



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 11:23 AM EST

PDB ID : 3DG5
EMDB ID : EMD-1302
Title : Coordinates of 16S and 23S rRNAs fitted into the cryo-EM map of RF3-bound termination complex
Authors : Gao, H.; LeBarron, J.; Frank, J.
Deposited on : 2008-06-12
Resolution : 15.50 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

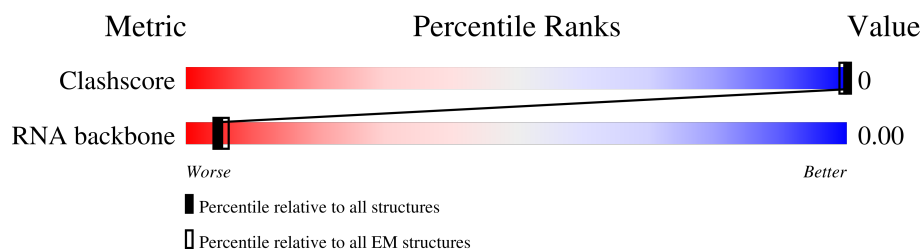
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

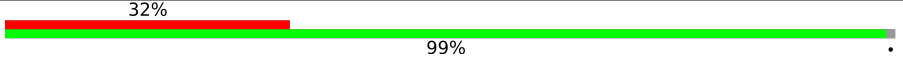
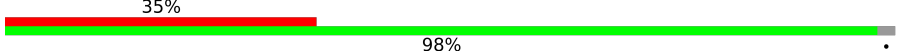
The reported resolution of this entry is 15.50 Å.

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		

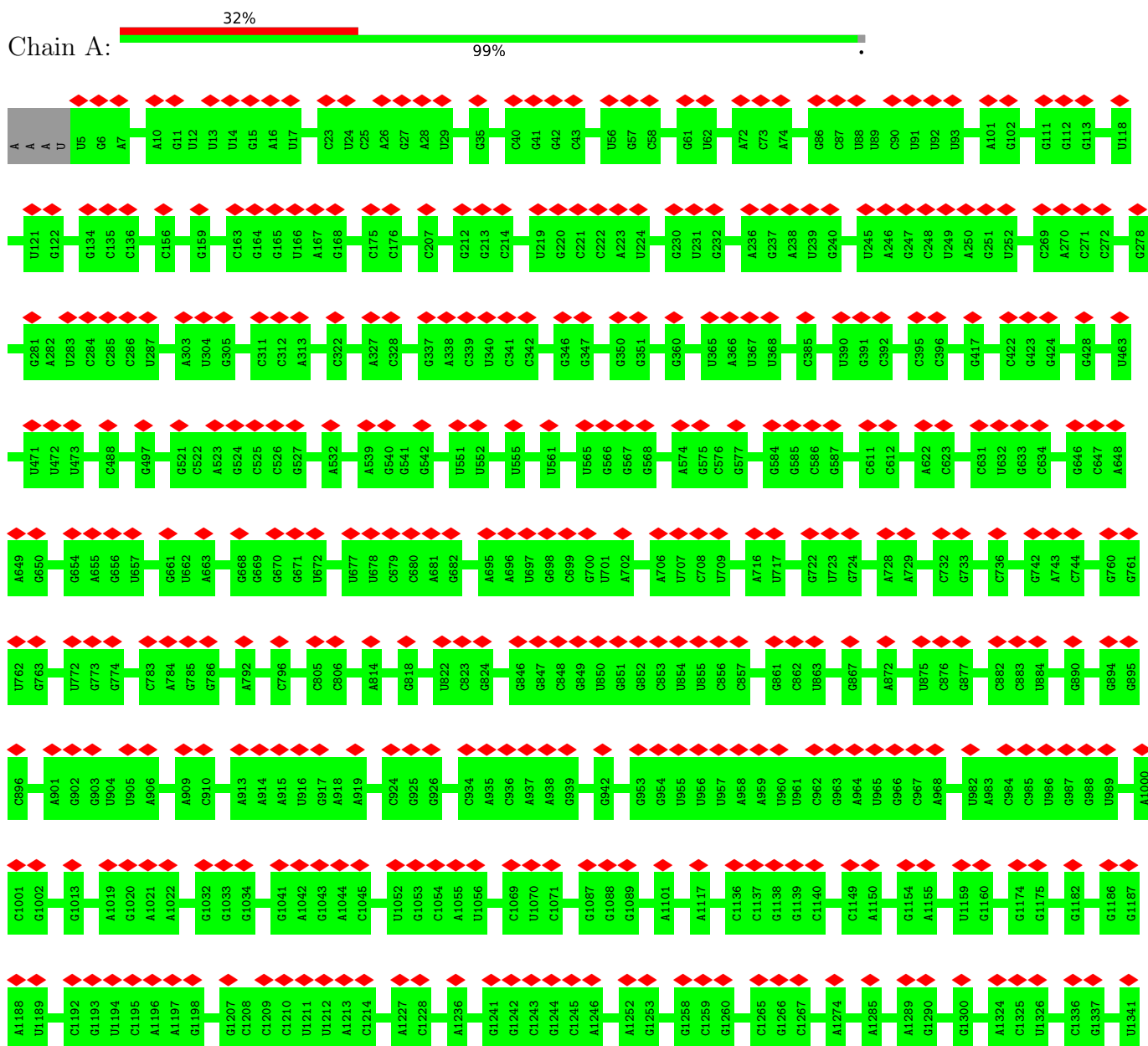
- Molecule 2 is a RNA chain called 23S Ribosomal RNA from E. coli.

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

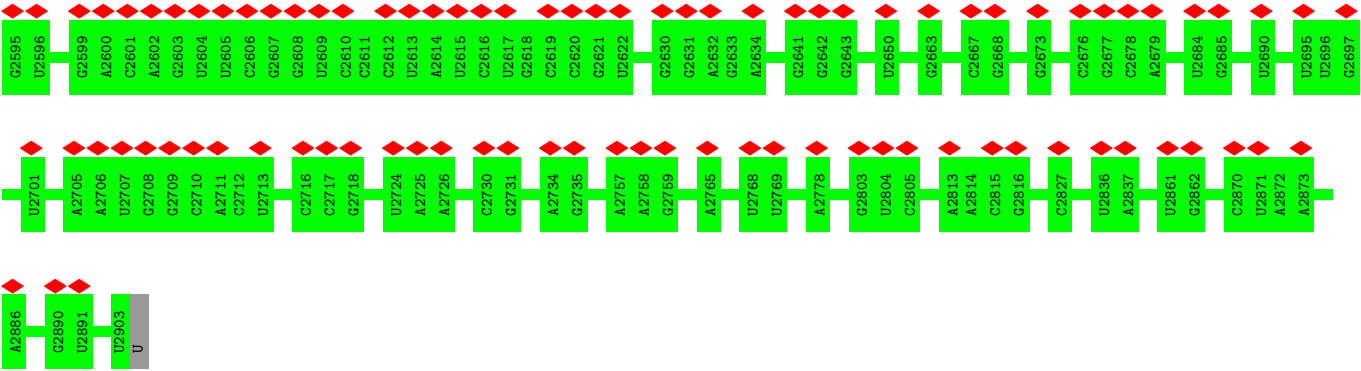
3 Residue-property plots

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



A2482	C2483	G2484	G2487	G2490	U2491	U2492	U2493	G2494	G2495	G2496	A2497	G2505	U2506	G2509	C2510	U2511	C2512	G2524	G2525	A2534	G2535	G2536	U2537	C2538	C2539	C2540	G2545	U2546	A2547	U2548	G2553	C2556	G2557	C2558	C2559	A2560	U2561	U2562	U2563	G2567	U2568	G2569	G2583	U2584	U2585	U2586	A2587		
G2382	G2383	U2387	A2388	G2389	U2390	G2391	G2397	U2398	G2399	U2402	G2413	G2414	G2415	G2421	C2422	U2423	C2424	U2431	A2432	A2433	A2434	A2435	G2436	G2437	U2438	A2439	C2440	U2441	C2442	U2449	A2450	A2451	C2452	A2453	G2454	G2455	C2456	U2460	A2461	C2462	C2463	G2464	C2465	A2471	G2472	U2473	U2474	C2480	A2481
G2242	U2243	U2244	U2245	G2246	G2251	C2254	G2255	G2256	U2257	C2258	U2259	C2260	C2261	A2270	G2271	U2272	A2273	A2274	C2275	G2276	G2279	G2280	U2296	A2297	A2298	U2299	C2300	C2301	U2302	A2309	A2322	G2323	U2324	G2325	C2326	G2330	C2339	A2340	G2341	C2347	U2348	C2362	G2363	C2364	G2365	C2380	A2381		
C	G	A	C	C	U	U	G	A	A	A	A	A	U	A	C	C	A	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C		
U1982	G1983	G1984	C1985	C1986	A1987	G1988	G1989	C1990	U1993	C1994	U1995	C1996	C1997	A1998	C1999	C2000	C2001	G2004	C2008	A2009	U2016	A2020	G2024	A2030	A2033	U2034	G2035	A2042	C2045	G2046	C2047	C2050	A2051	A2059	A2060	C2063	C2064	C2065	C2066	G2067	U2068	C2069	A2070	U2076	A2077				
C2078	U2079	A2080	U2081	U2085	U2086	A2090	C2103	C2104	U2105	U2106	G2107	G2110	U	U	U	U	A	G	G	A	U	U	G	G	G	C	U	U	U	G2133	A2134	G2140	G2141	A2142	A2147	G2148	C2150	U2149	U2151	G2152	C2153	A2154	U2155	G2156	G2157	A	G	C	
G1907	C1908	C1909	G1910	U1911	A1912	A1913	C1914	U1915	A1916	U1917	A1918	G1922	U1923	C1924	C1925	U1926	G1930	U1931	A1932	G1933	C1934	A1937	A1938	U1939	C1942	U1943	C1947	G1948	G1949	G1950	U1951	A1952	U1956	C1957	C1958	G1959	A1960	U1963	A1966	G1972	C1973	C1974	G1975	U1976	A1977	U1978	U1979	G1980	A1981
C1800	A1801	A1805	C1806	G1807	A1808	U1812	U1820	A1821	C1822	G1831	C1832	C1833	U1834	G1835	C1836	C1837	G1840	U1841	G1842	C1843	G1849	G1850	A1853	A1854	G1861	G1862	G1875	G1878	C1879	U1880	C1881	U1882	U1883	G1884	A1885	U1886	C1887	G1888	C1893	C1894	C1895	G1896	A1899	A1900	A1901	C1902	G1903		
U1692	U1693	C1694	G1695	G1696	G1697	A1698	G1699	G1702	G1703	C1706	G1707	C1708	U1709	A1713	U1720	G1721	G1733	G1734	A1735	G1738	A1744	A1745	U1746	U1747	C1748	A1749	G1750	U1758	C1761	A1762	C1768	U1769	G1770	C1771	A1772	A1773	U1777	A1785	A1786	A1787	C1788	C1793	A1794	C1795	U1796				
G1587	G1588	U1589	A1590	A1591	C1592	A1608	A1609	G1613	G1619	G1620	U1624	C1625	A1626	G1627	G1631	A1637	G1642	G1643	C1644	G1645	C1646	A1650	G1651	A1652	G1653	A1654	A1655	C1656	G1659	G1660	G1661	U1662	G1663	A1664	A1665	G1674	C1675	A1676	A1677	G1681	G1682	U1683	G1684	C1685	C1686	G1687	C1691		
C1289	C1290	C1291	U1294	C1295	A1301	A1302	C1305	G1311	U1312	C1323	G1324	G1334	C1335	A1336	C1348	C1349	C1350	A1354	G1355	G1356	C1357	G1368	G1369	G1374	A1378	A1384	A1383	U1396	G1407	G1408	U1409	G1418	A1419	G1420	G1421	G1422	G1425	C1428	G1429	A1430	A1431								
G1432	A1433	A1434	G1435	G1436	C1437	U1440	U1443	C1446	C1461	G1464	G1465	U1466	U1467	U1468	G1478	A1490	C1498	C1499	G1500	G1501	A1504	U1513	G1514	G1529	C1536	G1537	G1538	U1539	G1540	C1541	A1548	A1552	G1555	C1556	U1559	G1560	C1565	A1569	U1576										
A1147	U1148	C1149	C1150	C1167	G1168	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	A1189	G1195	U1199	C1200	G1215	G1216	U1217	G1218	U1219	A1226	C1229	A1230	U1231	C1243	A1244	G1245	A1246	A1247	G1248	U1255	G1256	C1257	U1258	G1259	A1260	A1274	A1275	A1276	G1277	A1286	A1287	G1288		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45000	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	242.787	Depositor
Minimum map value	-80.434	Depositor
Average map value	5.959	Depositor
Map value standard deviation	23.236	Depositor
Recommended contour level	57.2	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	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 [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.

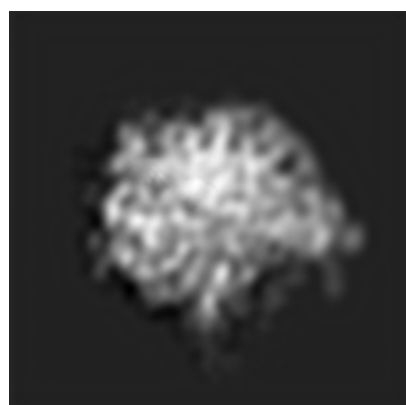
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1302. These allow visual inspection of the internal detail of the map and identification of artifacts.

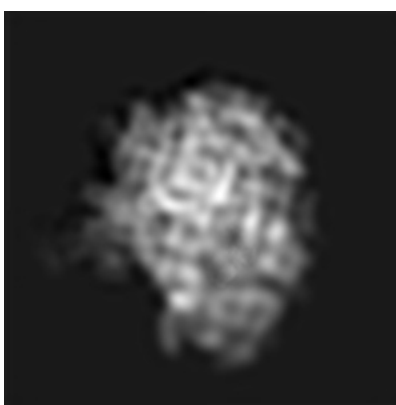
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

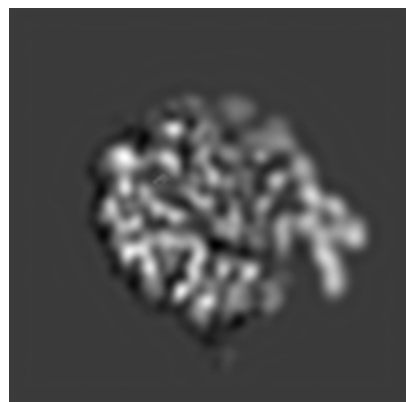


Z

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

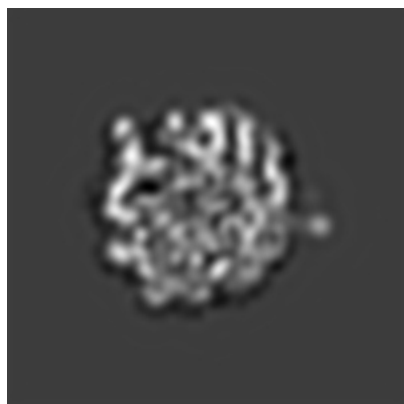


Z Index: 65

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: 81



Y Index: 68

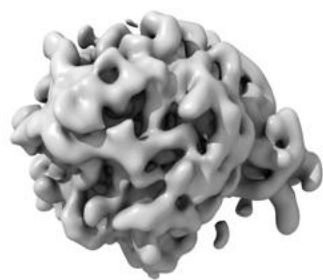


Z Index: 80

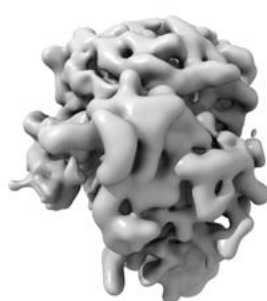
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

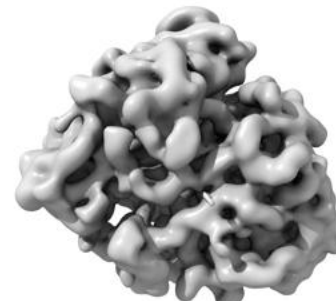
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 57.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

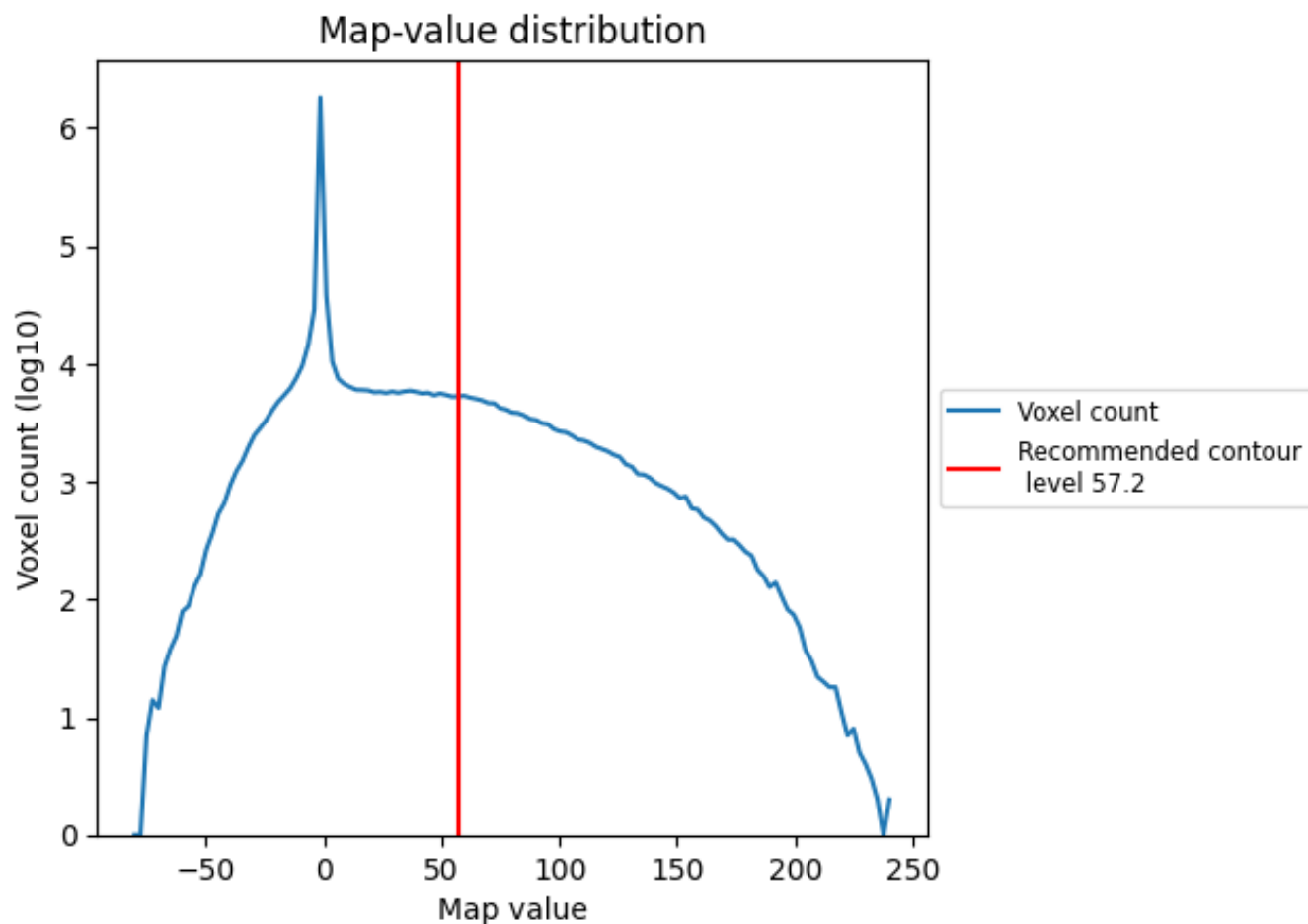
6.5 Mask visualisation

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

7 Map analysis [i](#)

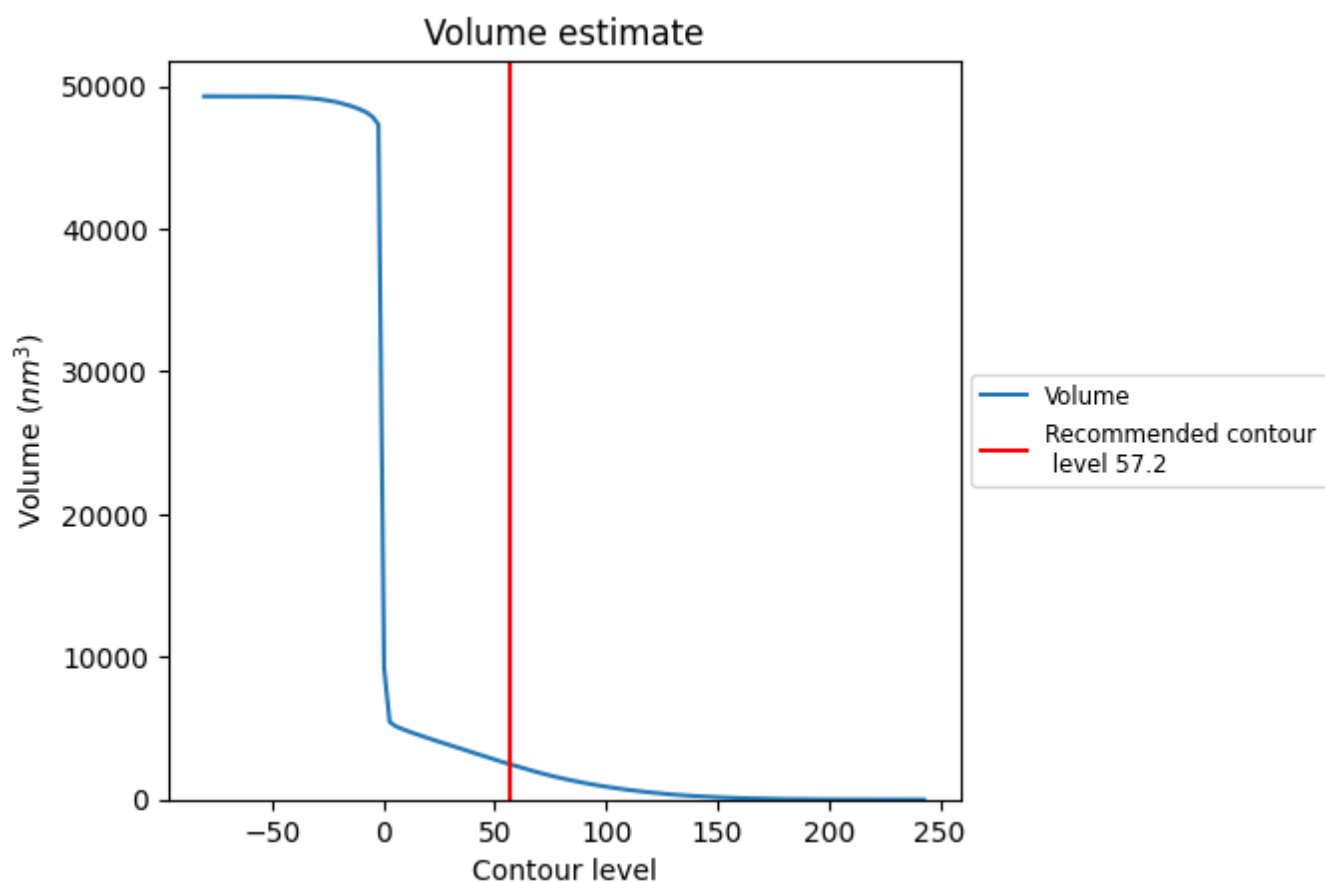
This section contains the results of statistical analysis of the map.

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.

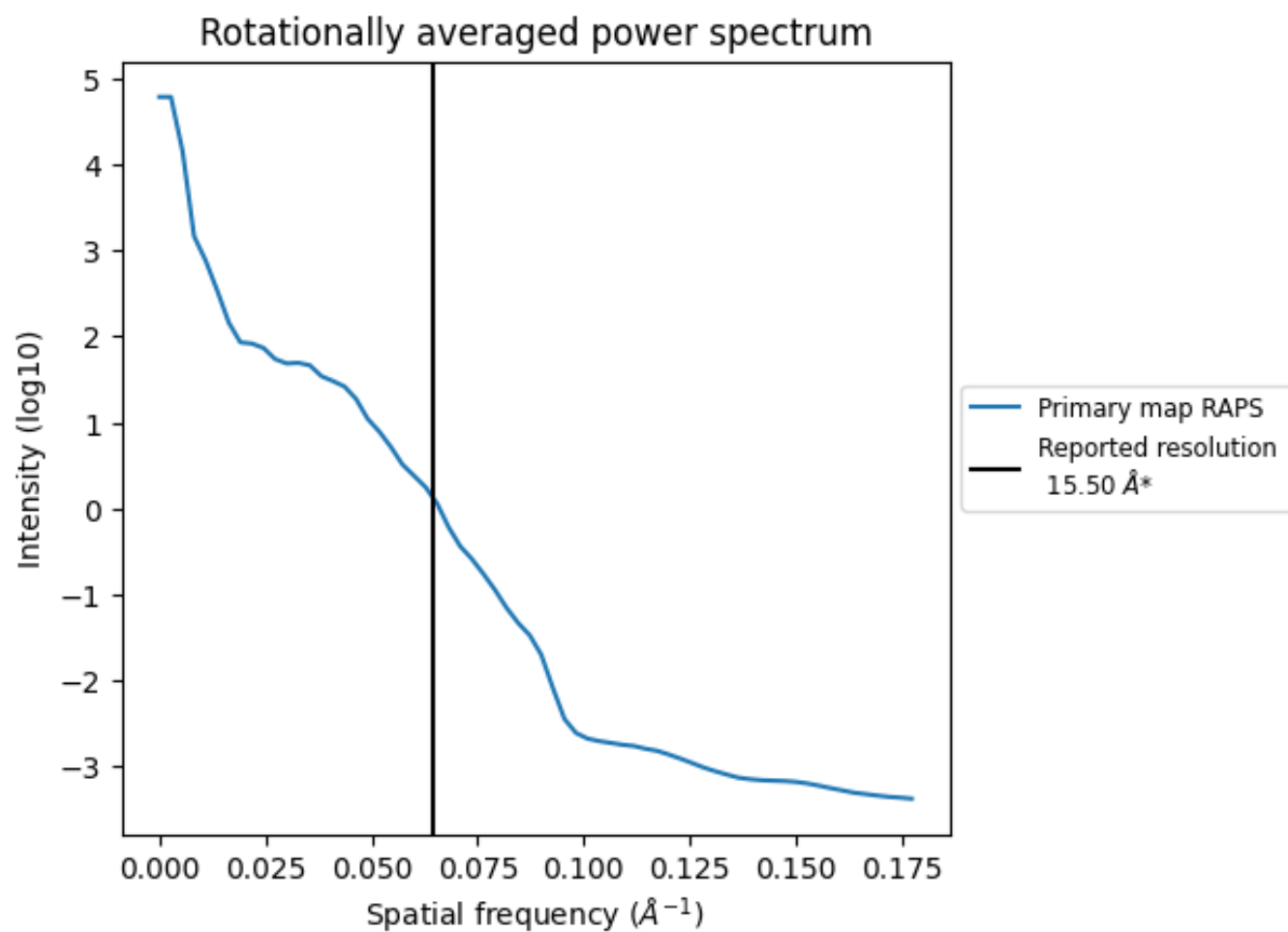
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2459 nm³; this corresponds to an approximate mass of 2221 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 0.065 Å⁻¹

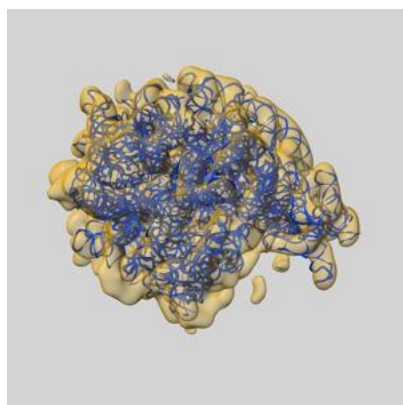
8 Fourier-Shell correlation

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

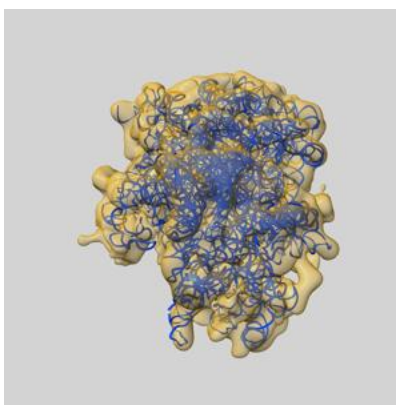
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1302 and PDB model 3DG5. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

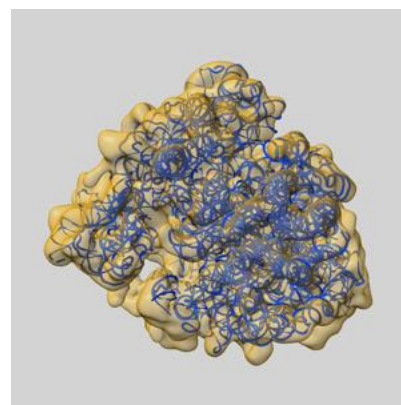
9.1 Map-model overlay [i](#)



X



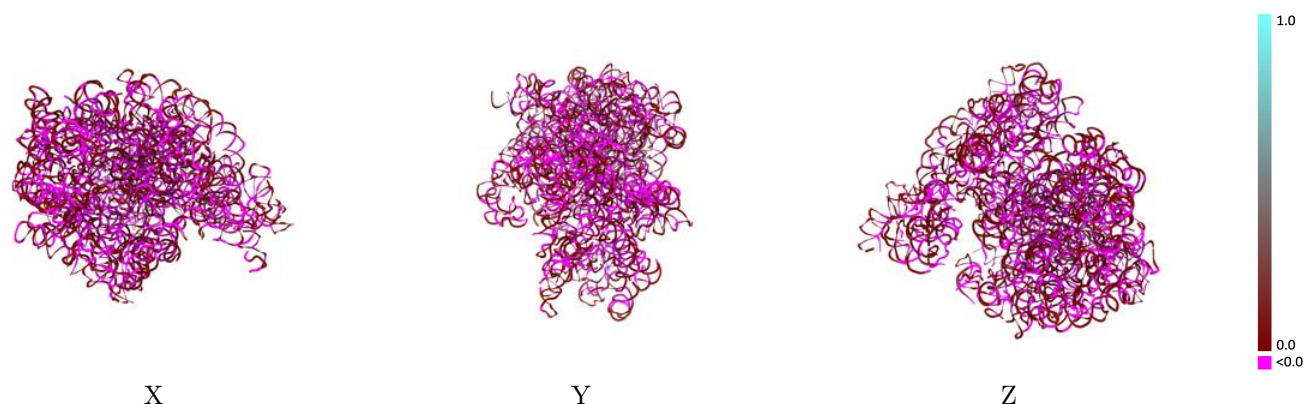
Y



Z

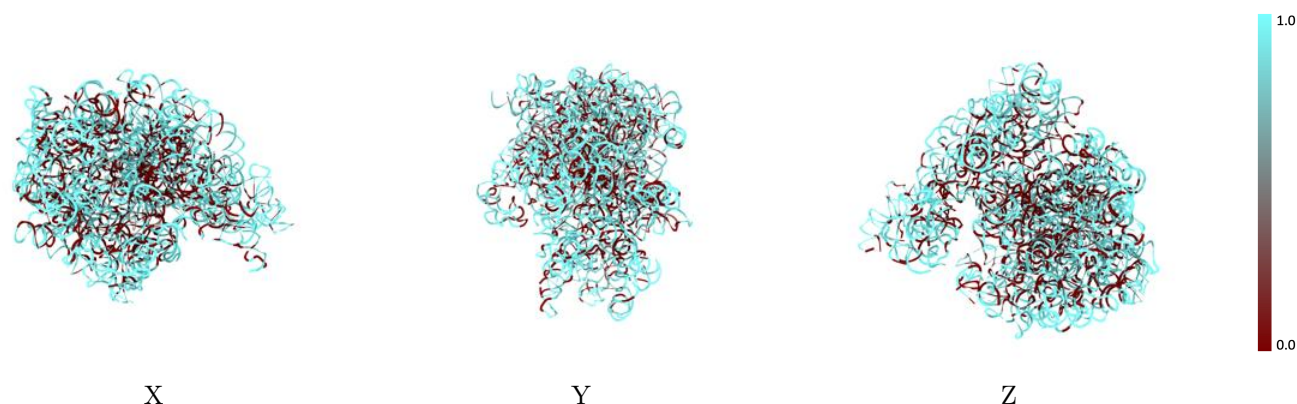
The images above show the 3D surface view of the map at the recommended contour level 57.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



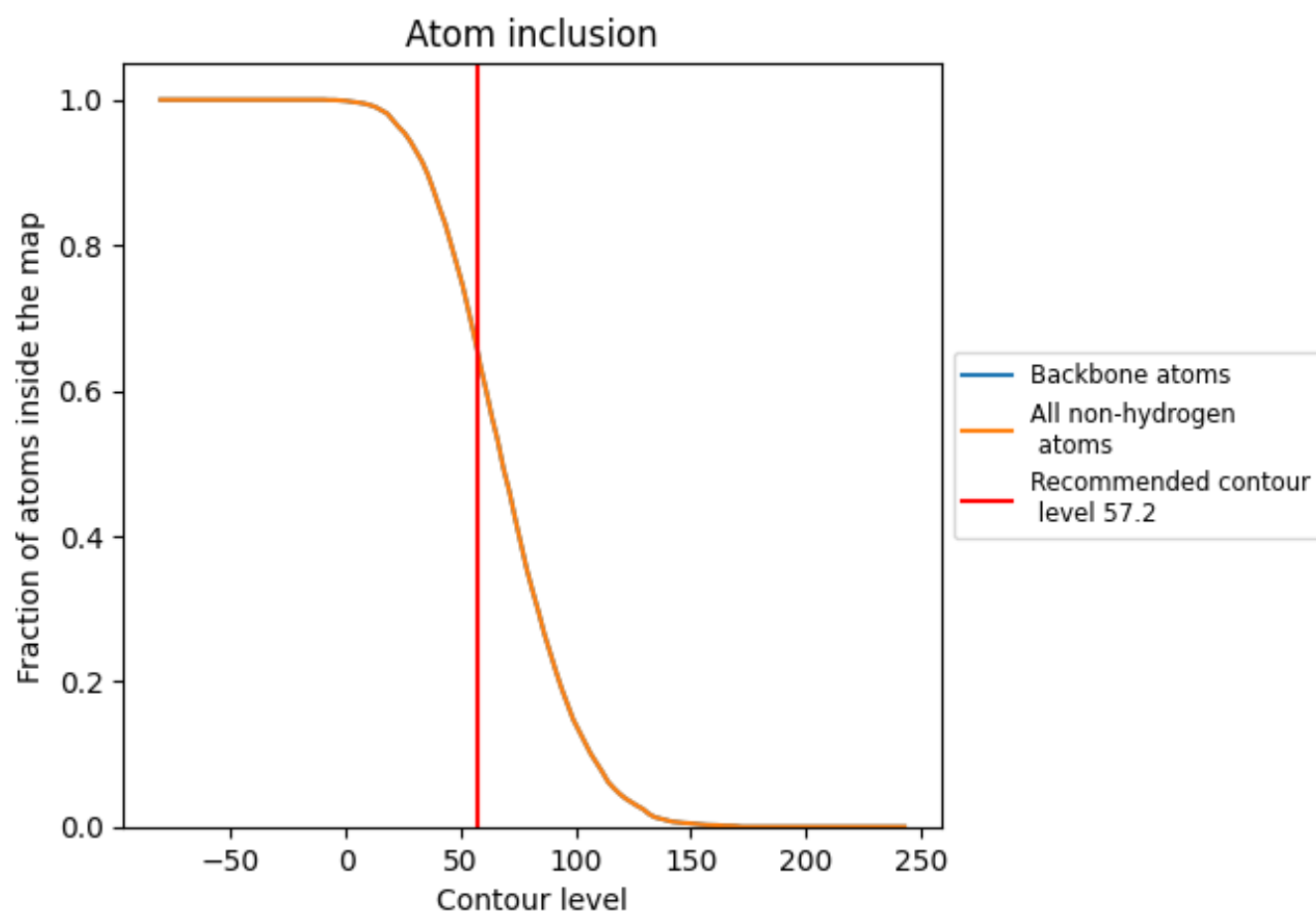
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (57.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (57.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6559	<div></div> 0.0040
A	<div></div> 0.6745	<div></div> 0.0030
B	<div></div> 0.6459	<div></div> 0.0050

