Full wwPDB EM Validation Report ⓘ

Mar 13, 2024 – 12:16 PM JST

PDB ID	:	3DG0
EMDB ID	:	EMD-1363
Title	:	Coordinates of 16S and 23S rRNAs fitted into the cryo-EM map of EF-G-bound translocation complex
Authors	:	Gao, H.; LeBarron, J.; Frank, J.
Deposited on	:	2008-06-12
Resolution	:	10.80 Å(reported)
Based on initial models	:	2AVY, 2AW4

This is a Full wwPDB EM Validation 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:

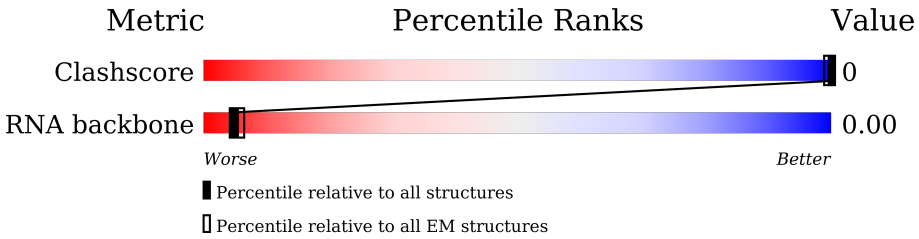
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.80 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	A	1542	33% 99%
2	B	2904	28% 98%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4371 atoms, of which 0 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 Ribosomal RNA from E. coli.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	1530	Total	P	0	1530
			1530	1530		

- Molecule 2 is a RNA chain called 23S Ribosomal RNA from E. coli.

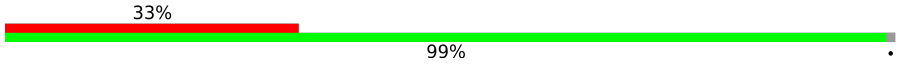
Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	2841	Total	P	0	2841
			2841	2841		

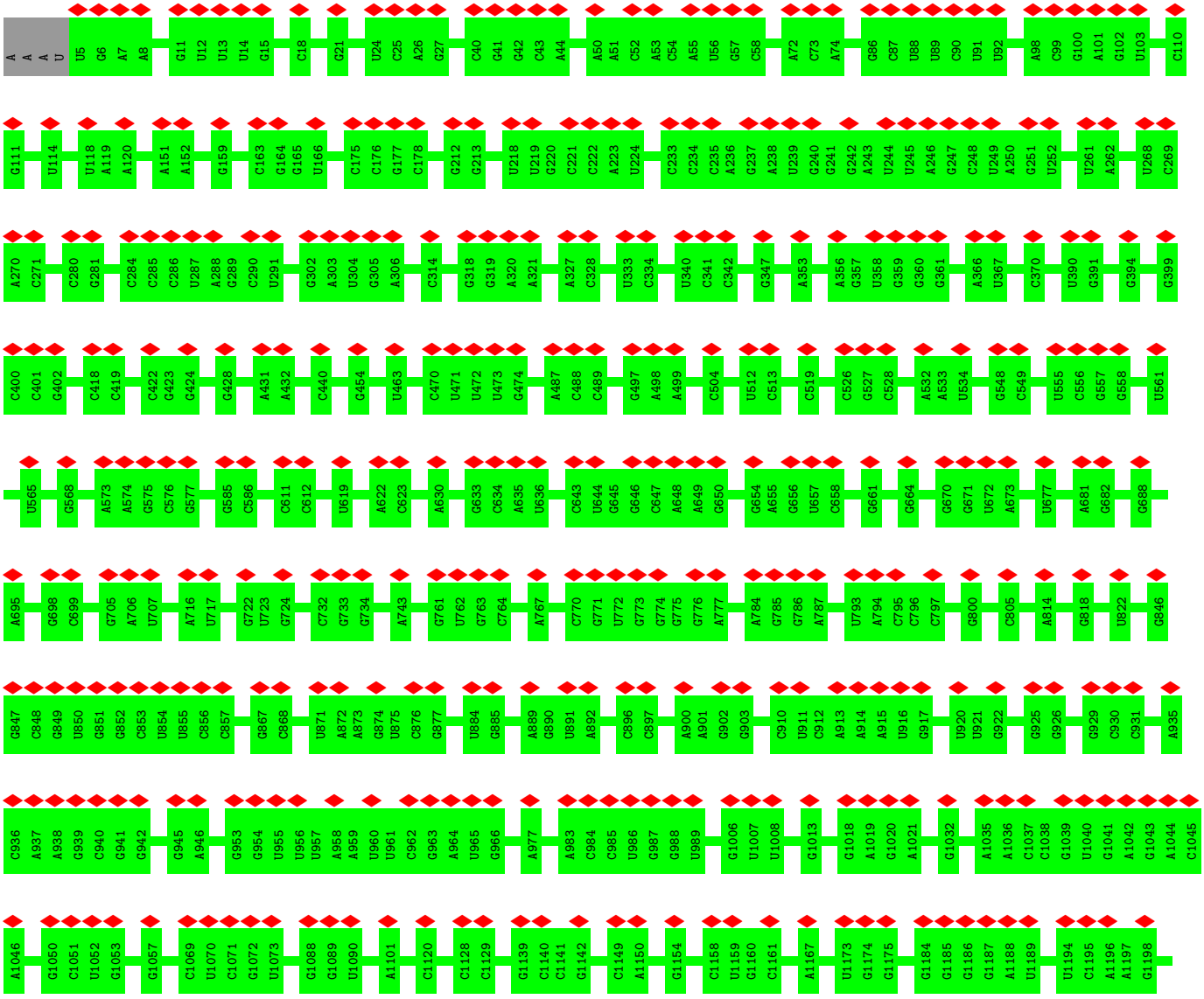
3 Residue-property plots (i)

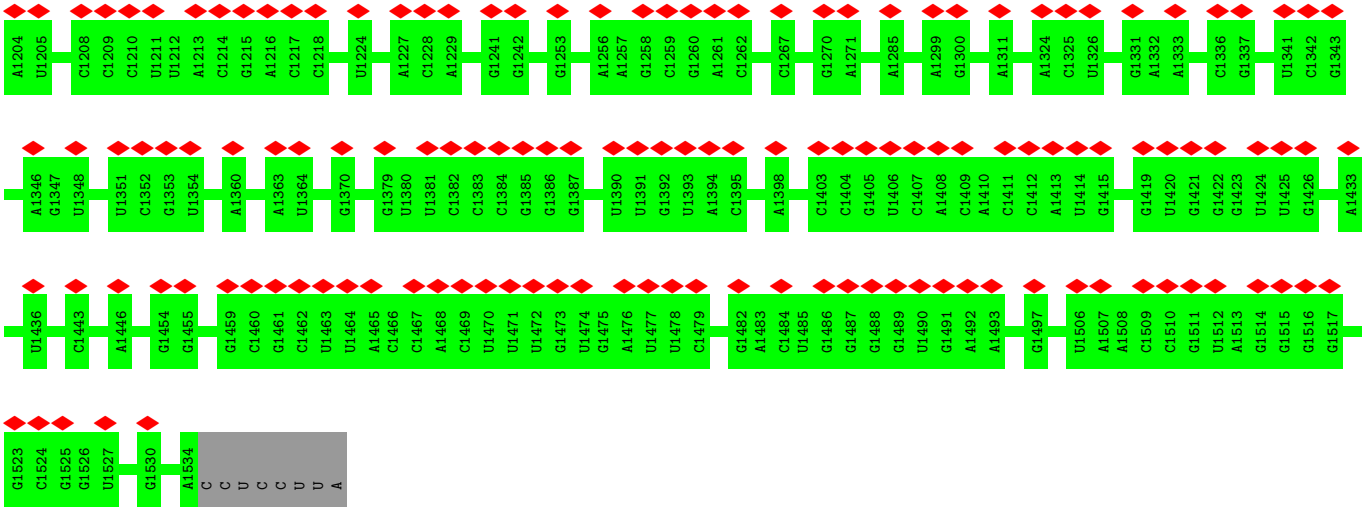
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 Ribosomal RNA from E. coli

Chain A:

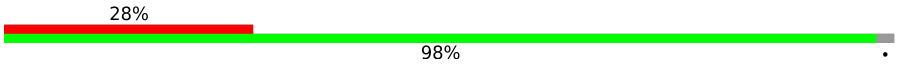


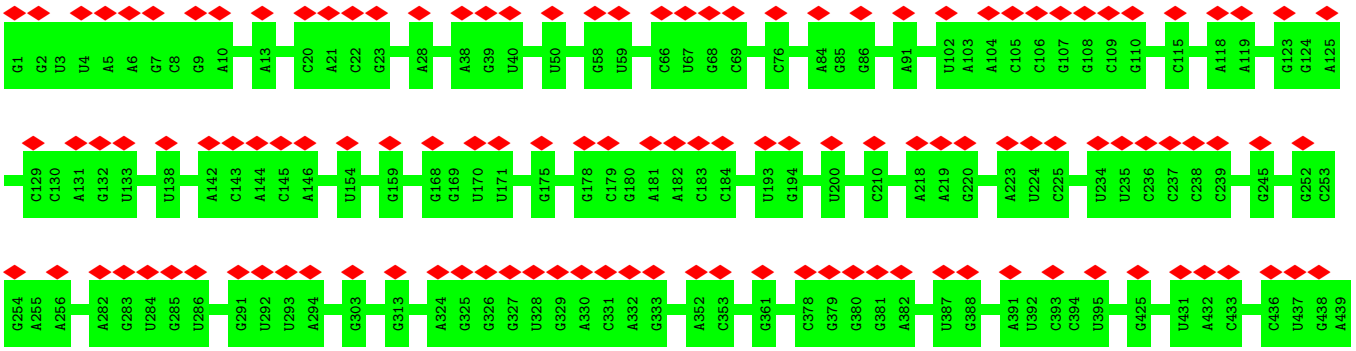




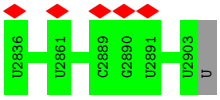
• Molecule 2: 23S Ribosomal RNA from E. coli

Chain B:






G1128 A1129 U1130 A1133 G1136 C1145 G1149 C1150 C1167 U1176 G1177 C1178 G1179 U1180 U1181 U1184 G1185 G1193 A1194 G1195 C1200 G1218 U1219 G1220 A1226 G1227 A1230 U1231 A1237 U1240 A1241 U1242 A1247 G1248 U1249 A1253 G1259 A1260 C1261 A1262 U1267
C1270 U1273 A1274 A1275 A1276 C1289 C1290 C1291 G1292 C1293 U1294 C1295 G1296 C1297 C1298 A1301 A1302 C1315 A1322 C1323 G1324 C1330 G1334 C1335 A1336 G1346 A1347 C1348 C1349 G1355 G1356 C1357 G1361 G1368 G1369 C1370 G1371 U1372 A1378 G1382 U1396 G1418 A1419 A1420 G1421
G1422 G1423 C1428 G1432 A1433 A1434 G1435 G1436 U1443 G1464 G1465 U1466 U1467 U1468 A1469 A1470 G1471 G1478 U1481 G1482 A1490 G1500 C1501 A1502 G1516 C1517 C1518 G1537 G1538 U1539 A1551 A1552 A1553 U1554 G1555 C1556 U1559 G1560 C1564 C1565 G1588 U1589 A1590 A1591 C1592
A1608 A1609 G1613 G1619 G1623 U1624 G1627 C1638 C1646 A1650 A1654 A1655 G1659 G1660 G1661 U1662 G1663 A1672 G1673 G1674 C1675 A1676 A1677 U1683 G1684 C1691 U1692 U1693 C1694 G1695 G1699 G1702 G1703 C1706 G1707 C1708 U1720 G1721 C1730 G1733 G1734 A1735
A1744 A1745 A1746 U1747 C1748 A1749 G1750 U1758 C1761 A1762 G1763 C1764 C1768 U1769 G1770 C1771 A1772 A1773 G1776 U1777 A1787 C1788 A1794 C1795 U1796 C1800 A1801 G1807 A1810 G1811 U1812 U1820 A1821 C1822 G1826 A1829 C1833 U1834 G1835 G1840 U1841 G1849 G1873
C1874 G1875 A1876 A1877 G1878 C1879 U1880 C1881 U1882 U1883 G1884 G1888 A1889 A1890 G1891 C1892 C1893 C1894 A1899 A1900 A1901 G1904 C1908 C1909 G1910 U1911 C1914 U1915 A1916 U1917 A1918 U1923 C1924 C1925 U1931 G1935 A1936 A1937 A1938 U1939 U1943 C1957 C1958 G1959 A1960 U1963 G1968
G1973 C1974 G1975 U1976 A1977 A1978 U1979 G1984 A1987 C1990 U1993 C1996 C1997 A1998 C2001 G2004 G2012 A2020 G2024 G2027 U2028 G2029 A2030 A2033 U2034 G2035 C2045 G2046 C2047 G2048 G2049 C2050 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 A2070 C2073
C2078 U2079 A2080 U2081 U2085 U2086 C2103 C2104 U2105 U2106 C2107 A2108 U2109 G2110 U G U A G G A U A G G G U G G G A G G C U U U G2133 A2134 G2141 A2142 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A G C C
G A C C U U G A A A U A C C A C C C2179 U2180 U2181 U2185 G2186 U2187 U2188 U2189 G2190 G2193 U2194 U2195 G2201 A2205 U2213 C2214 C2215 G2216 G2217 G2218 A2227 G2228 U2229 G2230 U2231 C2232 U2233 G2239 U2240 A2241 G2242 U2243 G2246 C2254
G2255 G2256 U2257 C2258 A2270 G2271 U2272 A2273 A2274 G2279 G2280 U2296 A2297 A2298 U2299 C2300 C2301 U2302 A2309 A2322 G2323 U2324 G2325 C2326 A2327 G2330 C2338 C2339 A2340 G2341 U2356 G2357 A2358 G2363 C2364 C2380 A2381 G2382 G2383 U2387 G2391 U2402 G2413 G2414 G2415 C2416
C2417 G2421 C2422 A2433 A2434 A2435 G2436 G2437 C2440 U2441 C2442 C2443 U2449 A2450 A2451 C2452 G2455 C2462 C2463 G2472 G2481 A2482 C2483 G2484 G2485 C2486 G2487 G2490 U2491 U2492 U2493 G2494 G2505 U2506 C2510 U2511 C2512 U2519 C2520 G2525 G2535 G2536 C2539 C2540
G2543 G2544 G2545 U2546 A2547 U2548 G2549 G2553 C2556 C2559 A2566 G2567 U2568 G2569 G2582 G2583 U2584 U2585 U2586 A2587 G2595 G2599 A2600 C2601 A2602 G2603 U2604 U2605 C2606 G2607 G2608 U2609 C2610 U2613 A2614 U2615 C2616 U2617 U2622 G2625 G2630 G2631 A2632 A2635 C2636 G2642 G2643
G2644 U2650 C2667 G2673 G2677 C2678 A2679 U2684 G2685 U2689 U2690 C2691 U2701 U2707 G2708 G2709 U2713 C2716 C2717 A2721 U2724 A2725 A2726 U2739 G2744 A2757 A2764 A2765 U2768 U2769 C2773 A2778 G2803 U2804 C2805 A2813 A2823


U2836
U2861
C2889
G2890
U2891
U2903
U

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	CTF correction of 3D map	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	49696	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	253.154	Depositor
Minimum map value	-116.942	Depositor
Average map value	2.691	Depositor
Map value standard deviation	25.799	Depositor
Recommended contour level	56.8	Depositor
Map size (Å)	366.6, 366.6, 366.6	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.82, 2.82, 2.82	Depositor

5 Model quality

5.1 Standard geometry

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	A	1530	0	0	0	0
2	B	2841	0	0	0	0
All	All	4371	0	0	0	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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	0/1542	-	-
2	B	0/2904	-	-
All	All	0/4446	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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.

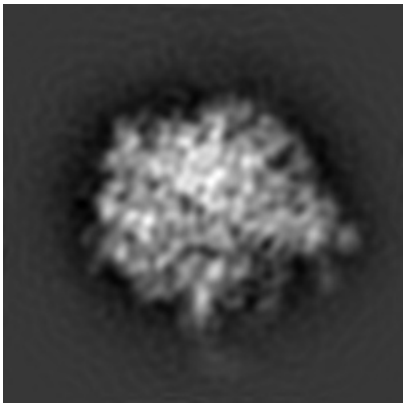
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1363. These allow visual inspection of the internal detail of the map and identification of artifacts.

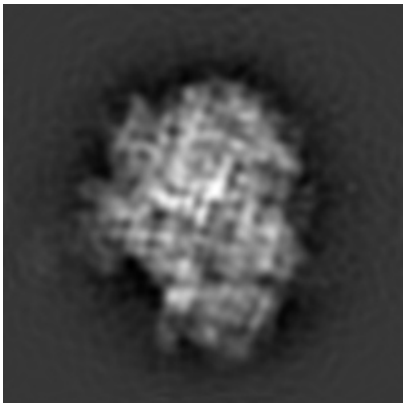
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

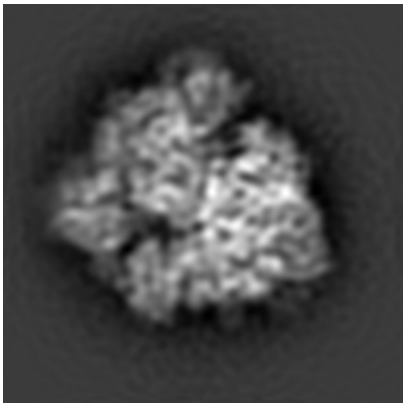
6.1.1 Primary map



X



Y

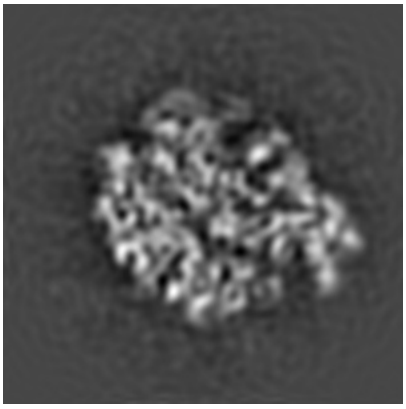


Z

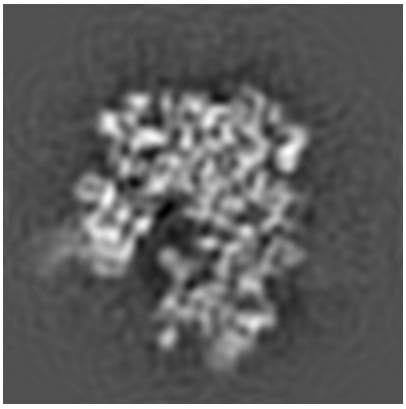
The images above show the map projected in three orthogonal directions.

6.2 Central slices

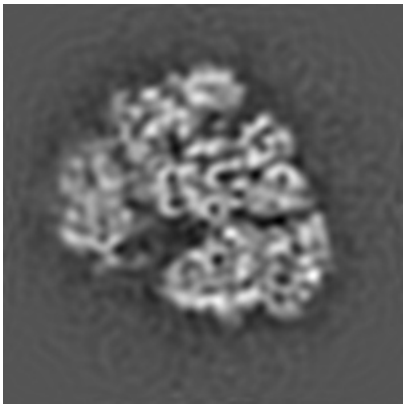
6.2.1 Primary map



X Index: 65



Y Index: 65

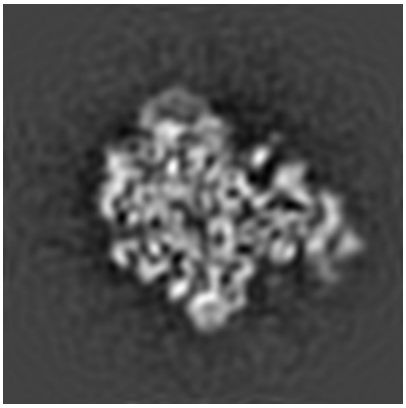


Z Index: 65

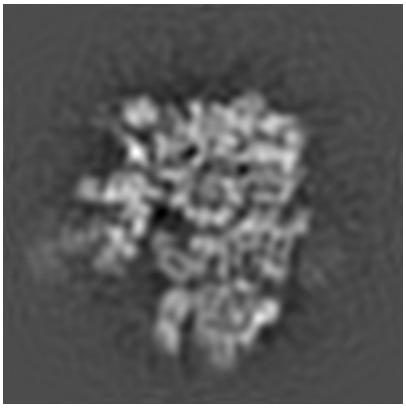
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

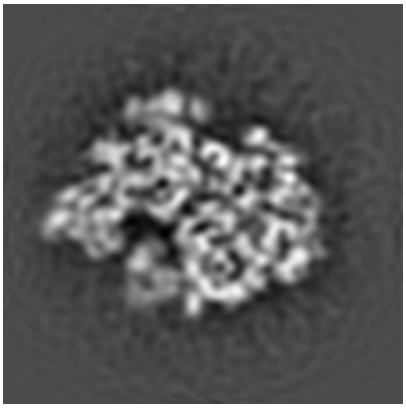
6.3.1 Primary map



X Index: 67



Y Index: 68

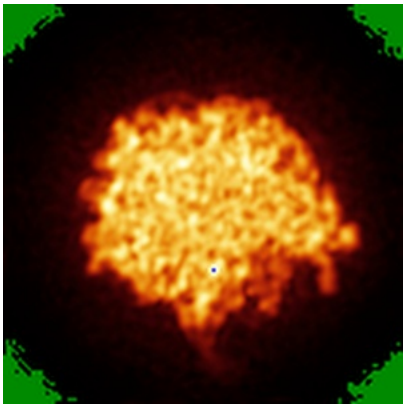


Z Index: 79

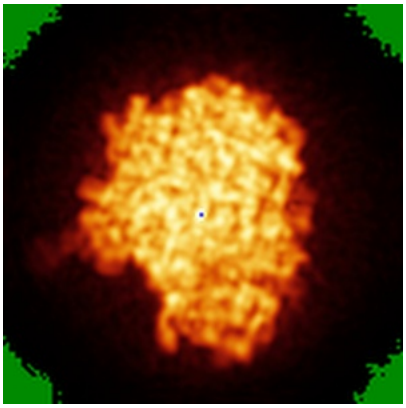
The images above show the largest variance slices of the map in three orthogonal directions.

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

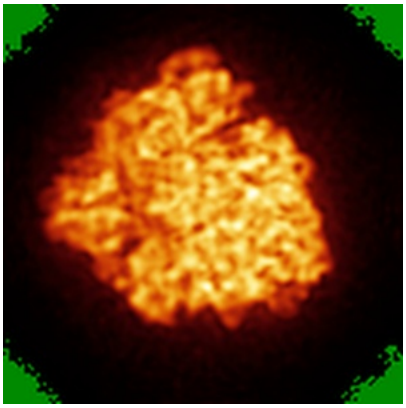
6.4.1 Primary map



X



Y

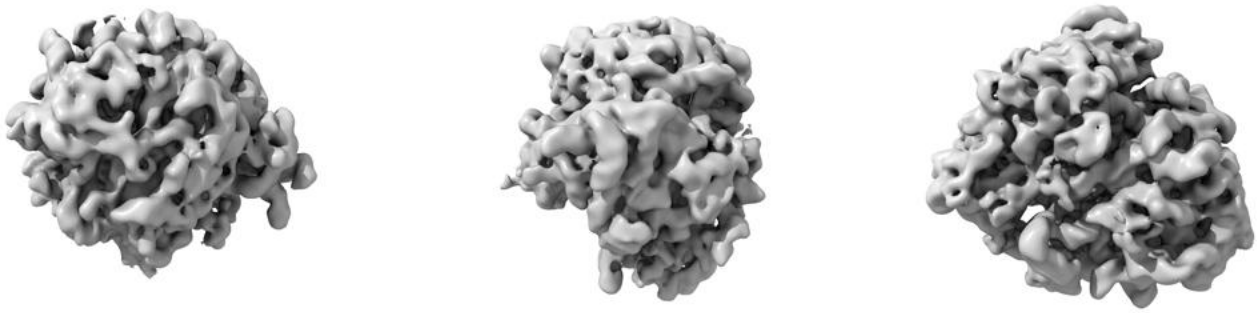


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 56.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

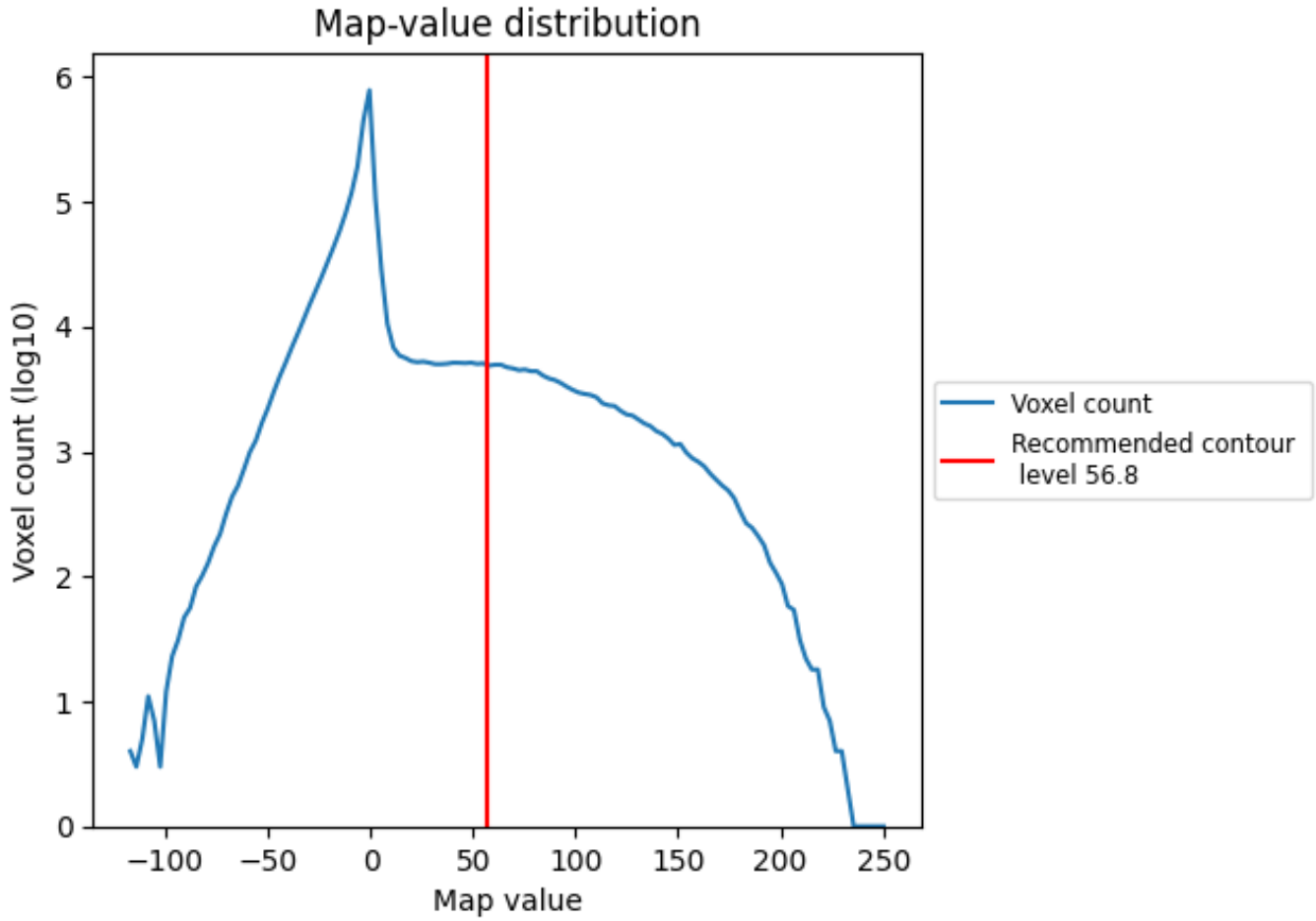
6.6 Mask visualisation (i)

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

7 Map analysis

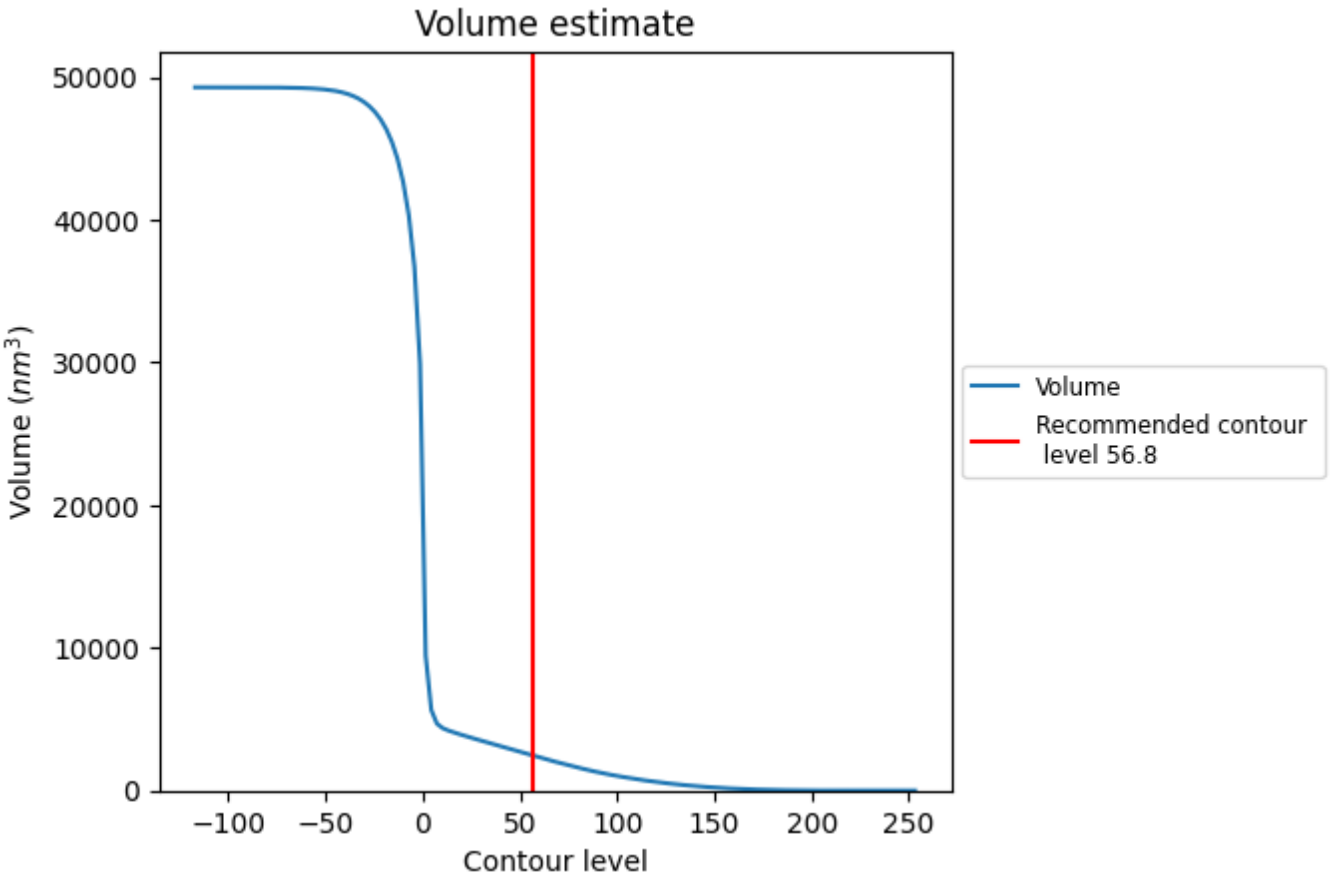
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

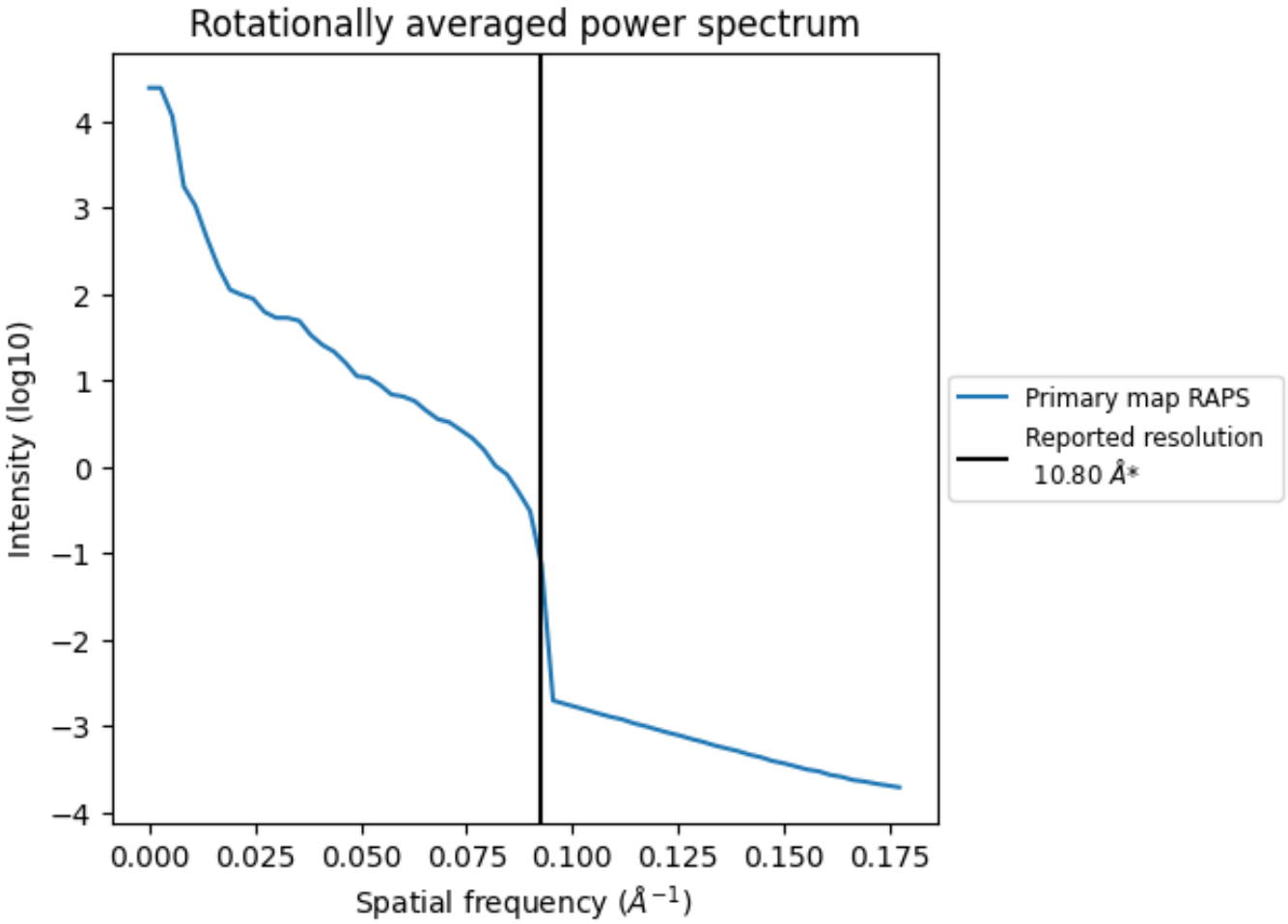
7.2 Volume estimate



The volume at the recommended contour level is 2453 nm^3; this corresponds to an approximate mass of 2216 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 0.093 Å^{-1}

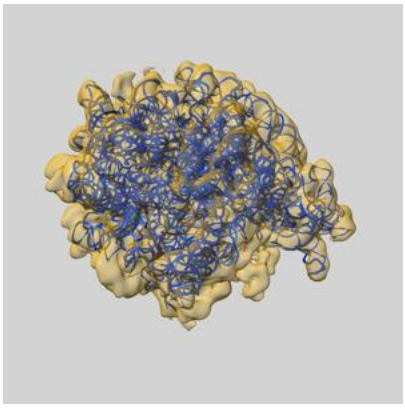
8 Fourier-Shell correlation (i)

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

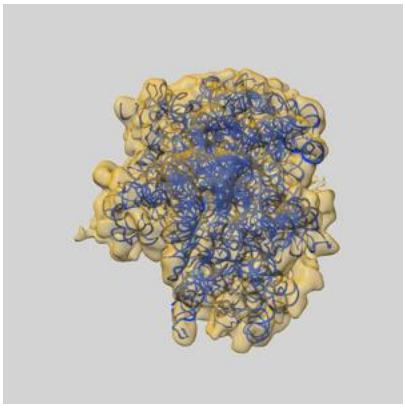
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1363 and PDB model 3DG0. Per-residue inclusion information can be found in section 3 on page 4.

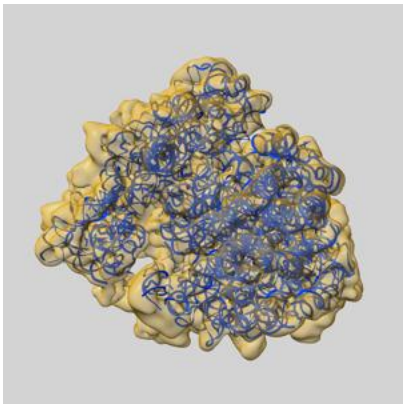
9.1 Map-model overlay



X



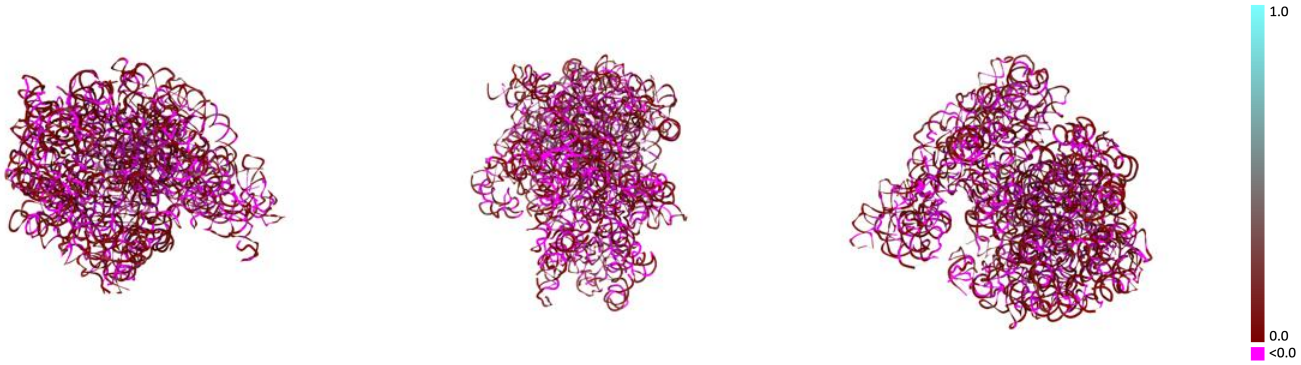
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 56.8 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.

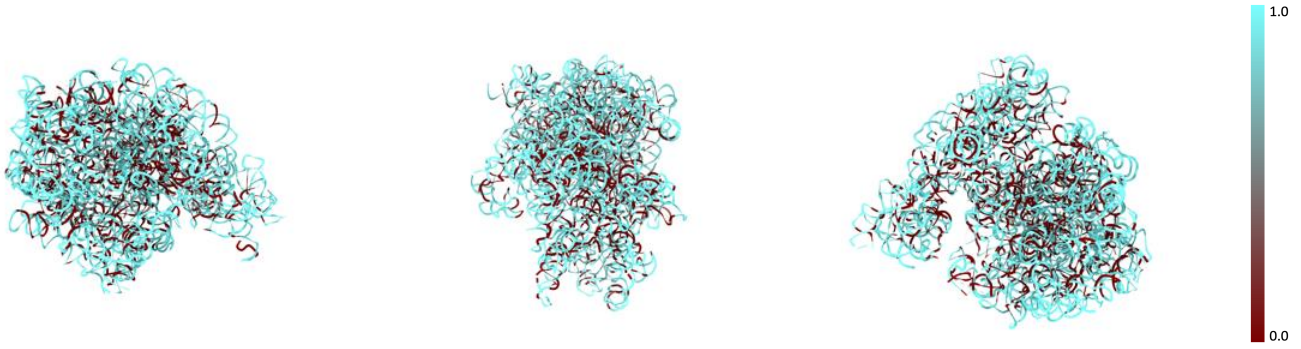
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

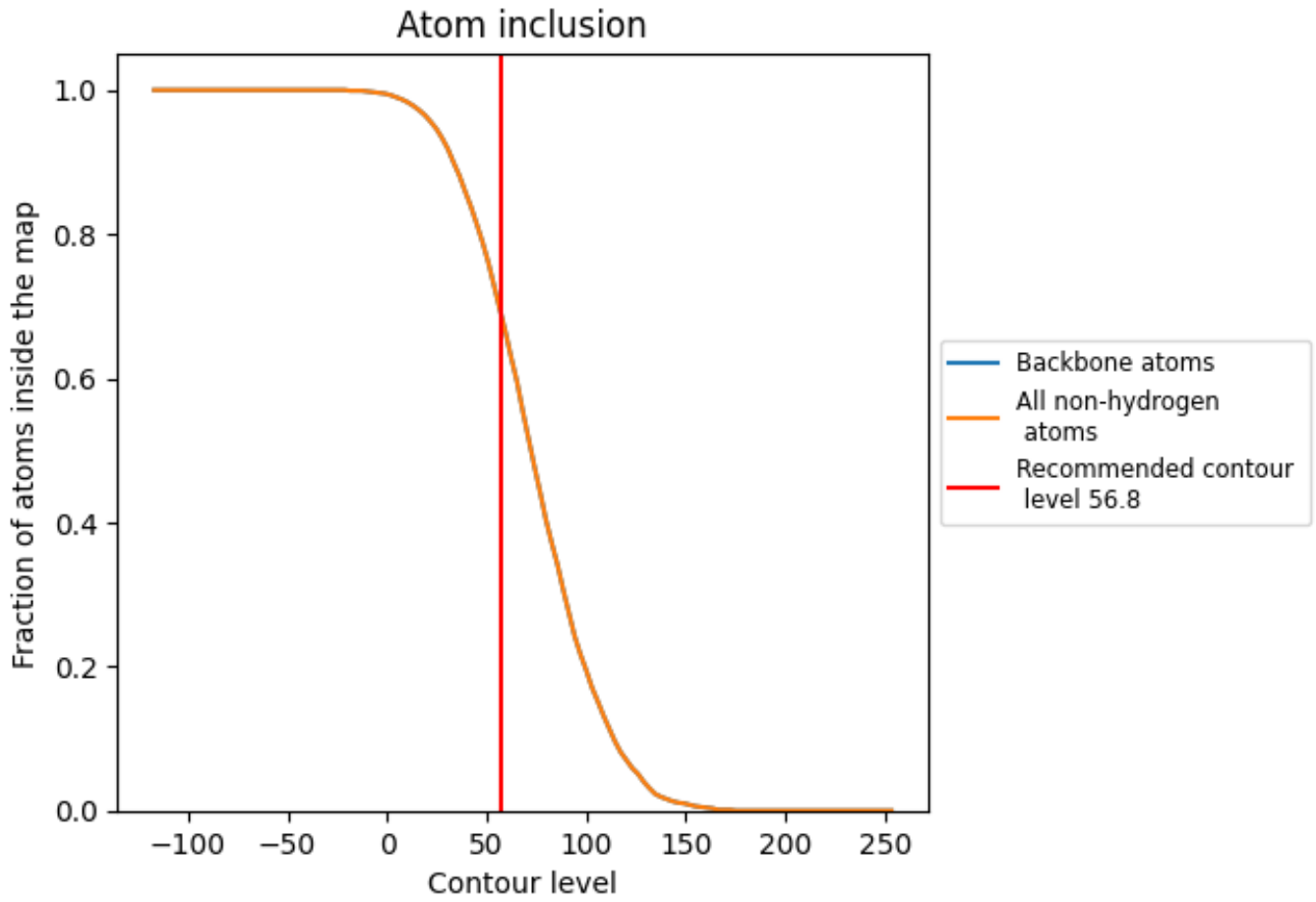
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (56.8).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 69% 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 (56.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.0270
A	0.6630	0.0240
B	0.7100	0.0290