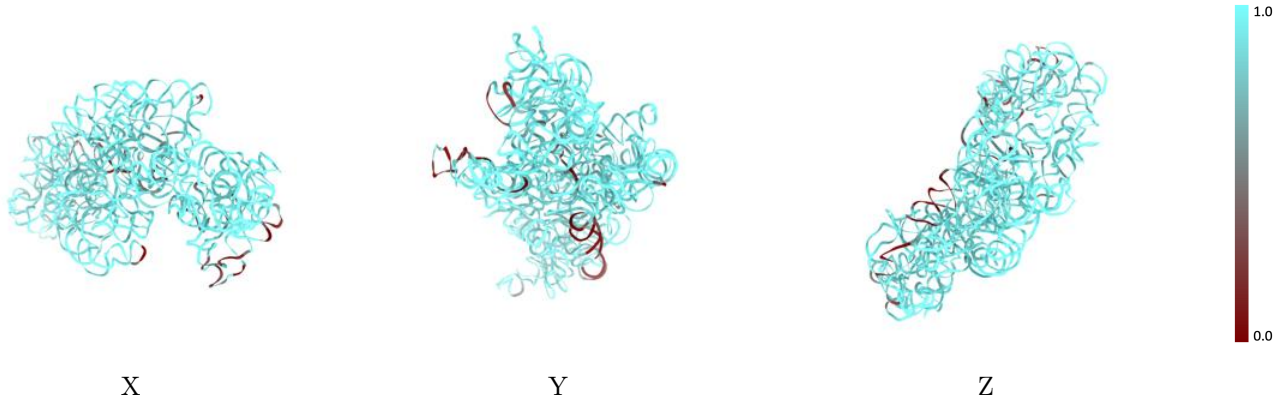
The images above show the 3D surface view of the map at the recommended contour level -2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



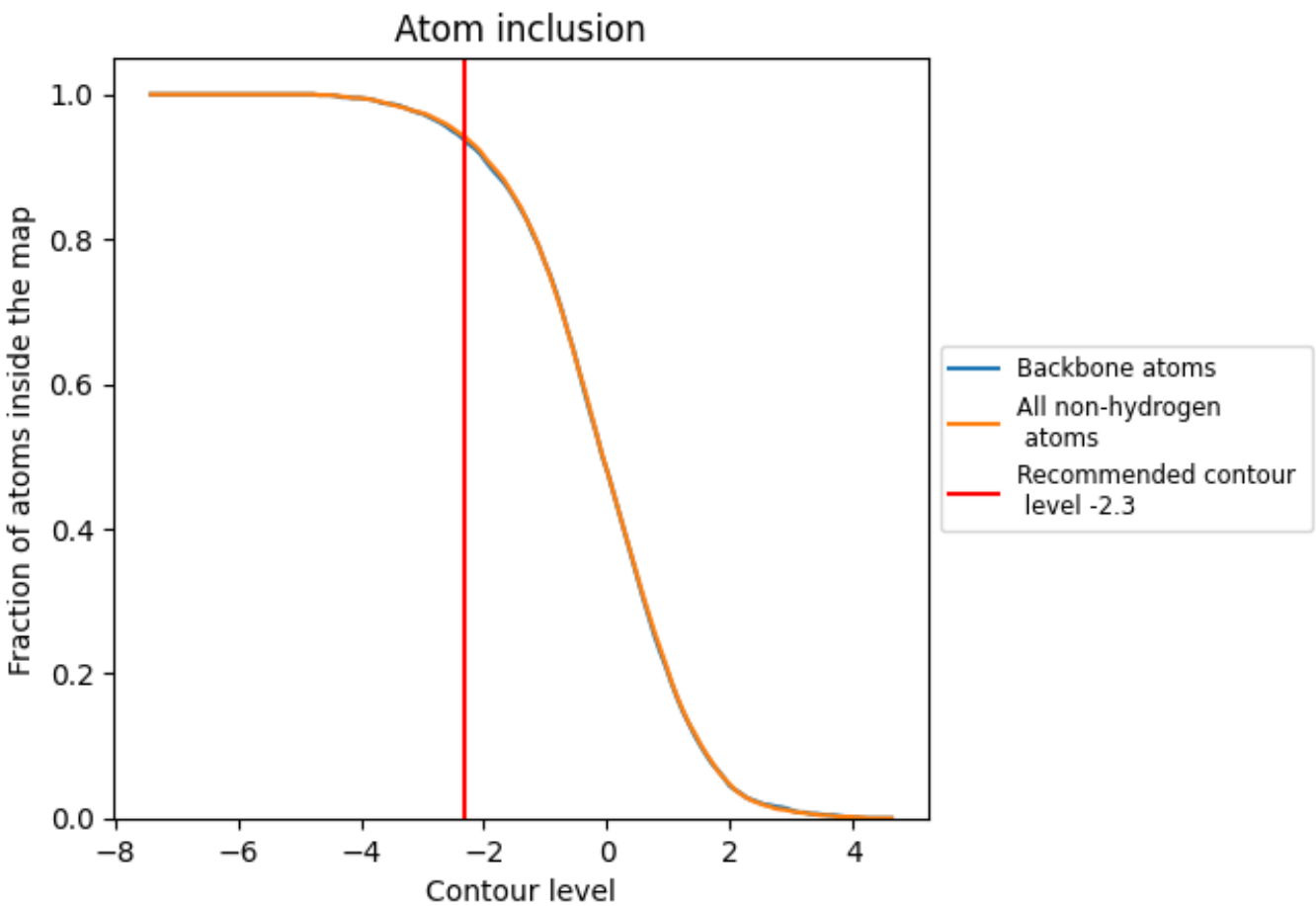
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.9410	0.0780
N	0.9420	0.0780