



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 11:00 AM EST

PDB ID : 3DG2
EMDB ID : EMD-1056
Title : Coordinates of 16S and 23S rRNAs fitted into the cryo-EM map of a pre-translocation complex
Authors : Gao, H.; LeBarron, J.; Frank, J.
Deposited on : 2008-06-12
Resolution : 10.00 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

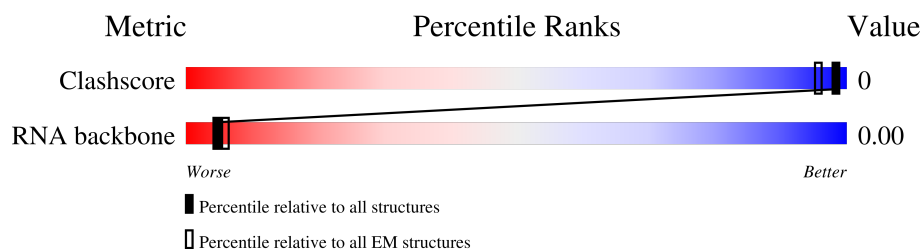
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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	<div> <div>35%</div> <div>99%</div> </div>
2	B	2904	<div> <div>43%</div> <div>98%</div> </div>

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		

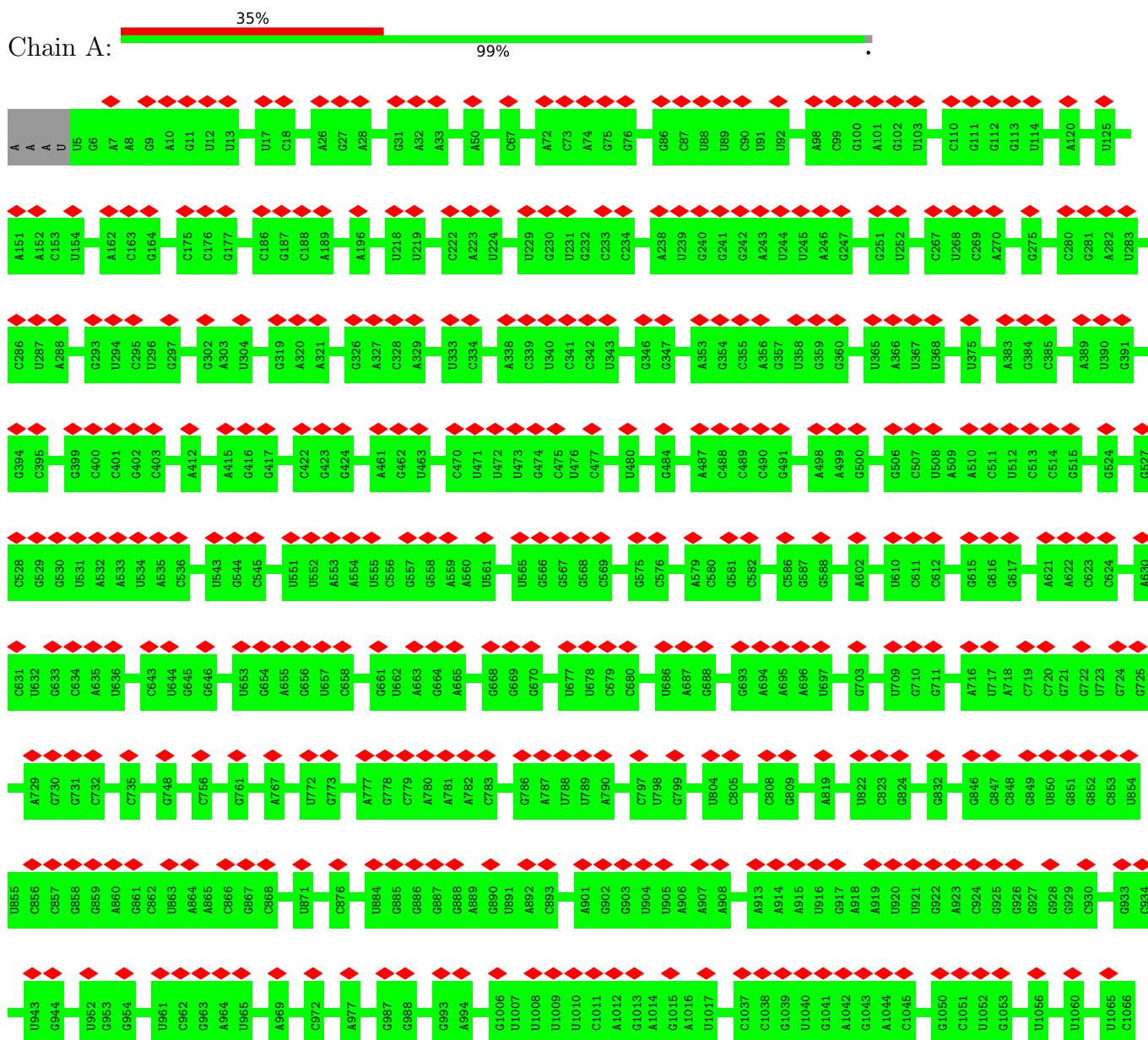
- Molecule 2 is a RNA chain called 23S Ribosomal RNA from E. coli.

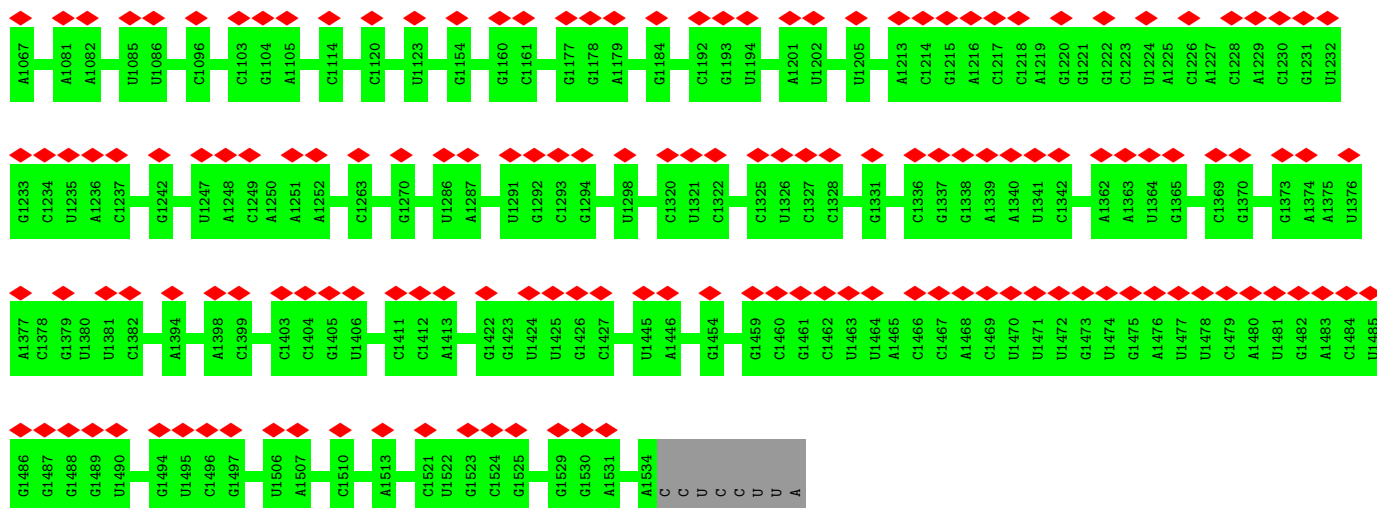
Mol	Chain	Residues	Atoms		AltConf	Trace
2	B	2841	Total	P	0	2841
			2841	2841		

3 Residue-property plots

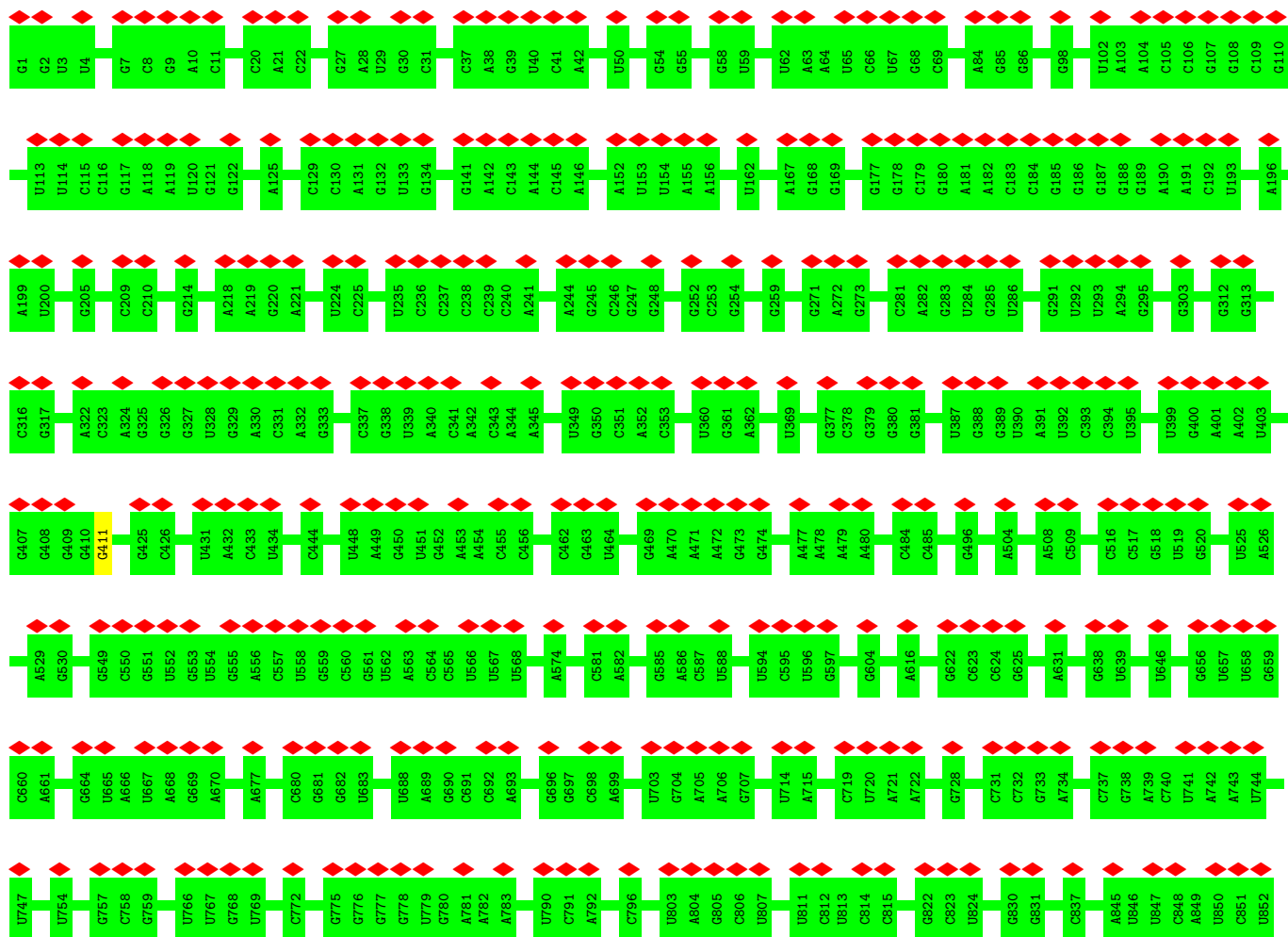
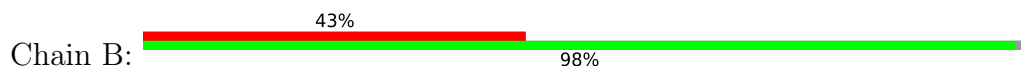
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



C1958	C1959	A1960	U1963	G1964	C1965	C1966	C1967	A1970	G1975	U1976	A1977	C1985	C1986	A1987	G1988	G1989	C1996	G2004	A2005	C2006	U2007	C2008	A2009	G2012	U2017	G2018	C2023	G2024	C2025	U2026	G2027	U2028	C2029	A2030	A2033	U2034	G2035	C2044	C2045	G2046	C2047	G2048	G2049	C2050	G2053	A2054			
A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	C2067	U2068	C2069	A2070	C2072	C2073	U2074	U2075	U2076	A2077	G1988	G1989	C1996	G2004	A2005	C2006	U2007	C2008	A2009	G2012	U2017	G2018	C2023	G2024	C2025	U2026	G2027	U2028	C2029	A2030	A2033	U2034	G2035	C2044	C2045	G2046	C2047	G2048	G2049	C2050	G2053	A2054
C1874	A1877	G1878	C1879	G1884	A1885	U1886	C1887	G1888	A1889	A1890	C1893	C1894	C1895	C1896	G1897	U1898	A1899	A1900	A1901	C1909	G1910	U1911	A1912	A1913	C1914	U1915	A1916	U1917	G1921	G1922	U1926	G1929	G1930	U1931	A1932	G1933	C1934	G1935	U1943	U1946	C1947	G1948	G1949	G1950	A1953	G1954	U1955	U1956	C1957
G1770	C1771	A1772	A1773	A1784	A1785	A1786	A1787	C1788	A1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	C1804	A1805	C1806	G1807	A1808	A1809	A1810	G1811	U1812	U1820	A1821	G1826	A1829	C1830	G1831	C1832	C1833	U1834	G1835	C1838	G1839	G1840	U1841	G1842	C1843	G1850	U1851	U1859	G1860	G1861	G1862	G1863	G1873
U1680	G1681	U1682	U1683	G1684	C1685	C1686	G1687	U1688	A1689	A1690	C1691	U1692	G1695	G1702	G1703	C1706	G1707	C1708	U1709	A1713	G1718	G1719	U1720	G1721	G1731	C1732	G1733	G1734	A1735	U1736	G1737	G1738	A1739	G1740	A1745	A1746	U1747	C1748	A1749	G1750	U1751	C1752	A1755	U1759	G1762	G1767	C1768	U1769	
C1592	A1593	A1597	A1598	G1601	U1602	A1603	A1608	A1609	C1612	G1613	A1618	G1619	G1620	G1623	U1624	C1625	A1626	G1627	G1628	U1629	A1632	U1636	G1645	C1646	U1647	U1648	G1649	A1650	A1654	A1655	C1656	G1659	G1660	G1661	U1662	G1663	G1666	G1667	A1668	A1669	G1673	G1674	C1675	A1676	A1677				
G1479	C1480	U1481	G1482	G1483	A1489	A1490	G1491	G1492	A1495	A1496	A1502	A1503	A1504	A1505	U1506	G1514	G1527	A1528	G1529	C1536	G1537	G1538	C1541	C1547	A1548	A1549	C1550	A1551	A1552	A1553	U1554	G1555	C1556	U1559	G1560	U1563	C1564	G1565	A1566	G1567	A1570	A1571	A1572	G1588	U1589	A1590	A1591		
A1275	A1276	G1288	C1289	G1292	C1293	U1294	C1295	G1296	C1297	C1298	A1301	A1302	G1303	A1308	G1309	G1310	G1311	C1315	A1322	C1323	G1324	U1325	U1326	A1327	G1333	G1334	C1335	A1336	G1337	U1344	C1345	G1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	C1357	G1361	C1362	C1363	G1364	A1365	G1369
A1169	C1172	A1175	U1176	U1177	C1178	U1179	U1180	U1184	G1185	G1193	C1200	U1209	G1215	G1216	U1217	G1218	U1219	G1220	C1221	A1226	A1237	U1240	A1241	U1242	C1243	A1244	G1245	A1246	A1247	G1248	U1249	A1254	U1255	G1256	U1257	U1258	G1259	A1260	C1261	A1265	A1268	A1269	C1270	U1273	A1274				
A1050	G1051	C1052	G1055	C1064	U1065	U1066	A1067	G1068	G1074	C1075	C1076	A1077	U1078	C1079	A1080	A1090	G1091	C1092	G1093	U1094	A1095	A1096	U1105	C1114	G1115	G1116	C1117	C1118	U1119	G1120	C1121	G1122	A1126	A1127	G1128	A1129	A1133	G1136	G1137	G1138	G1139	C1146	A1147	U1148	G1149	C1150	C1167	G1168	
G949	G950	C951	G952	G953	G954	U955	G956	C957	U958	A959	C968	A975	G976	A980	A981	C982	A983	C986	C987	G993	C994	C995	A996	U999	A1000	A1001	G1002	G1003	U1004	C1005	C1013	A1021	G1022	U1023	G1024	G1025	C1030	G1031	A1032	U1033	G1034	G1041	G1042	C1043	C1044	G1047	A1048	C1049	
C953	C954	G955	G958	G959	C965	A966	C967	U968	G969	U970	U971	U972	C973	G974	A978	G	G	G	C	U	C	A	U	C	C998	C902	A911	C912	U913	G914	U934	C935	A936	C937	G940	A941	C944	A945	C946	A947	C948								



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52181	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	250.773	Depositor
Minimum map value	-142.587	Depositor
Average map value	1.513	Depositor
Map value standard deviation	24.331	Depositor
Recommended contour level	43.4	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	2.88	0.72

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.

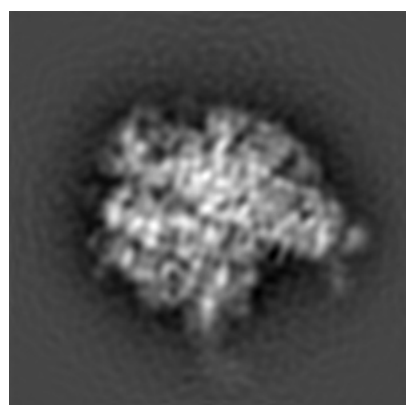
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1056. These allow visual inspection of the internal detail of the map and identification of artifacts.

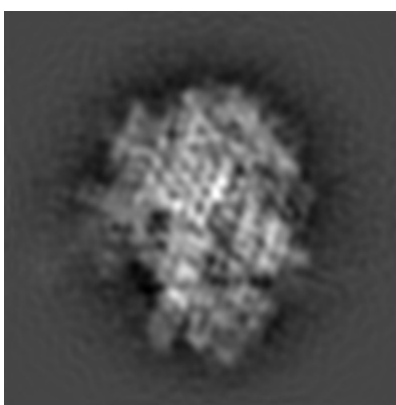
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

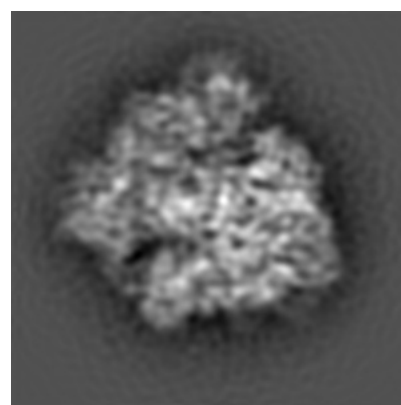
6.1.1 Primary map



X



Y

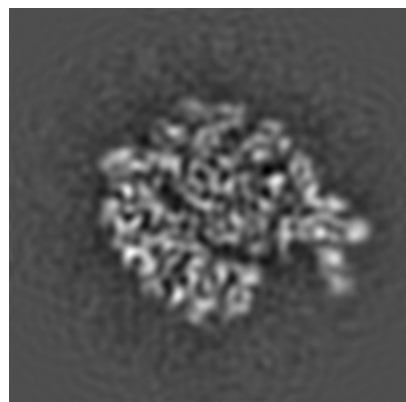


Z

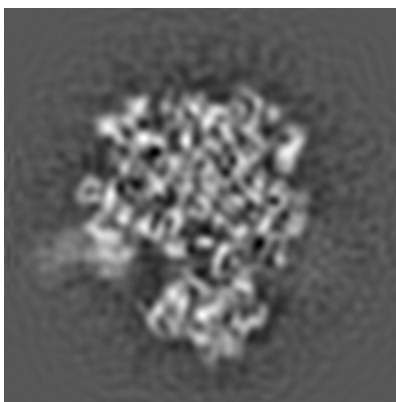
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

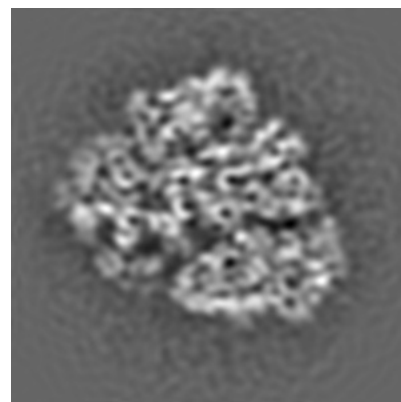
6.2.1 Primary map



X Index: 65



Y Index: 65

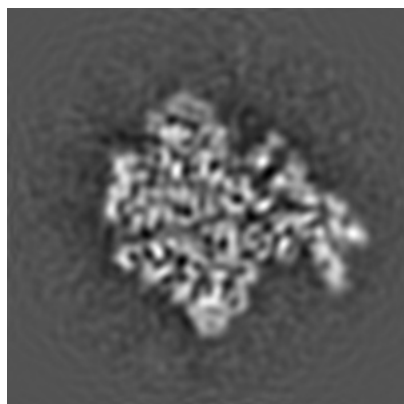


Z Index: 65

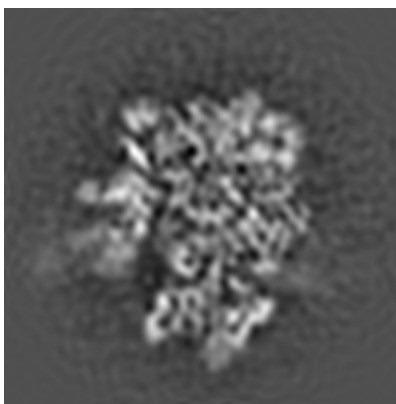
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

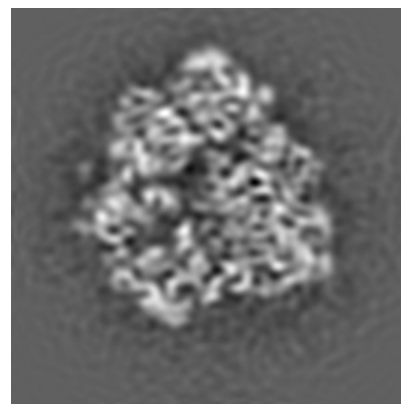
6.3.1 Primary map



X Index: 68



Y Index: 68

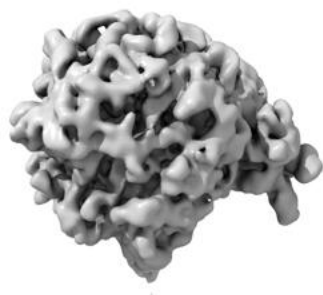


Z Index: 58

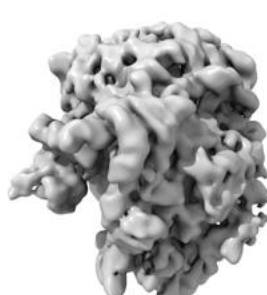
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

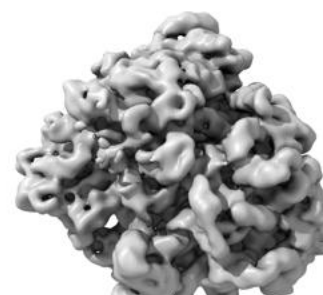
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 43.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

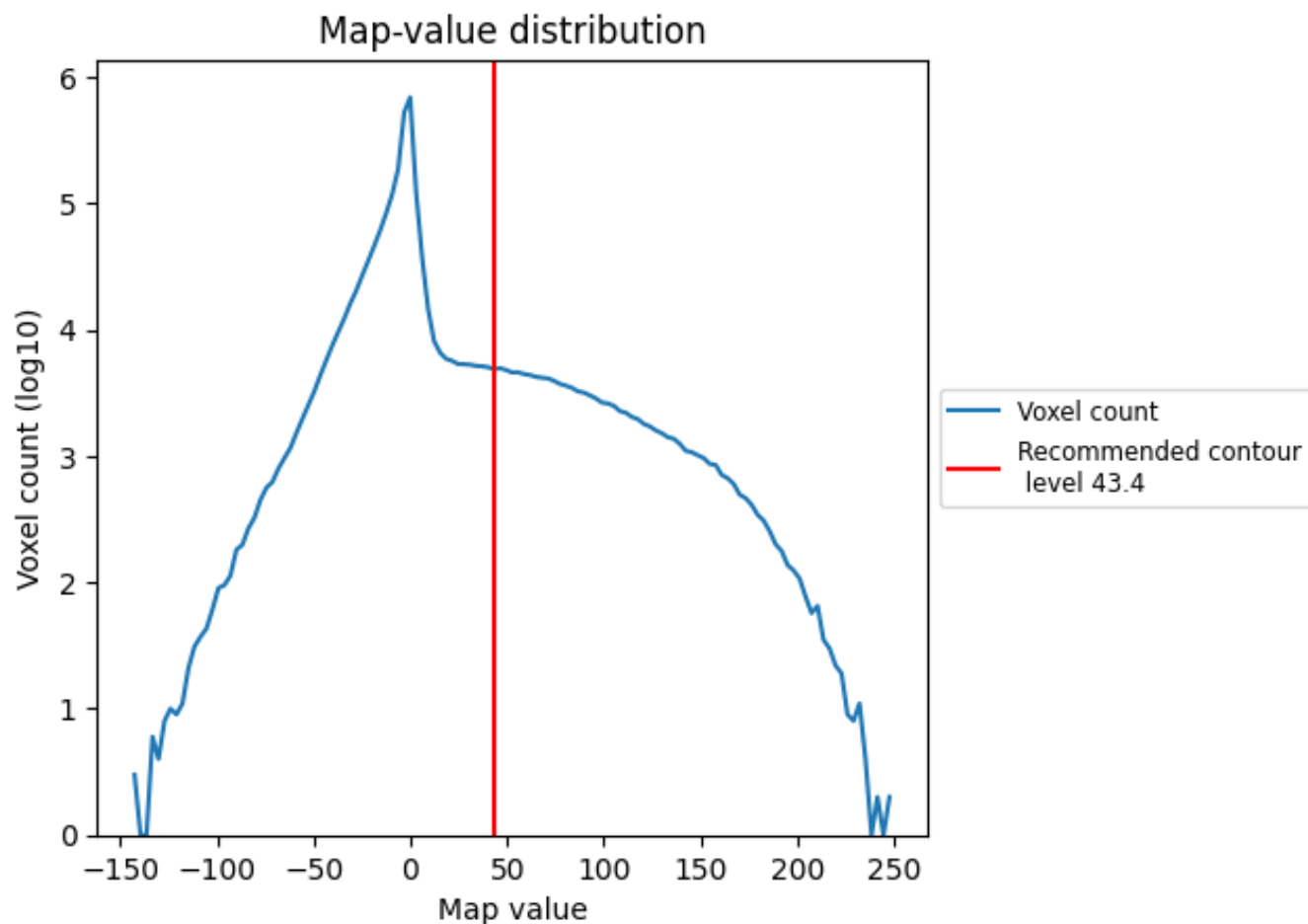
6.5 Mask visualisation

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

7 Map analysis [i](#)

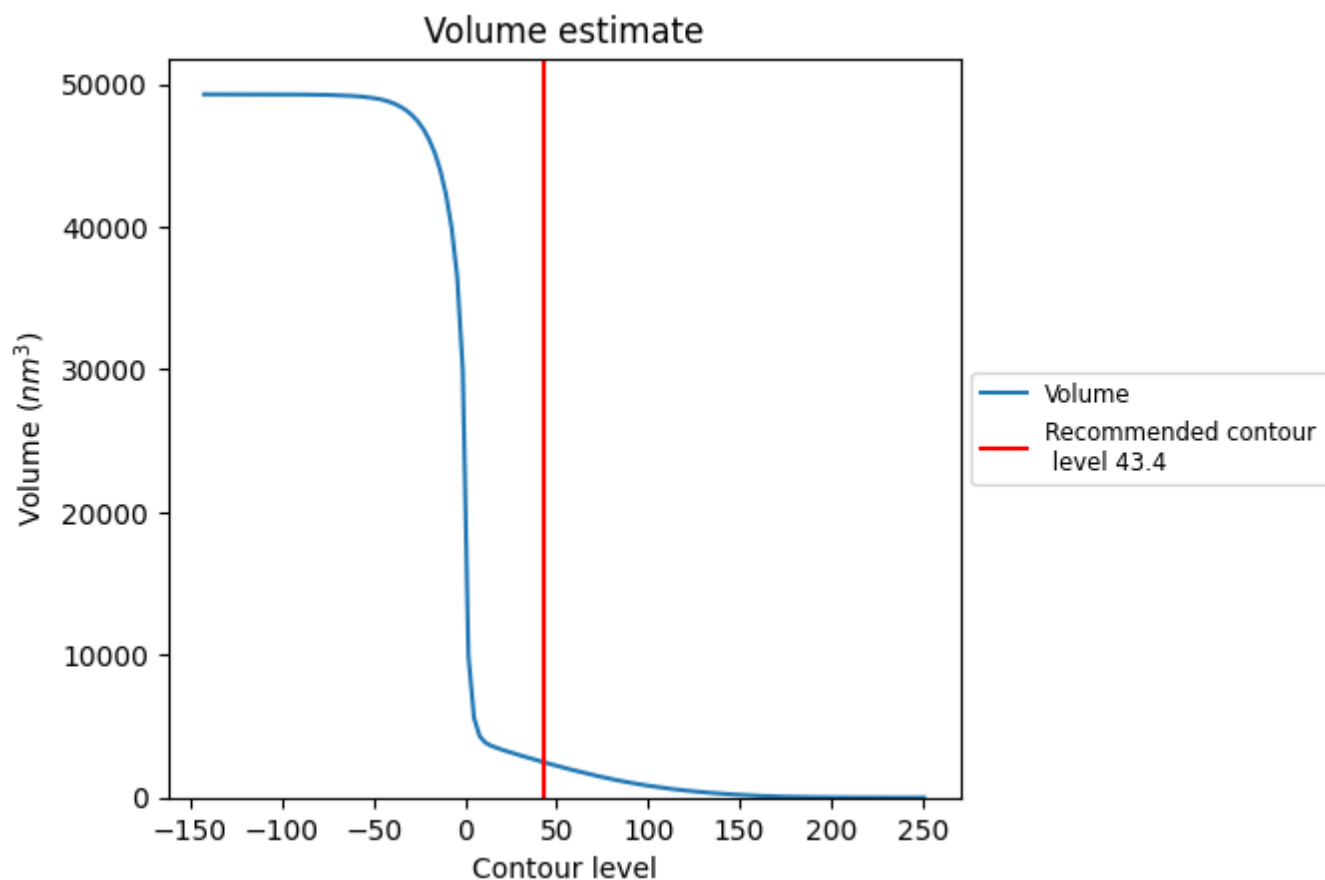
This section contains the results of statistical analysis of the map.

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.

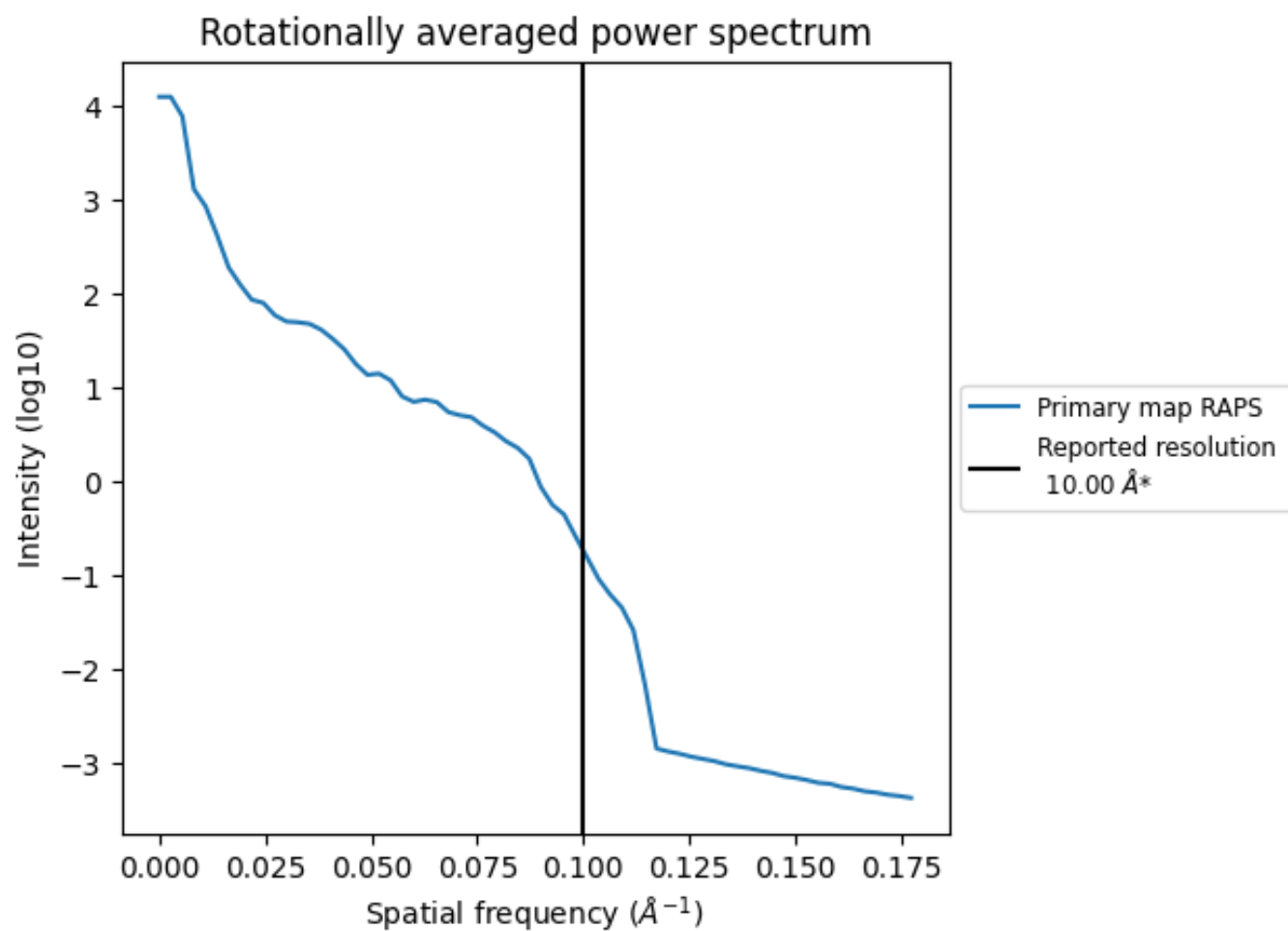
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2462 nm³; this corresponds to an approximate mass of 2224 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 0.100 Å⁻¹

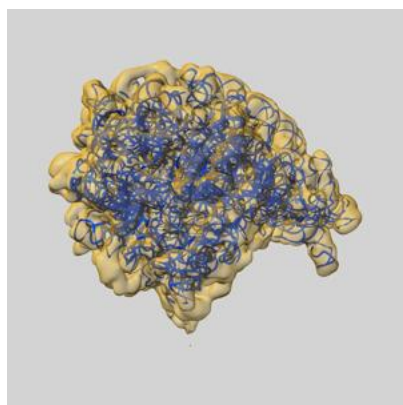
8 Fourier-Shell correlation

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

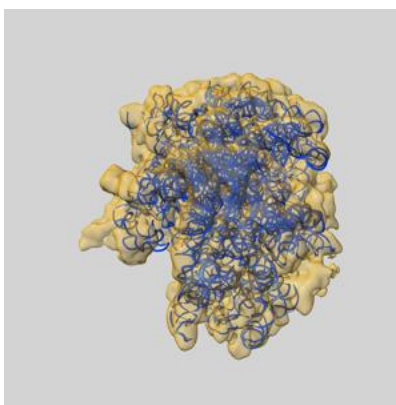
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1056 and PDB model 3DG2. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

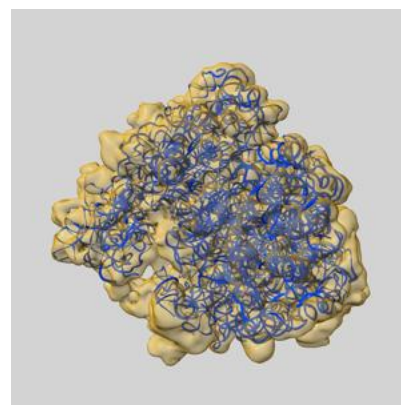
9.1 Map-model overlay [i](#)



X



Y



Z

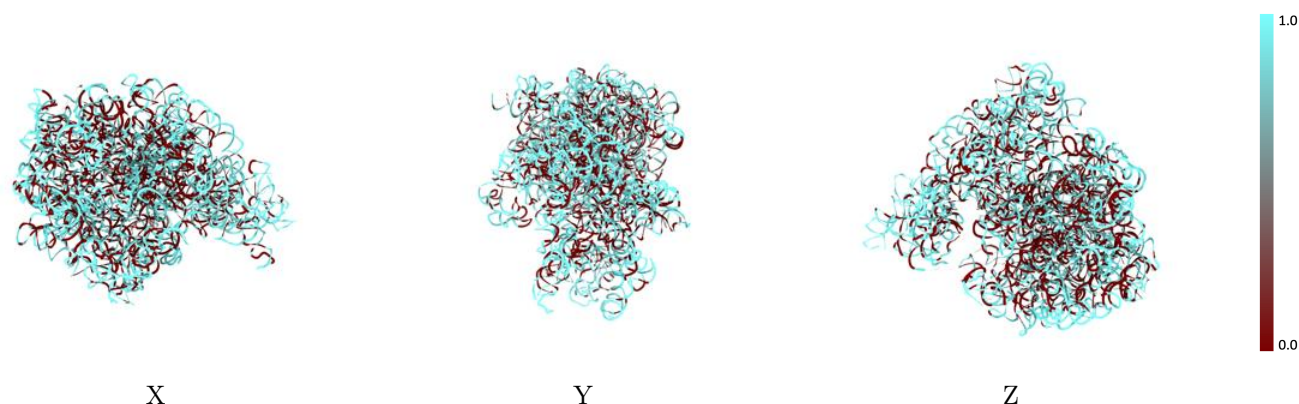
The images above show the 3D surface view of the map at the recommended contour level 43.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



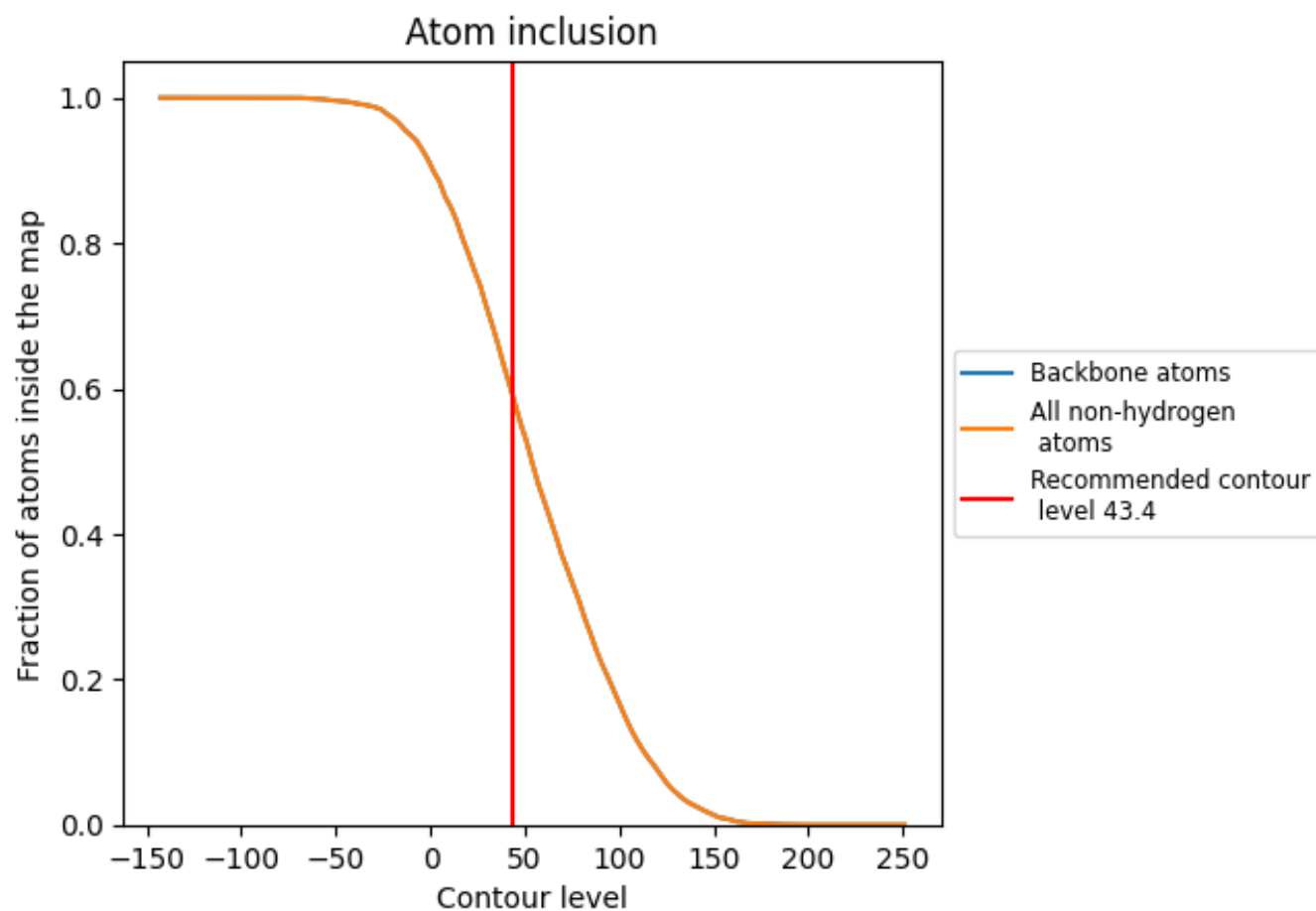
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (43.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% 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 (43.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5925	<div></div> 0.0280
A	<div></div> 0.6451	<div></div> 0.0320
B	<div></div> 0.5642	<div></div> 0.0260

