



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 11:01 AM EST

PDB ID : 3DG4
EMDB ID : EMD-1184
Title : Coordinates of 16S and 23S rRNAs fitted into the cryo-EM map of RF1-bound termination complex
Authors : Gao, H.; LeBarron, J.; Frank, J.
Deposited on : 2008-06-12
Resolution : 12.80 Å (reported)
Based on initial models : 2AVY, 2AW4

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

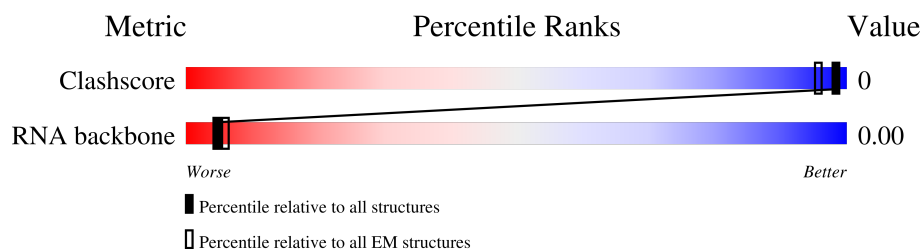
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

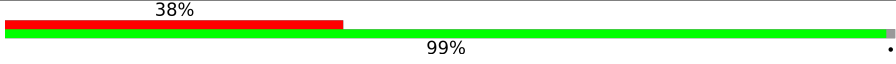
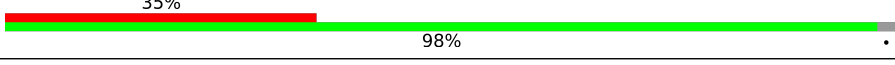
The reported resolution of this entry is 12.80 Å.

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 $\leq 5\%$. 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	A	1542	
2	B	2904	

2 Entry composition

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		

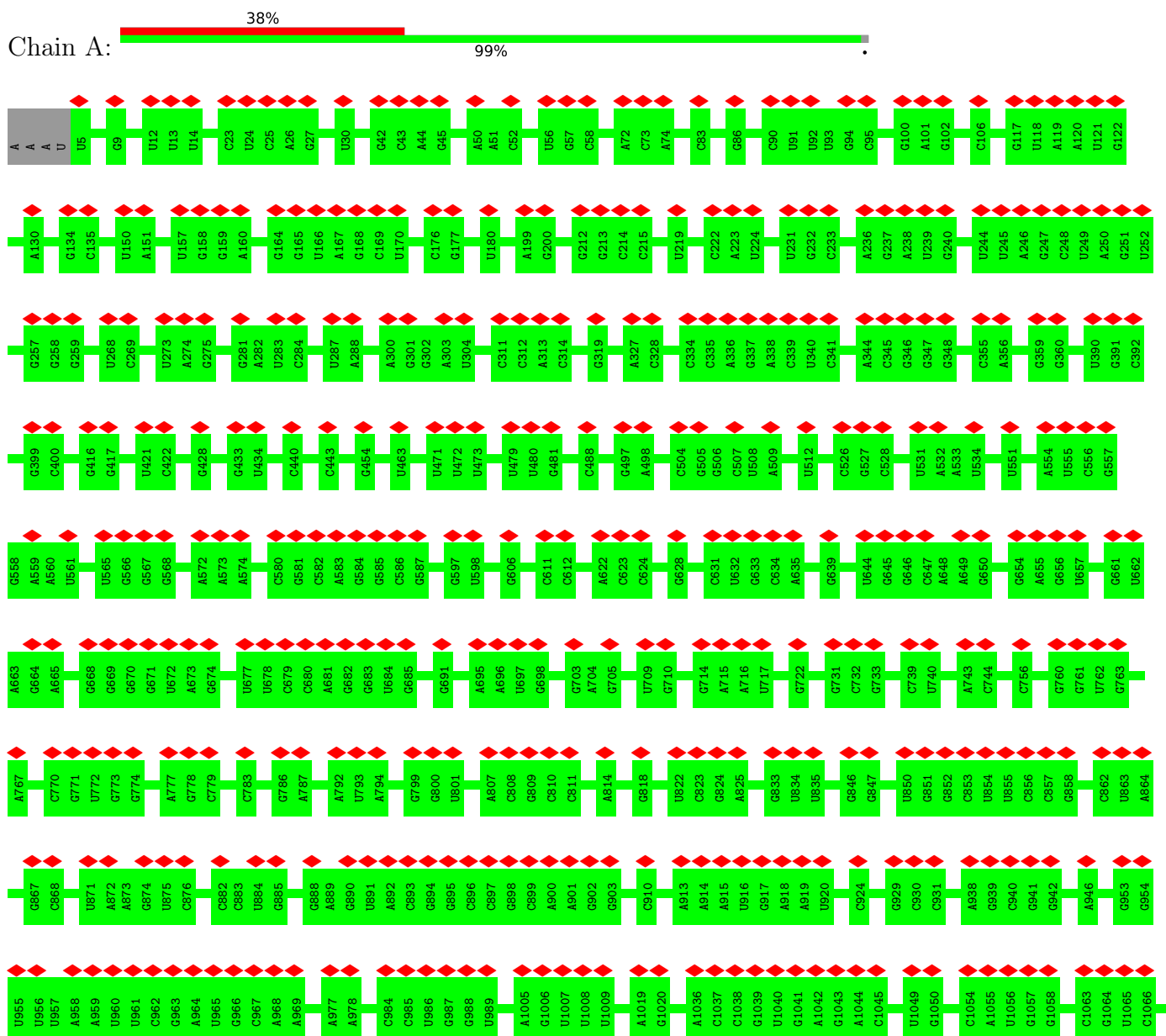
- Molecule 2 is a RNA chain called 23S RibosomaL RNA from E. coli.

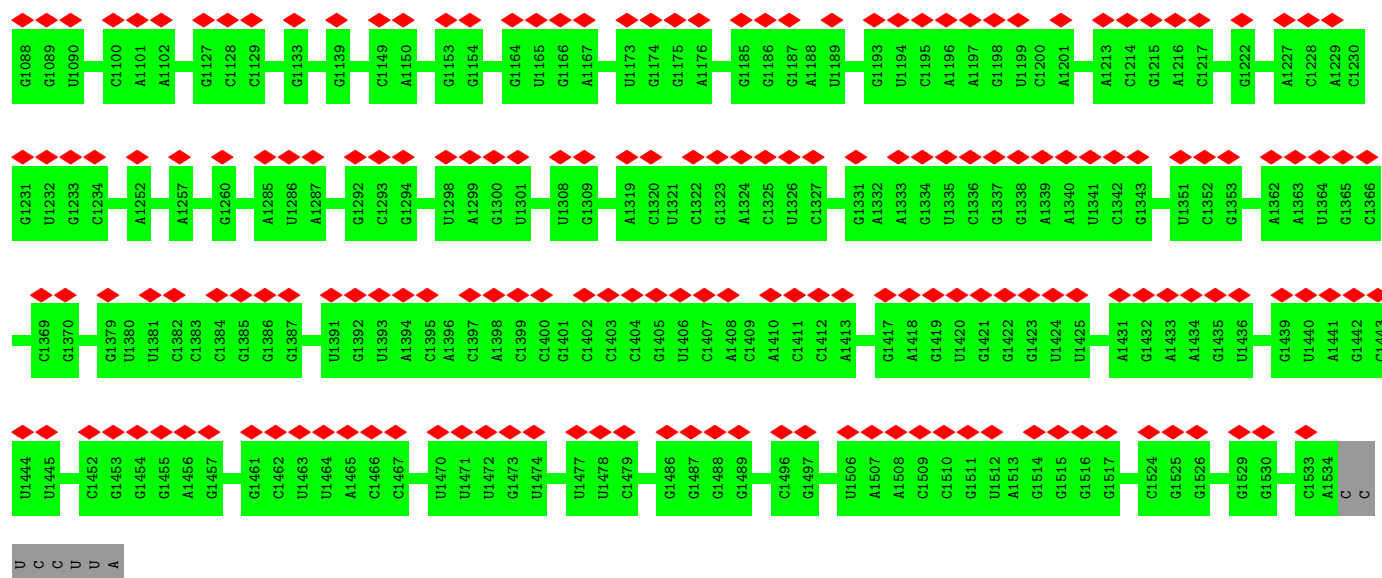
Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	2841	Total	P	0	2841
			2841	2841		

3 Residue-property plots

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



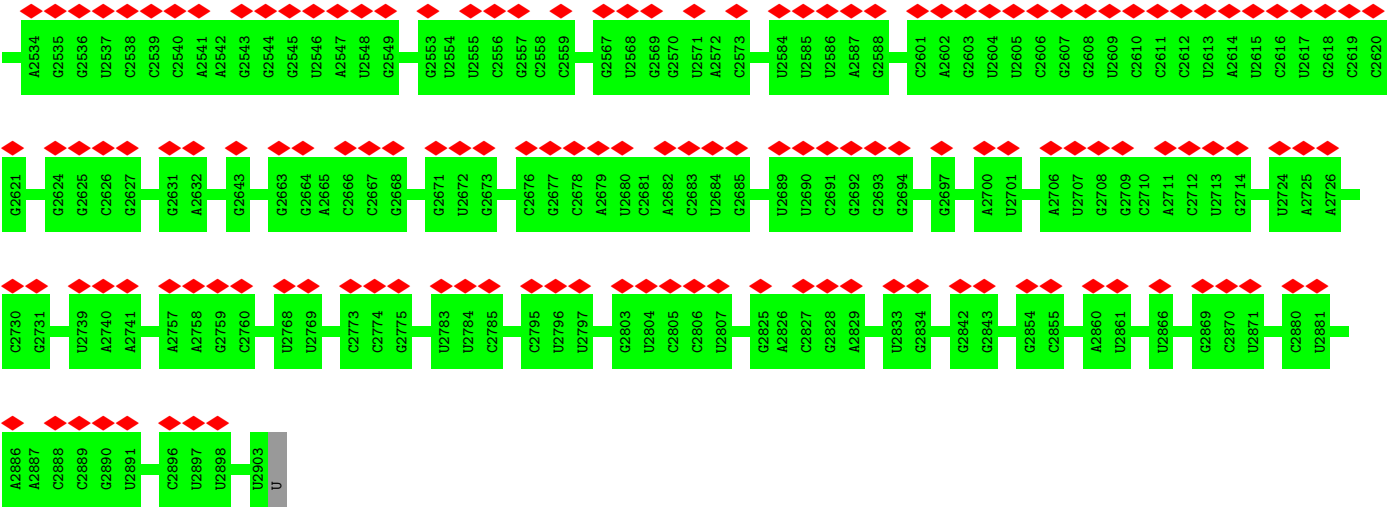


• Molecule 2: 23S Ribosomal RNA from E. coli

Chain B: 35% 98% .



U1066	G1179	G1421	G1560	G1699	C1822	U2007	G2110	C	A2274	U2431
A1067	U1180	G1426	A1591	G1703	G1823	C2008	U	C	C2275	A2432
G1068	U1181	A1427	C1592	G1707	G1824	G2012	G	U	G2276	A2433
A1073	G1187	C1428	C1593	G1708	U1825	A2019	A	A	U2296	A2434
G1074	U1188	G1429	U1594	C1709	G1826	A2020	C	C	A2297	A2435
C1075	A1189	A1430	A1608	U1720	G1831	C2023	U	U	A2309	G2436
C1076	G1190	A1431	A1609	G1721	C1832	G2024	A	A	C2313	A2439
U1077	G1191	A1432	G1613	G1724	U1833	C2025	G	G	A2314	U2440
U1078	G1193	A1433	A1614	G1724	U1834	C2025	U	U	G2323	U2441
C1079	A1194	G1436	C1615	G1724	G1835	A2030	G	G	G2324	C2442
U1080	G1195	C1437	G1619	C1730	G1836	G2033	A	A	U2193	C2443
A1090	C1196	U1440	G1620	G1734	G1840	U2034	C	C	U2194	U2449
G1091	U1197	U1441	C1625	A1735	U1841	G2035	U	U	A2198	C2452
C1092	G1198	U1442	A1626	G1744	C1843	G2038	C	C	G2204	A2453
G1093	U1199	U1442	G1627	A1745	U1844	C2047	U	U	G2210	G2454
U1094	C1200	G1446	U1628	A1746	G1845	C2048	G	G	A2211	G2455
C1104	U1201	C1447	U1629	U1747	G1846	C2049	C2133	U	U2210	A2461
U1105	A1204	C1448	G1640	C1748	A1847	C2050	G2140	G	A2212	C2462
C1114	A1205	G1449	A1641	A1749	G1857	C2055	G2141	C	U2213	G2463
G1115	G1206	G1450	G1642	U1758	U1858	C2055	A2142	U	G2217	C2464
G1116	C1207	G1456	A1643	C1761	U1859	A2059	G2143	C	C2222	C2465
C1117	G1218	G1464	G1644	A1762	G1860	A2060	G2144	U	A2227	U2472
G1118	U1219	G1465	C1645	G1763	U1880	C2061	U2148	G	G2228	U2473
U1119	G1220	U1481	C1646	C1764	G1884	A2062	U2149	C	U2229	C2480
G1120	C1221	U1481	G1660	C1768	C1884	C2063	C2150	U	C2230	G2481
C1121	G1229	G1481	G1661	C1768	C1884	C2064	U2151	C	U2231	A2482
G1125	A1230	G1482	U1662	G1769	C1893	C2065	G2152	U	G2239	G2484
A1126	G1232	G1483	U1663	G1770	C1894	C2066	A2154	C	U2240	G2485
A1127	G1233	U1484	G1663	C1771	U1898	G2069	C2155	U	A2241	C2486
G1128	C1233	U1485	G1663	A1772	A1899	C2073	G2157	A	G2246	G2487
A1133	G1248	U1486	U1671	A1773	A1900	U2074	G	C	A2247	A2490
A1134	U1255	U1487	A1672	U1777	A1901	U2074	C	C	C2248	U2491
C1145	G1258	C1488	C1675	U1778	C1902	U2079	U	U	U2249	U2492
C1146	U1259	C1489	A1676	A1787	G1903	A2080	C	C	G2250	G2493
A1147	A1260	U1513	A1677	C1793	U1907	U2081	A	A	C2251	A2494
G1148	G1261	G1514	C1677	A1794	C1908	U2081	U	U	G2252	G2495
G1149	A1262	A1515	U1682	C1795	C1909	U2082	G	G	G2253	C2496
C1150	U1263	G1516	U1683	U1796	G1910	C1990	A	A	C2254	G2396
G1160	G1263	C1536	G1682	U1800	U1911	U1993	U	U	G2255	C2397
C1161	A1273	G1537	U1684	C1801	A1912	C1994	C	C	G2256	U2398
A1165	A1274	G1538	C1685	A1808	A1916	U1995	U	U	U2257	G2399
G1166	A1275	U1541	U1688	A1809	U1917	C1996	A	A	A2407	A2407
C1167	A1276	C1541	U1693	A1810	A1918	C1997	C	C	G2414	G2414
G1168	C1290	A1552	U1695	G1811	A1919	A1998	U	U	G2415	G2415
U1173	G1291	A1553	G1696	G1812	C1920	C2000	C	C	C2416	C2416
U1174	G1292	A1554	G1697	G1813	G1925	A2003	A	A	A2418	A2418
A1175	C1293	U1554	A1698	A1821	U1926	G2004	C	C	C2422	C2422
U1176	U1294	C1556	G1697	G1821	C1934	A2005	A	A		
G1177	A1302	C1557	A1698							
G1178	G1303	U1559								



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24622	Depositor
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 ($e^-/\text{\AA}^2$)	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	225.713	Depositor
Minimum map value	-115.182	Depositor
Average map value	4.811	Depositor
Map value standard deviation	21.585	Depositor
Recommended contour level	50.8	Depositor
Map size (\AA)	366.6, 366.6, 366.6	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.82, 2.82, 2.82	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).

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 [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	A	1530	0	0	0	0
2	B	2841	0	0	1	0
All	All	4371	0	0	1	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.

All (1) 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)
2:B:411:G:P	2:B:2407:A:P	3.16	0.44

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	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 [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-1184. These allow visual inspection of the internal detail of the map and identification of artifacts.

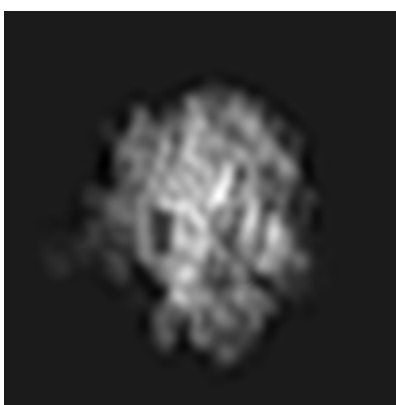
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 65



Y Index: 65

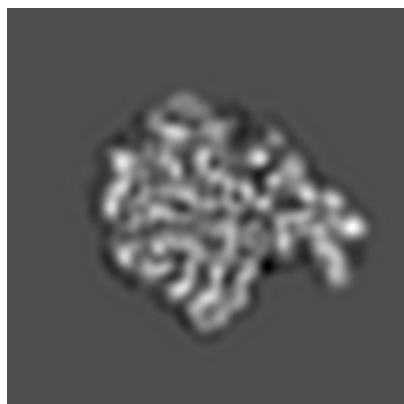


Z Index: 65

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: 67

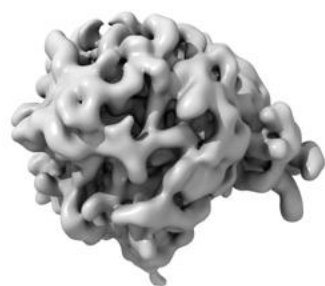


Z Index: 60

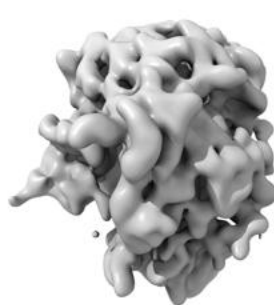
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

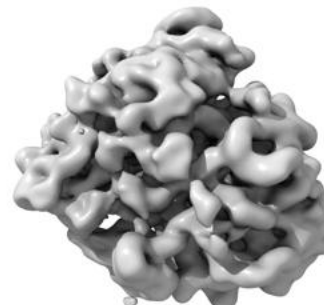
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 50.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

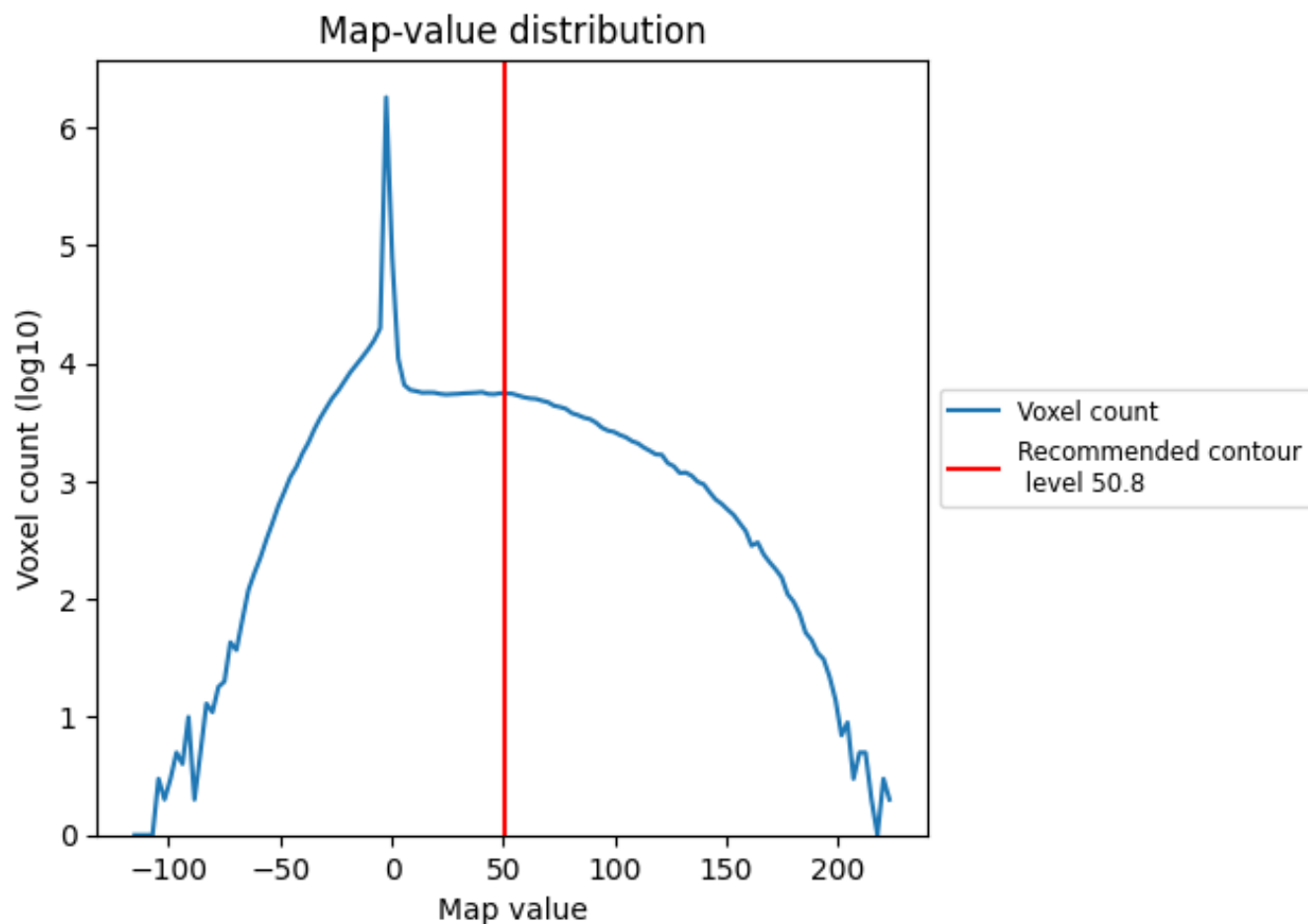
6.5 Mask visualisation

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

7 Map analysis [i](#)

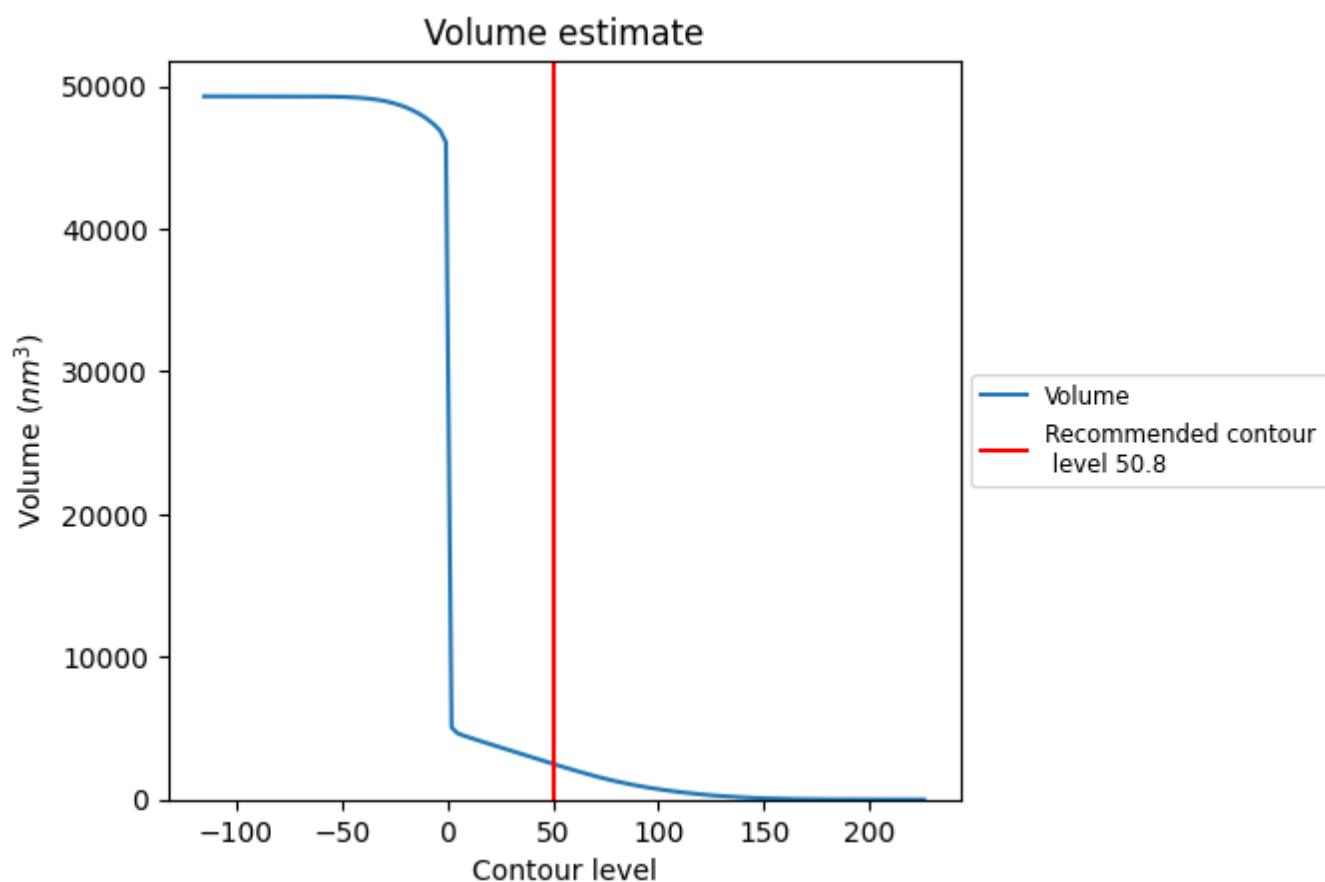
This section contains the results of statistical analysis of the map.

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.

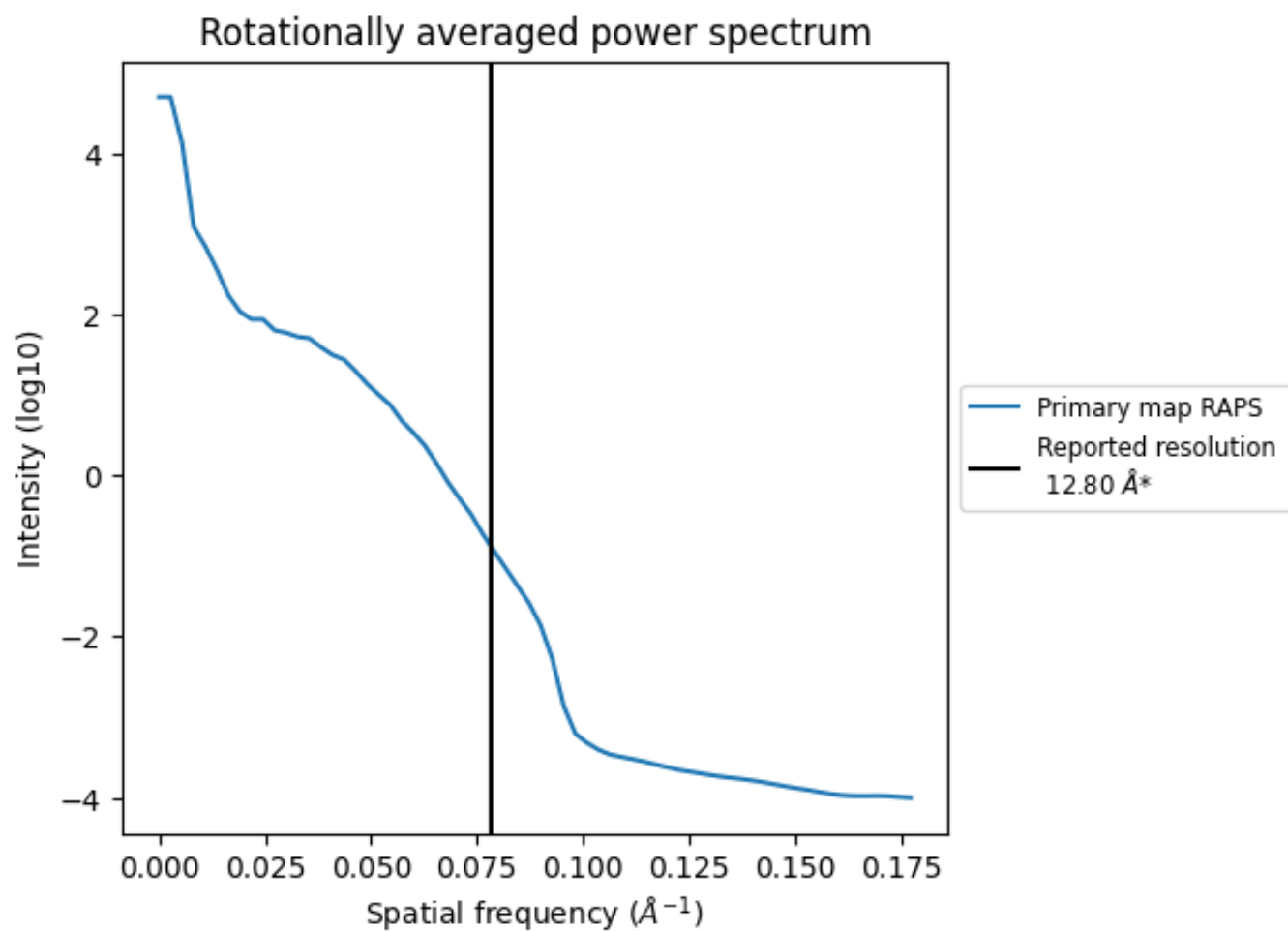
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2469 nm³; this corresponds to an approximate mass of 2230 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 0.078 Å⁻¹

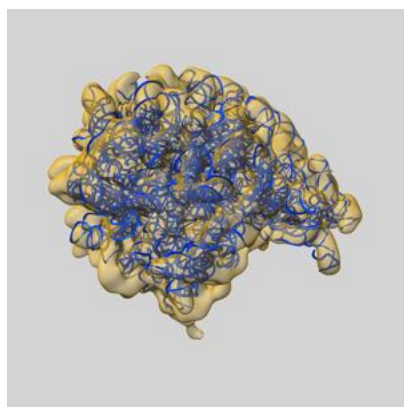
8 Fourier-Shell correlation

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

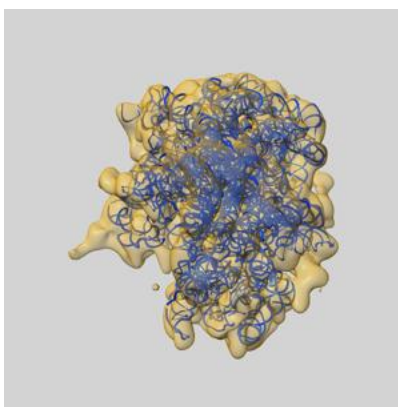
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1184 and PDB model 3DG4. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

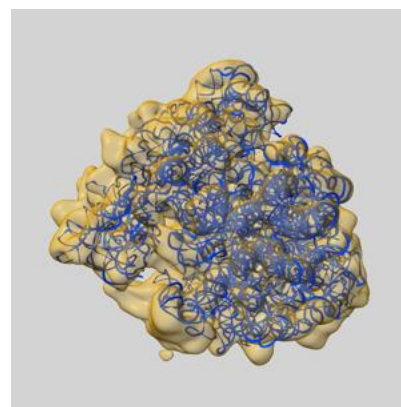
9.1 Map-model overlay [i](#)



X



Y



Z

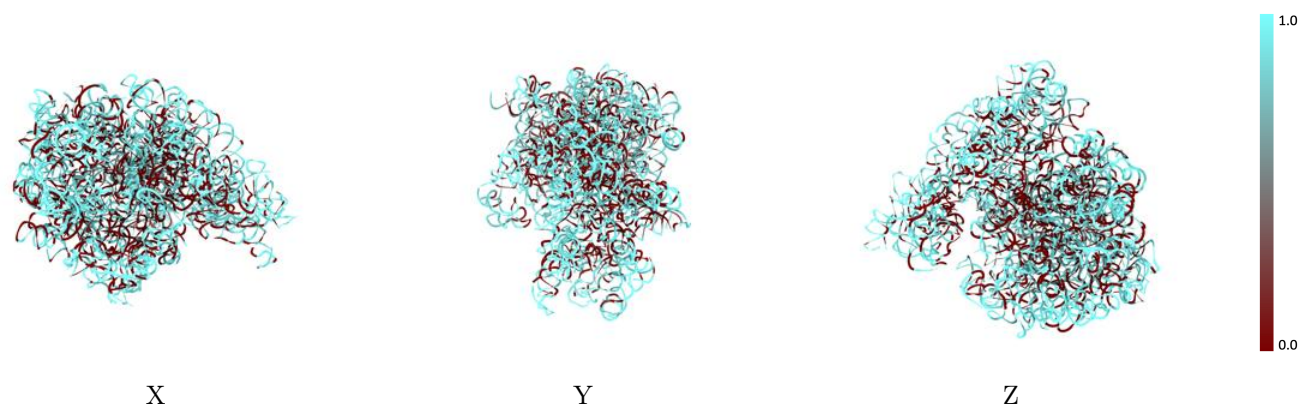
The images above show the 3D surface view of the map at the recommended contour level 50.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



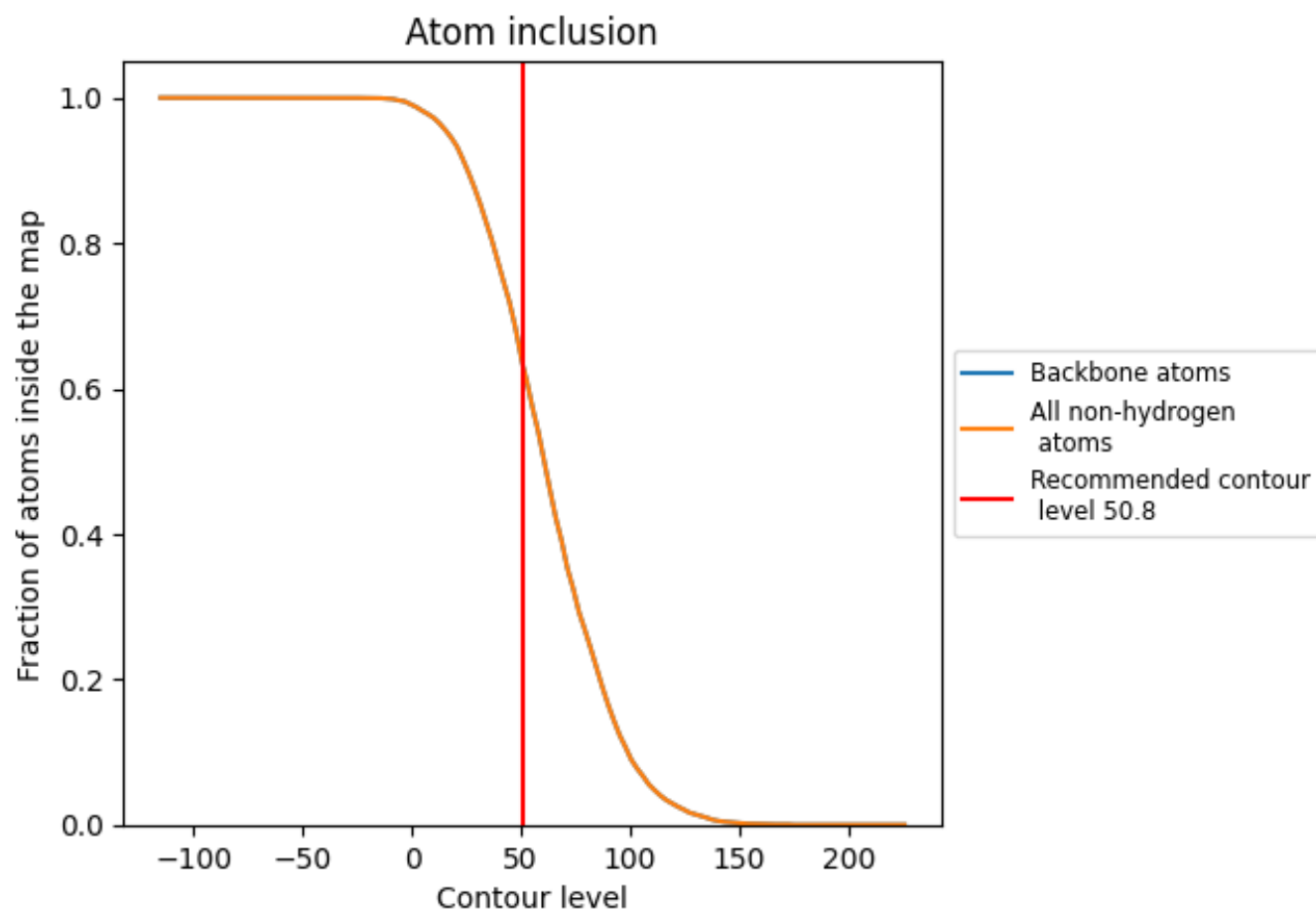
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (50.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 63% 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 (50.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6319	<div></div> 0.0020
A	<div></div> 0.6183	<div></div> 0.0010
B	<div></div> 0.6392	<div></div> 0.0030

