



## wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 03:55 PM EST

PDB ID : 3J3W  
EMDB ID : EMD-5643  
Title : Atomic model of the immature 50S subunit from *Bacillus subtilis* (state II-a)  
Authors : Li, N.; Guo, Q.; Zhang, Y.; Yuan, Y.; Ma, C.; Lei, J.; Gao, N.  
Deposited on : 2013-04-28  
Resolution : 10.70 Å (reported)  
Based on initial models : 2AW4, 2J01

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The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

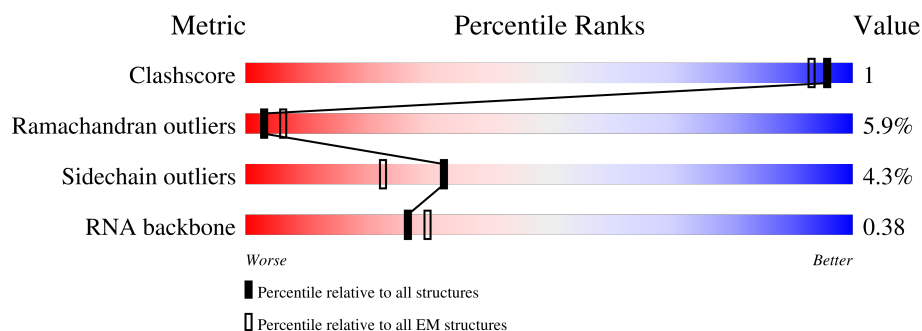
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.70 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.




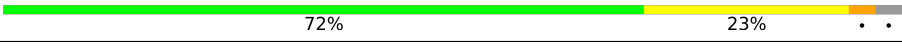
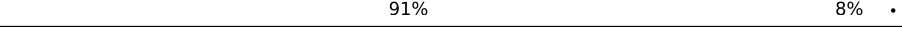

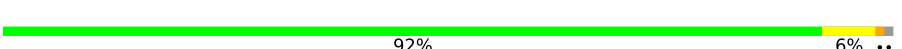


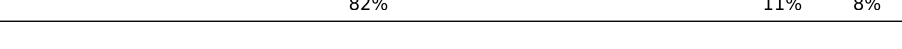

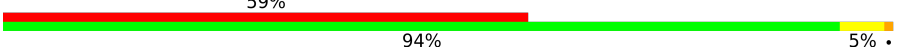



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	2927	
2	O	59	
3	C	277	
4	N	120	
5	G	179	
6	J	145	
7	K	122	

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Mol	Chain	Length	Quality of chain
8	L	146	 88% 10% .
9	P	115	 72% 23% . .
10	Q	119	 91% 8% .
11	D	209	 91% 6% ..
12	R	102	 88% 11% .
13	S	113	 92% 6% ..
14	T	95	 86% 13% .
15	U	103	 83% 17% .
16	X	66	 82% 11% 8%
17	2	44	 91% 9%
18	5	232	 48% . 48%
19	6	141	 59% 94% 5% .
20	E	207	 86% 13%

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 76573 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 ribosome RNA 23S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2685	Total	C	N	O	P	0	0
			57639	25720	10638	18600	2681		

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	55	Total	C	N	O	S	0	0
			433	267	87	72	7		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	277	Total	C	N	O	S	0	0
			2129	1323	419	380	7		

- Molecule 4 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	120	Total	C	N	O	S	0	0
			962	588	187	182	5		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	163	Total	C	N	O	S	0	0
			1246	776	226	242	2		

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	143	Total	C	N	O	S	0	0
			1134	717	207	204	6		

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 9 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	P	112	Total	C	N	O	S	0	0
			916	584	178	154			

- Molecule 10 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 11 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	206	Total	C	N	O	S	0	0
			1568	984	289	290	5		

- Molecule 12 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

- Molecule 13 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	112	Total	C	N	O	S	0	0
			868	541	168	155	4		

- Molecule 14 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	95	Total	C	N	O	S	0	0
			767	480	139	144	4		

- Molecule 15 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	103	Total	C	N	O	S	0	0
			780	488	145	143	4		

- Molecule 16 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	61	Total	C	N	O	S	0	0
			504	312	97	93	2		

- Molecule 17 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 18 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	120	Total	C	N	O	S	0	0
			910	576	156	176	2		

- Molecule 19 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	141	Total	C	N	O	S	0	0
			1044	657	184	196	7		

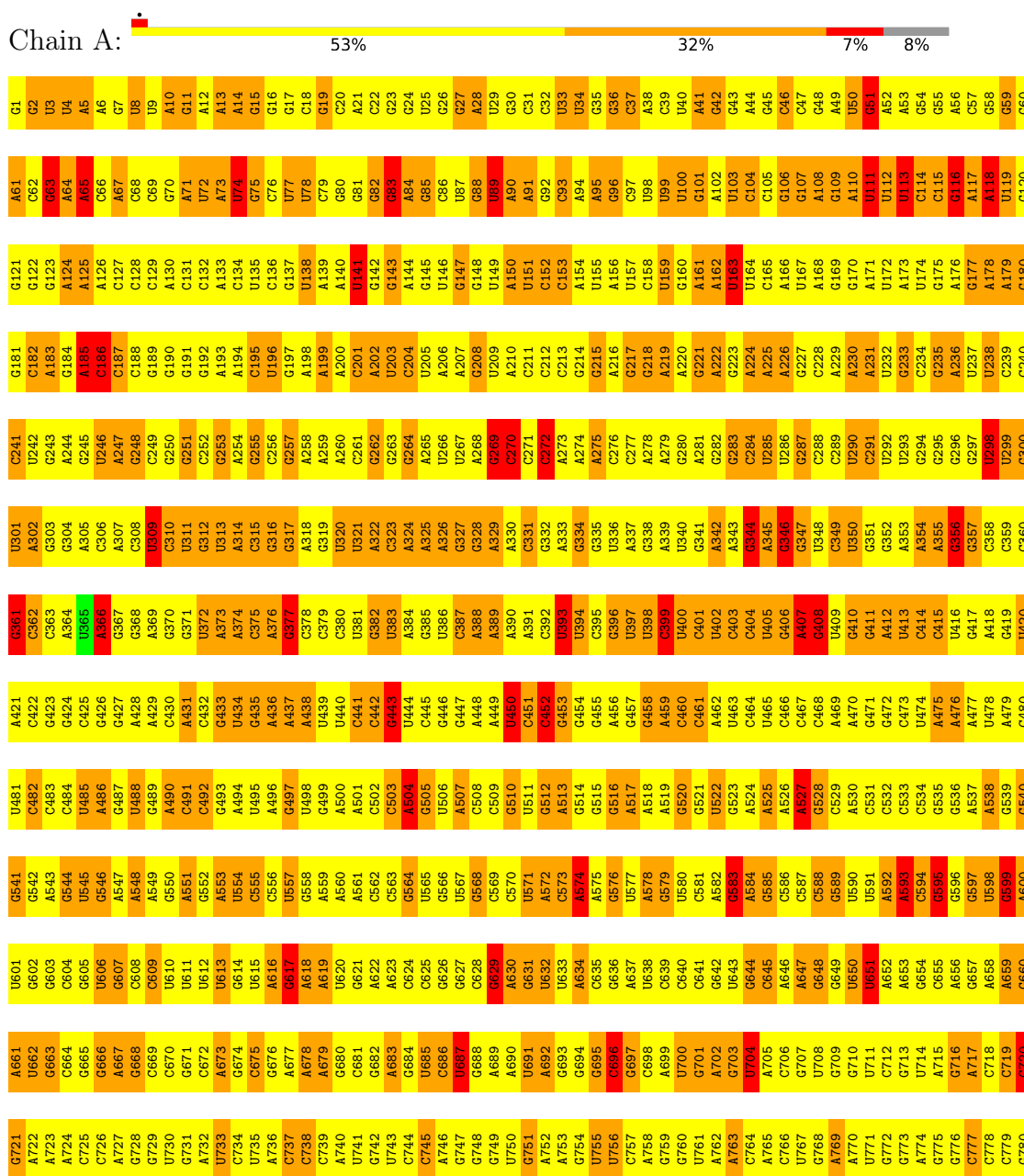
- Molecule 20 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

### 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.

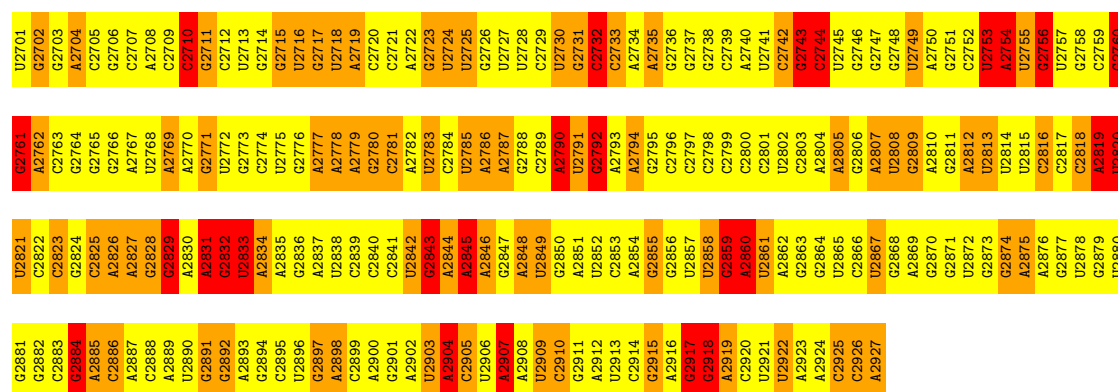
#### • Molecule 1: ribosome RNA 23S



A1681	C1682	C1683	A1684	C1685	A1686	A1687	C1688	A1689	A1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	A1708	A1709	A1710	C1711	C1712	A1713	A1714	C1715	C1716	C1717	C1718	C1719	C1720	A1721	C1722	A1723	A1724	C1725	C1726	A1727	C1728	C1729	C1730	C1731	C1732	C1733	A1734	A1735	C1736	C1737	A1738	C1739	A1680											
G1621	G1622	G1623	G1624	C1625	A1626	A1627	G1628	C1629	G1630	A1631	C1632	C1633	G1634	G1635	G1636	A1637	A1638	A1639	G1640	G1641	G1642	C1643	A1644	C1645	A1646	A1647	A1648	A1649	A1650	G1651	C1652	A1653	A1654	G1655	A1656	C1657	C1658	A1659	A1660	A1661	C1662	A1663	A1664	G1665	A1666	C1667	C1668	C1669	A1670	A1671	A1672	A1673	A1674	A1675	C1676	A1677	A1678	A1679	A1680	
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C961	C962	G963	A964	A965	U966	G967	C968	C969	A970	A971	U972	C973	A974	C975	U976	U977	A978	U979	C980	C981	A982	G983	G984	G985	A986	A987	G988	U989	C990	A991	G992	A993	C994	U995	G996	C997	G998	A999	G1000	U1001	G1002	A1003	U1004	A1005	A1006	G1007	A1008	U1009	C1010	C1011	U949	U950	C951	A952	G953	U954	C955	U956	A1019	A1020
A841	C842	G843	U844	G845	G846	A847	G848	A849	U850	A851	G852	C853	U854	G855	G856	U857	U858	C859	U860	C861	U862	C863	G864	G865	A866	A867	G868	U869	U899	C930	C931	C932	U874	U875	U876	G877	G878	G879	C880	U881	A882	G883	C884	C885	U886	G887	A888	A889	U890	A891	U892	A893	A894	G895	A896	G897	U898	C899	U900	
A761	A762	C763	C764	C765	C766	C767	G768	G769	A770	A771	G772	G773	U774	G775	A776	A777	U778	A779	U780	G802	C803	G804	G805	G806	G807	A808	U809	G810	A811	G812	G813	U814	U815	U816	G817	G818	G819	U820	A821	G822	G823	G824	G825	U826	G827	A828	A829	U830	U831	G832	C833	C834	A835	A836	U837	C838	G839	A840		



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U2642	G2582	U2522	A2462	A	C	G	C222	C2102	A2042	A	C	C	C1862	A1802	G1742
A2643	G2583	G2523	A2463	C	A	C	U223	A2103	A2043	G	A	C	U1863	G1803	A1743
U2644	U2584	G2524	A2464	G	U	C	U224	U2104	A2044	G	C	C	U1864	U1804	G1744
C2645	C2585	C2525	G2465	A	U	C	U225	A2105	U2045	U	A	G	C1865	A1805	A1745
C2646	C2586	G2526	G2466	A	C	U	U226	A2106	U2046	C	U	G	C	U1806	A1746
C2647	C2587	U2467	U2467	A	G	C	A227	C2107	A2047	C	U	C	C	U1807	G1747
U2648	C2588	A2468	A2468	G	C	C	A228	U2108	U2048	G	A	U	C	U1808	G1748
C2650	C2589	C2469	C2469	U	A	C	C229	C2109	A2049	A	A	A	G	U1809	G1749
C2651	A2590	C2470	C2470	C	G	C	C230	C2110	G2050	C	A	A	G	G1810	G1750
G2652	U2591	C2471	C2471	G	A	U	C231	A2111	U2051	C	C	C	C	C1811	U1751
C2653	U2592	C2472	G2472	G	G	C	G232	C2112	A2052	C	G	C	C	A1812	G1752
C2654	A2593	G2473	C2473	G	U	C	C233	C2113	C2053	G	U	U	G	A1813	C1753
C2655	G2474	G2474	C234	C	G	U	G234	C2114	C2054	C	C	G	G	A1814	U1754
G2656	U2595	G2475	G235	U	A	A	G235	U2115	U2055	C	U	G	G	A1815	C1755
G2657	G2596	G2476	G236	U	U	A	G236	G2116	G2056	C	U	G	G	A1816	U1756
A2658	C2597	A2477	U2477	A	A	A	C237	A2117	U2057	G	U	C	C	A1817	G1757
G2659	G2598	U2478	U2478	A	A	A	C238	U2118	G2058	G	U	C	C	A1818	U1758
G2660	G2599	A2479	U2479	G	G	C	U239	U2119	A2059	A1999	U	U	G	C1819	U1759
A2661	U2600	C2480	A2480	G	G	C	U240	U2120	A2060	A2000	U	U	U	A1820	U1760
C2662	C2602	C2481	A2481	C	U	A	A241	U2121	G2061	G2001	A	C	C	G1821	G1761
A2663	G2603	U2482	U2482	C	A	A	U242	G2122	A2062	G2002	A	A	A	G1822	G1762
U2664	G2604	G2483	G2483	A	C	C	C243	A2123	U2063	C2003	C	C	C	U1823	G1763
U2665	C2605	G2484	G2484	A	C	C	G244	A2124	G2064	G2004	G	C	G	C1824	U1764
U2666	G2606	G2485	G2485	A	G	G	G245	U2125	C2065	C2005	A	U	C	U1825	G1765
G2667	G2607	U2486	G2486	G	G	C	G246	G2126	A2066	A2006	G	G	G	C1826	C1766
A2668	C2608	U2487	U2487	G	G	C	C247	U2127	G2067	A2007	G	U	G	U1827	A1767
U2669	U2609	U2488	G2488	G	G	C	G248	U2128	G2068	C2008	A	U	C	G1828	A1768
A2670	G2610	G2489	G2489	G	A	C	G249	G2129	U2069	G2009	G	U	C	C1829	G1769
G2671	G2611	U2490	G2490	G	G	C	G250	C2130	U2070	A2010	C	U	C	G1830	C1770
C2672	G2612	U2491	U2491	C	C	U	G251	U2131	A2071	U2011	U	U	G	A1831	G1771
A2673	G2552	C2492	C2492	U	U	C	A252	C2132	C2072	C2012	C	C	C	A1832	C1772
U2674	G2553	C2493	C2493	U	C	C	G253	C2133	C2073	G2013	U	U	C	G1833	G1773
C2675	G2554	G2494	G2494	G	C	A	A254	A2134	C2074	G2014	C	U	U	C1834	A1774
U2676	G2555	C2495	C2495	A	C	A	G255	G2135	G2075	G2015	A	C	C	C1835	G1775
G2677	C2556	C2496	G2496	C	U	A	A256	C2136	C2076	G2016	G	C	C	G1836	A1776
U2678	U2557	A2497	U2557	G	G	C	G257	U2137	G2077	C2017	U	U	C	U1837	G1777
C2679	G2558	G2498	G2498	C	C	C	U258	U2138	A2078	A2018	G	G	C	A1838	A1778
U2680	U2559	A2499	G2499	G	G	C	G259	G2139	C2079	C2019	U	U	U	A1839	G1779
U2681	A2619	A2499	A2499	A	U	U	U260	U2140	A2080	U2020	A	A	C	G1840	C1780
U2682	U2621	G2499	G2499	A	U	C	C261	A2141	G2081	G2021	C	U	C	G1841	C1781
A2683	U2622	U2561	G2499	G	C	U	A262	C2142	G2082	U2022	C	U	C	C1842	G1782
C2684	C2623	U2562	G2501	A	C	C	G263	A2143	A2083	C2023	C	U	C	G1843	C1783
U2685	G2624	C2563	G2501	C	C	C	G264	G2144	C2084	U2024	G	G	C	A1844	A1784
A2686	U2625	U2502	U2502	C	U	U	U265	G2145	G2085	C2025	A	A	C	A1845	G1785
G2687	G2626	C2503	C2503	U	C	C	G266	A2146	G2086	A2026	A	A	C	G1846	U1786
G2688	A2627	G2566	G2566	A	A	A	G267	U2147	A2087	A2027	G	G	C	U1847	G1787
A2689	G2628	U2567	U2567	C	C	C	G268	A2148	A2088	C2028	A	U	C	A1848	A1788
G2690	A2629	C2568	U2568	A	A	A	C269	G2149	A2089	G2029	A	U	C	U1849	A1789
A2691	C2630	C2569	G2570	A	A	U	A270	U2150	G2090	A2030	U	U	C	A1850	U1790
G2692	A2631	A2570	A2507	G	U	U	G271	U2151	A2091	G2031	C	C	C	G1851	A1791
C2693	G2632	G2571	U2508	C	U	G	U272	A2152	C2092	A2032	C	C	G	G1852	G1792
A2694	U2633	U2572	U2508	C	C	U	U273	C2153	C2093	G2033	C	A	A	G1853	C1793
C2695	G2634	G2573	A2509	G	U	G	G274	G2154	C2094	A2034	C	A	A	G1854	C1794
G2696	C2635	U2574	G2510	A	U	U	U275	A2155	C2095	U2035	U	U	U	U1855	C1795
C2697	G2636	U2575	A2511	C	C	C	G276	G2156	G2096	U2036	G	U	C	G1856	C1796
G2698	G2637	U2576	G2456	C	C	C	A	C2157	U2097	C2037	U	U	C	G1857	A1797
C2699	U2638	G2577	G2457	A	A	A	C	U2158	G2098	G2038	C	C	A	A1858	G1798
U2700	G2639	G2578	G2458	G	A	U	U	U2159	G2099	G2039	G	G	C	G1859	C1799
			A2459	G	A	U	G	U2160	A2100	U2040	U	U	G	G1860	C1800



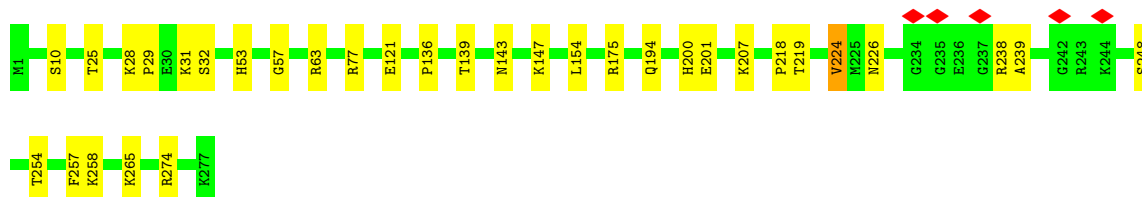
• Molecule 2: 50S ribosomal protein L32

Chain 0: 83% 10% 7%



• Molecule 3: 50S ribosomal protein L2

Chain C: 88% 12%



• Molecule 4: 50S ribosomal protein L17

Chain N: 96%



• Molecule 5: 50S ribosomal protein L6

Chain G: 84% 7% 9%



• Molecule 6: 50S ribosomal protein L13

Chain J: 87% 10% 3%




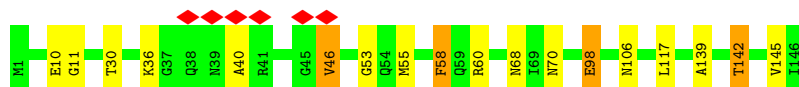
- Molecule 7: 50S ribosomal protein L14

Chain K:  93% 7%



- Molecule 8: 50S ribosomal protein L15

Chain L:  88% 10%



- Molecule 9: 50S ribosomal protein L19

Chain P:  72% 23%



- Molecule 10: 50S ribosomal protein L20

Chain Q:  91% 8%




- Molecule 11: 50S ribosomal protein L3

Chain D:  91% 6%




- Molecule 12: 50S ribosomal protein L21

Chain R:  88% 11%




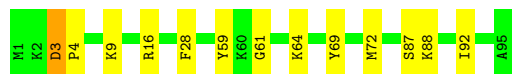
- Molecule 13: 50S ribosomal protein L22

Chain S:  92% 6%




- Molecule 14: 50S ribosomal protein L23

Chain T:  86% 13%




- Molecule 15: 50S ribosomal protein L24

Chain U:  83% 17%



- Molecule 16: 50S ribosomal protein L29

Chain X:  82% 11% 8%



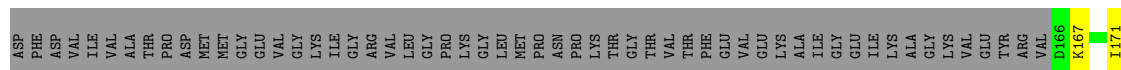
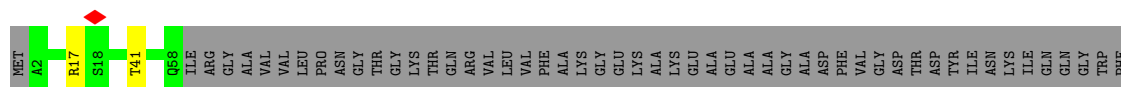
- Molecule 17: 50S ribosomal protein L34

Chain 2:  91% 9%




- Molecule 18: 50S ribosomal protein L1

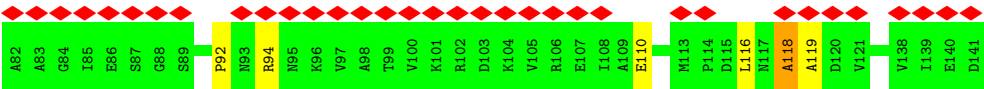
Chain 5:  48% 48%



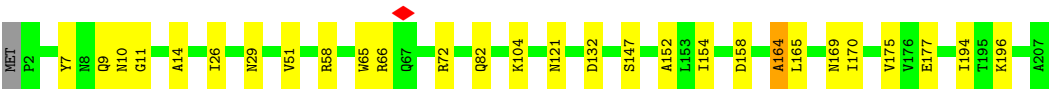
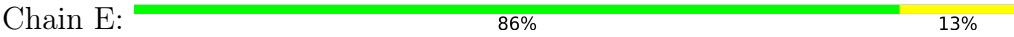
- Molecule 19: 50S ribosomal protein L11

Chain 6:  59% 94% 5%





• Molecule 20: 50S ribosomal protein L4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27652	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	10.909	Depositor
Minimum map value	-3.262	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size ( $\text{\AA}$ )	384.0, 384.0, 384.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.5, 1.5, 1.5	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.68	83/64560 (0.1%)	2.67	8132/100715 (8.1%)
2	O	1.04	0/440	1.20	2/584 (0.3%)
3	C	1.00	0/2166	1.09	0/2902
4	N	1.09	0/969	1.05	0/1294
5	G	0.97	0/1264	1.04	0/1709
6	J	0.95	0/1157	1.08	2/1557 (0.1%)
7	K	1.02	0/928	1.05	0/1245
8	L	0.97	0/1094	1.10	2/1457 (0.1%)
9	P	1.10	0/929	1.17	2/1243 (0.2%)
10	Q	1.05	0/952	1.06	2/1266 (0.2%)
11	D	0.96	0/1590	1.09	2/2130 (0.1%)
12	R	0.92	0/806	1.13	1/1080 (0.1%)
13	S	1.01	0/877	1.10	0/1179
14	T	1.01	0/774	1.15	2/1030 (0.2%)
15	U	0.87	0/790	1.16	3/1054 (0.3%)
16	X	1.04	0/505	1.01	0/671
17	2	1.26	0/371	1.04	0/483
18	5	0.87	0/921	1.05	2/1239 (0.2%)
19	6	0.92	0/1058	1.06	1/1427 (0.1%)
20	E	0.97	0/1586	1.10	1/2139 (0.0%)
All	All	1.55	83/83737 (0.1%)	2.43	8154/126404 (6.5%)

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	A	0	320
4	N	0	1
8	L	0	2
9	P	0	2
14	T	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	U	0	1
20	E	0	2
All	All	0	330

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1339	A	O3'-P	-7.12	1.52	1.61
1	A	1831	A	N7-C5	-6.74	1.35	1.39
1	A	52	A	N7-C5	-6.72	1.35	1.39
1	A	653	A	N7-C5	-6.68	1.35	1.39
1	A	1839	A	N7-C5	-6.64	1.35	1.39

The worst 5 of 8154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1339	A	P-O3'-C3'	34.26	160.81	119.70
1	A	313	U	P-O3'-C3'	20.76	144.62	119.70
1	A	178	A	P-O3'-C3'	20.05	143.75	119.70
1	A	74	U	P-O3'-C3'	19.98	143.68	119.70
1	A	375	C	P-O3'-C3'	19.92	143.60	119.70

There are no chirality outliers.

5 of 330 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	G	Sidechain
1	A	27	G	Sidechain
1	A	28	A	Sidechain
1	A	33	U	Sidechain
1	A	5	A	Sidechain

## 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	57639	0	29016	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	0	433	0	454	0	0
3	C	2129	0	2225	4	0
4	N	962	0	995	0	0
5	G	1246	0	1273	2	0
6	J	1134	0	1178	0	0
7	K	921	0	977	0	0
8	L	1082	0	1132	0	0
9	P	916	0	987	5	0
10	Q	940	0	1005	0	0
11	D	1568	0	1635	0	0
12	R	795	0	838	0	0
13	S	868	0	930	0	0
14	T	767	0	813	2	0
15	U	780	0	838	0	0
16	X	504	0	541	1	0
17	2	368	0	410	1	0
18	5	910	0	944	0	0
19	6	1044	0	1098	1	0
20	E	1567	0	1652	1	0
All	All	76573	0	48941	116	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 1.

The worst 5 of 116 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:A:1245:G:H1	1:A:1281:C:H41	1.25	0.84
1:A:898:U:H3	1:A:973:G:H1	1.41	0.68
1:A:2557:U:H3	1:A:2564:A:H61	1.41	0.68
1:A:1799:G:H1	1:A:2011:U:H3	1.46	0.63
1:A:2543:U:H3	1:A:2599:G:H1	1.48	0.62

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0	53/59 (90%)	43 (81%)	6 (11%)	4 (8%)	1	13
3	C	275/277 (99%)	217 (79%)	40 (14%)	18 (6%)	1	16
4	N	118/120 (98%)	101 (86%)	14 (12%)	3 (2%)	5	32
5	G	161/179 (90%)	148 (92%)	7 (4%)	6 (4%)	3	24
6	J	141/145 (97%)	124 (88%)	9 (6%)	8 (6%)	1	18
7	K	120/122 (98%)	106 (88%)	9 (8%)	5 (4%)	3	22
8	L	144/146 (99%)	100 (69%)	30 (21%)	14 (10%)	0	10
9	P	110/115 (96%)	76 (69%)	20 (18%)	14 (13%)	0	5
10	Q	115/119 (97%)	101 (88%)	9 (8%)	5 (4%)	2	22
11	D	204/209 (98%)	175 (86%)	21 (10%)	8 (4%)	3	23
12	R	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	1	17
13	S	110/113 (97%)	97 (88%)	10 (9%)	3 (3%)	5	31
14	T	93/95 (98%)	77 (83%)	11 (12%)	5 (5%)	2	19
15	U	101/103 (98%)	70 (69%)	20 (20%)	11 (11%)	0	8
16	X	59/66 (89%)	55 (93%)	2 (3%)	2 (3%)	3	26
17	2	42/44 (96%)	37 (88%)	4 (10%)	1 (2%)	6	33
18	5	116/232 (50%)	97 (84%)	13 (11%)	6 (5%)	2	19
19	6	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	3	25
20	E	204/207 (99%)	161 (79%)	25 (12%)	18 (9%)	1	11
All	All	2405/2594 (93%)	1981 (82%)	282 (12%)	142 (6%)	3	17

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	0	19	HIS
3	C	219	THR

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Mol	Chain	Res	Type
7	K	30	ARG
7	K	73	ASP
8	L	117	LEU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	0	49/53 (92%)	48 (98%)	1 (2%)	55	74
3	C	225/225 (100%)	215 (96%)	10 (4%)	28	53
4	N	100/100 (100%)	99 (99%)	1 (1%)	76	86
5	G	138/151 (91%)	135 (98%)	3 (2%)	52	71
6	J	122/123 (99%)	111 (91%)	11 (9%)	9	30
7	K	101/101 (100%)	98 (97%)	3 (3%)	41	63
8	L	110/110 (100%)	105 (96%)	5 (4%)	27	52
9	P	97/100 (97%)	90 (93%)	7 (7%)	14	39
10	Q	96/98 (98%)	93 (97%)	3 (3%)	40	62
11	D	167/170 (98%)	159 (95%)	8 (5%)	25	51
12	R	84/84 (100%)	78 (93%)	6 (7%)	14	39
13	S	93/93 (100%)	87 (94%)	6 (6%)	17	42
14	T	85/85 (100%)	82 (96%)	3 (4%)	36	59
15	U	87/87 (100%)	82 (94%)	5 (6%)	20	45
16	X	54/57 (95%)	50 (93%)	4 (7%)	13	38
17	2	39/39 (100%)	37 (95%)	2 (5%)	24	48
18	5	98/185 (53%)	97 (99%)	1 (1%)	76	86
19	6	110/110 (100%)	109 (99%)	1 (1%)	78	87
20	E	169/170 (99%)	162 (96%)	7 (4%)	30	55
All	All	2024/2141 (94%)	1937 (96%)	87 (4%)	33	53

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	R	98	GLU
15	U	101	LEU
13	S	20	VAL
14	T	64	LYS
16	X	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
20	E	169	ASN
19	6	34	ASN
13	S	57	ASN
18	5	172	HIS
12	R	90	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2681/2927 (91%)	823 (30%)	200 (7%)

5 of 823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	8	U
1	A	10	A

5 of 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1590	C
1	A	2050	G
1	A	2918	G
1	A	1606	A
1	A	1711	G

## 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.

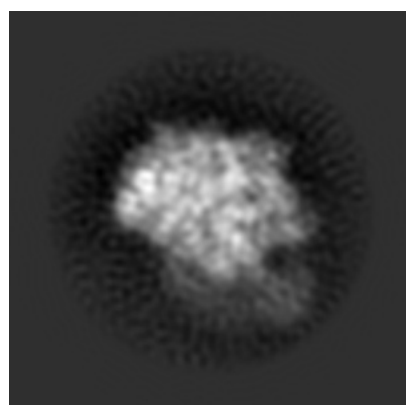
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5643. These allow visual inspection of the internal detail of the map and identification of artifacts.

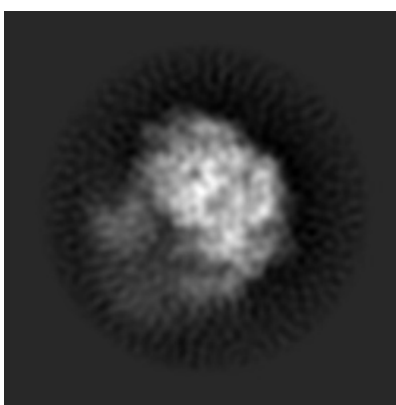
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

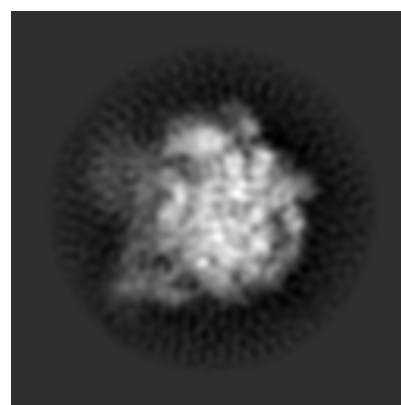
#### 6.1.1 Primary map



X



Y

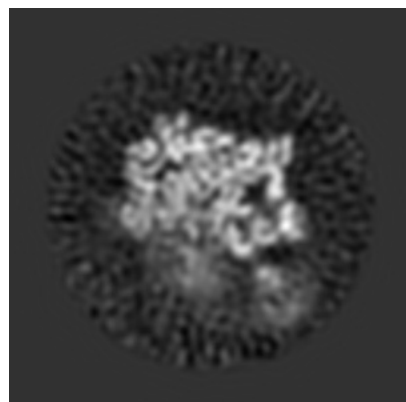


Z

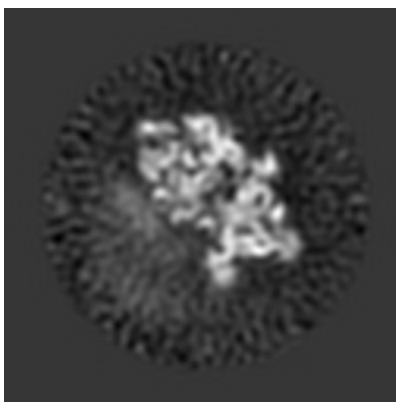
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

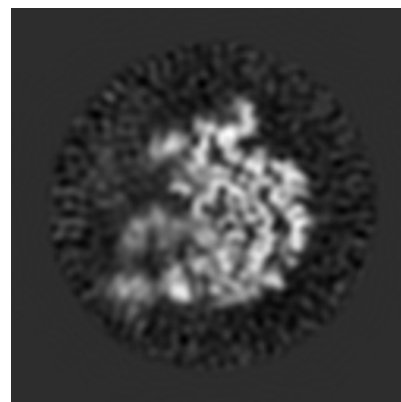
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

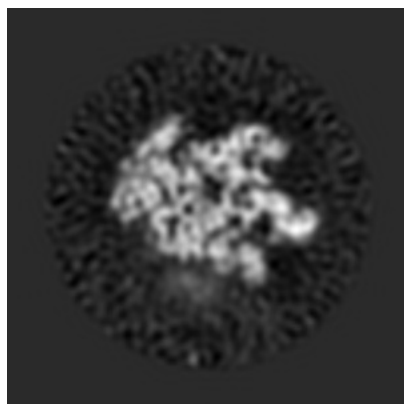


Z Index: 128

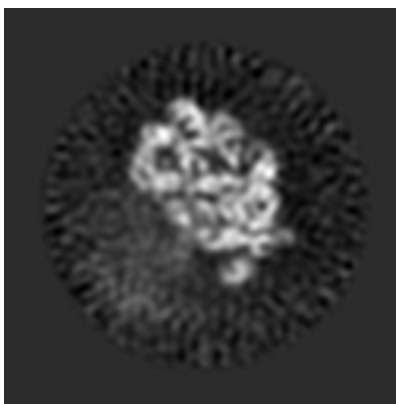
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 140



Y Index: 139

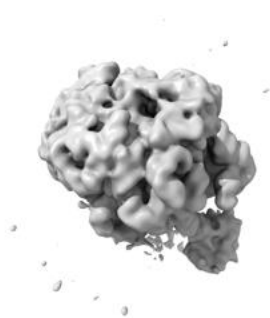


Z Index: 148

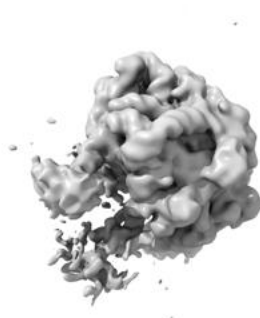
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

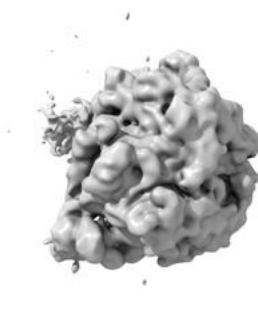
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

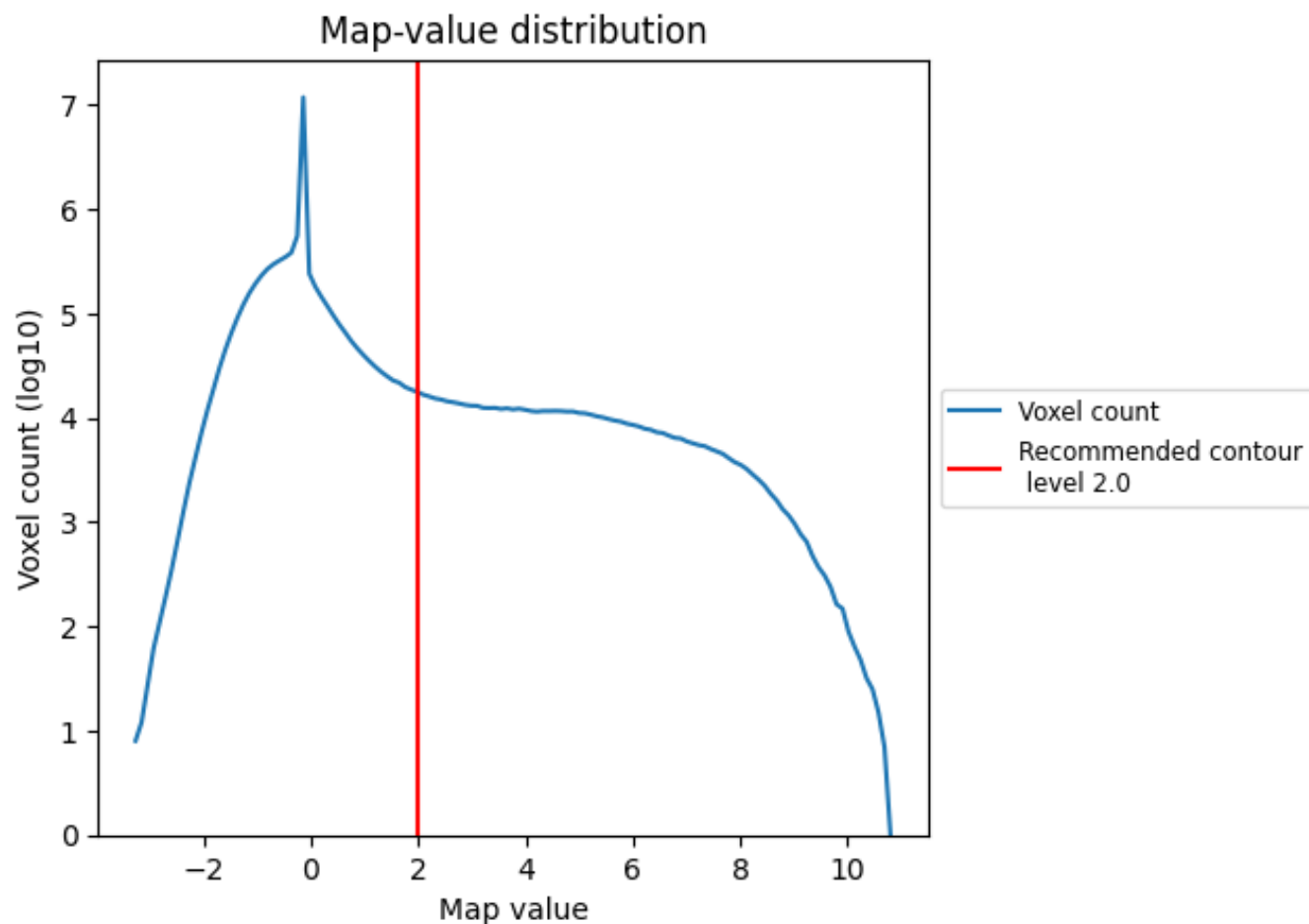
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

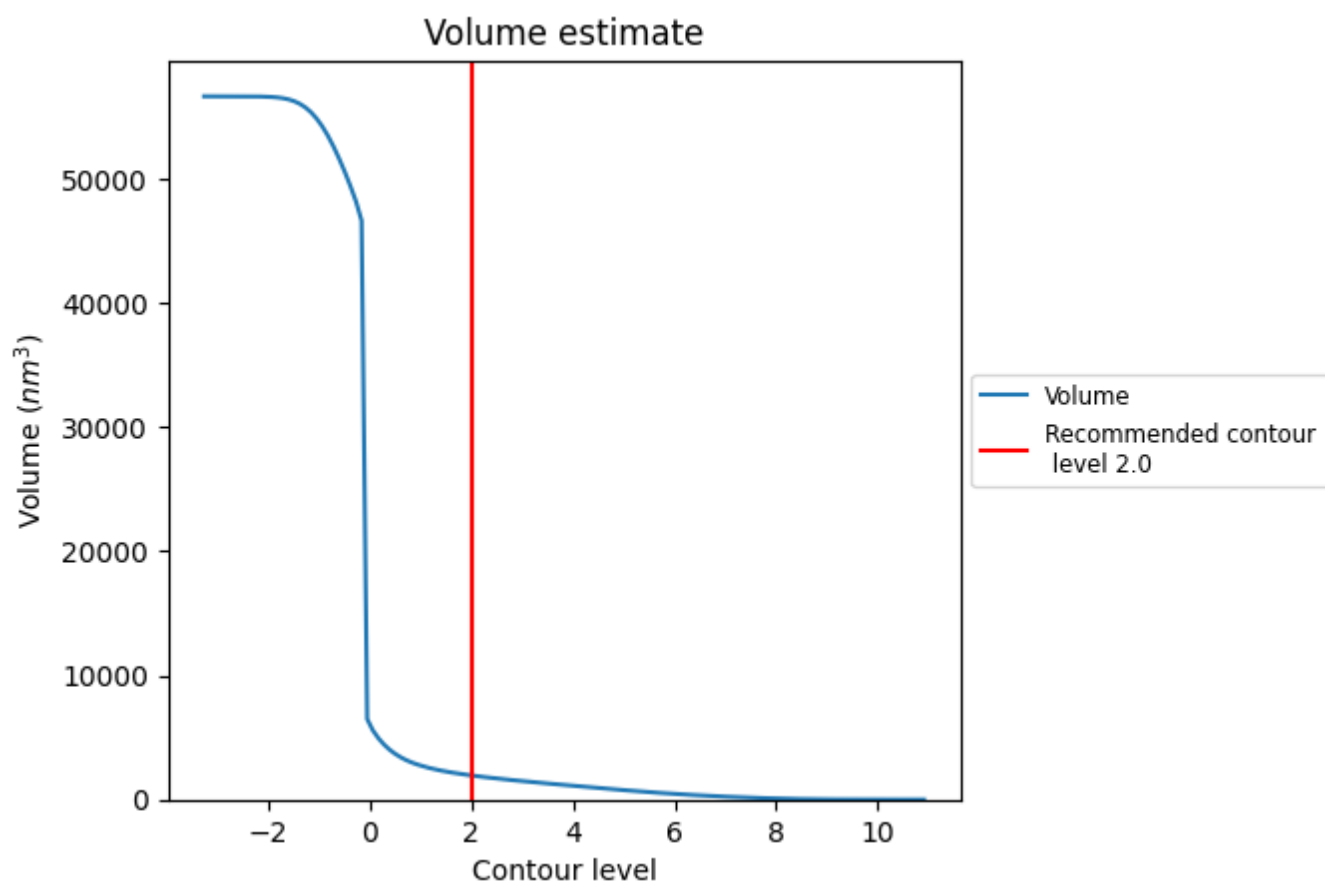
This section contains the results of statistical analysis of the map.

### 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.

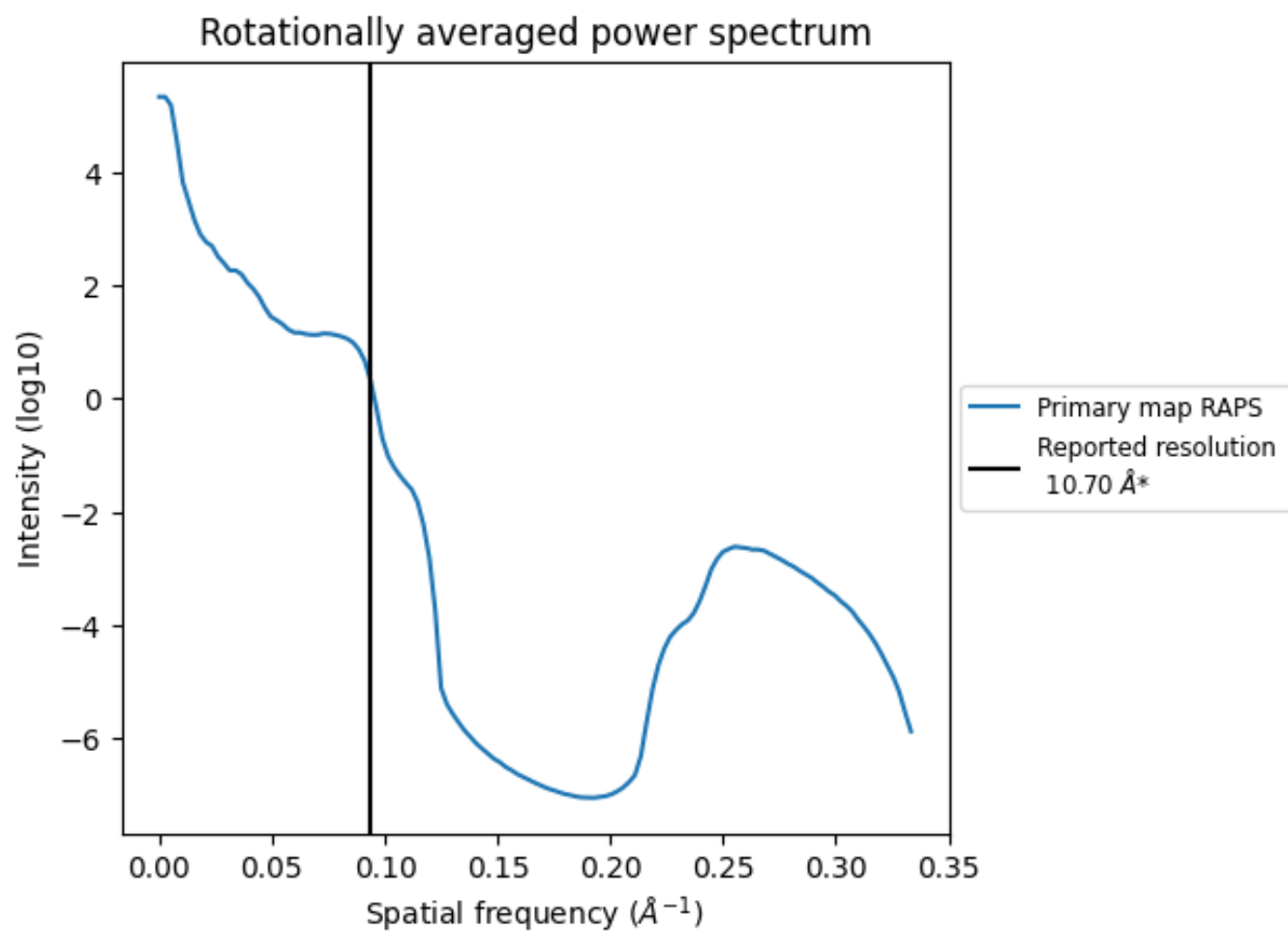
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1942  $\text{nm}^3$ ; this corresponds to an approximate mass of 1754 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<sup>-1</sup>

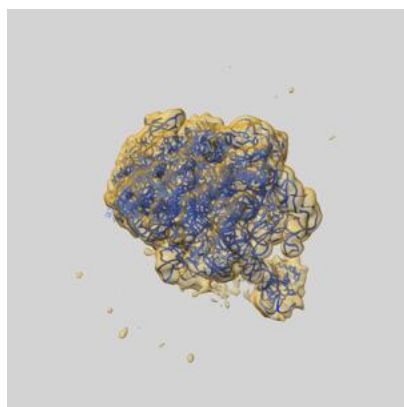
## 8 Fourier-Shell correlation

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

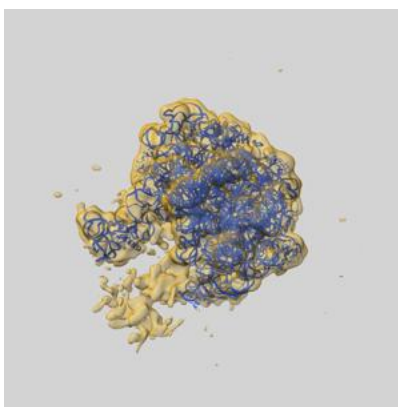
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5643 and PDB model 3J3W. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

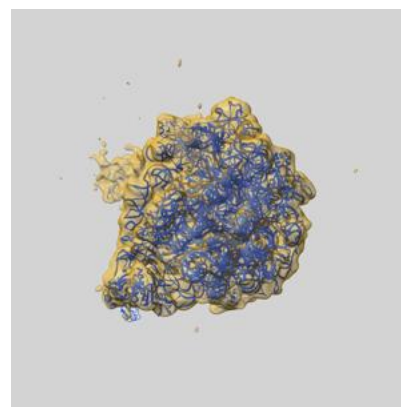
### 9.1 Map-model overlay [i](#)



X



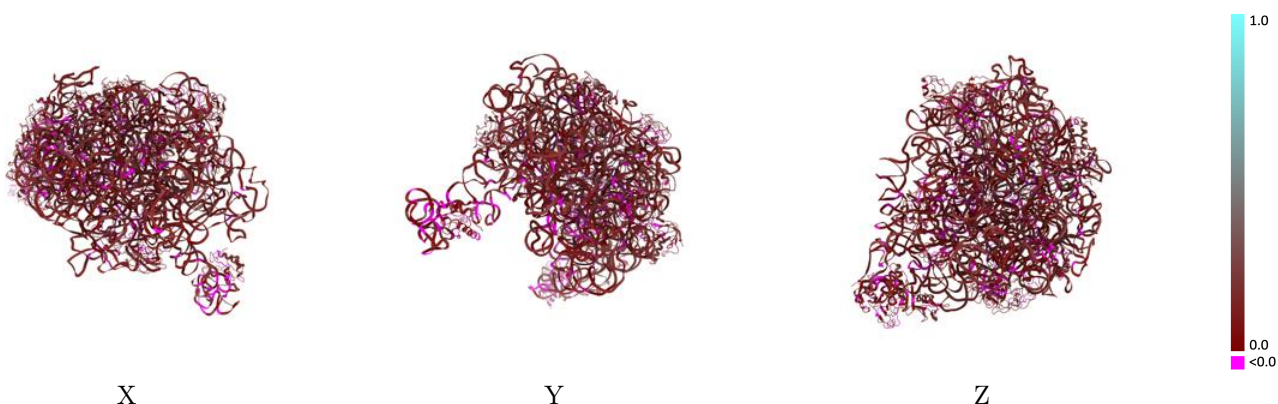
Y



Z

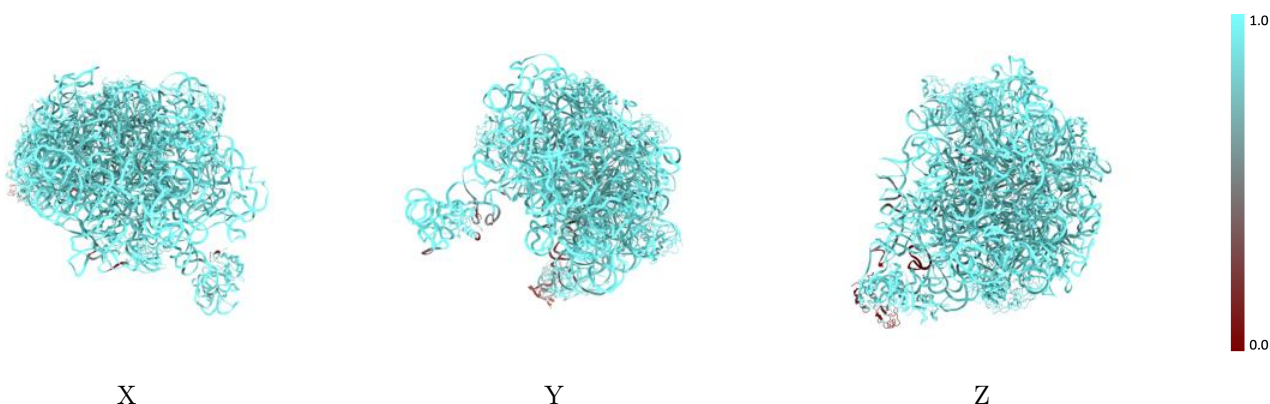
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



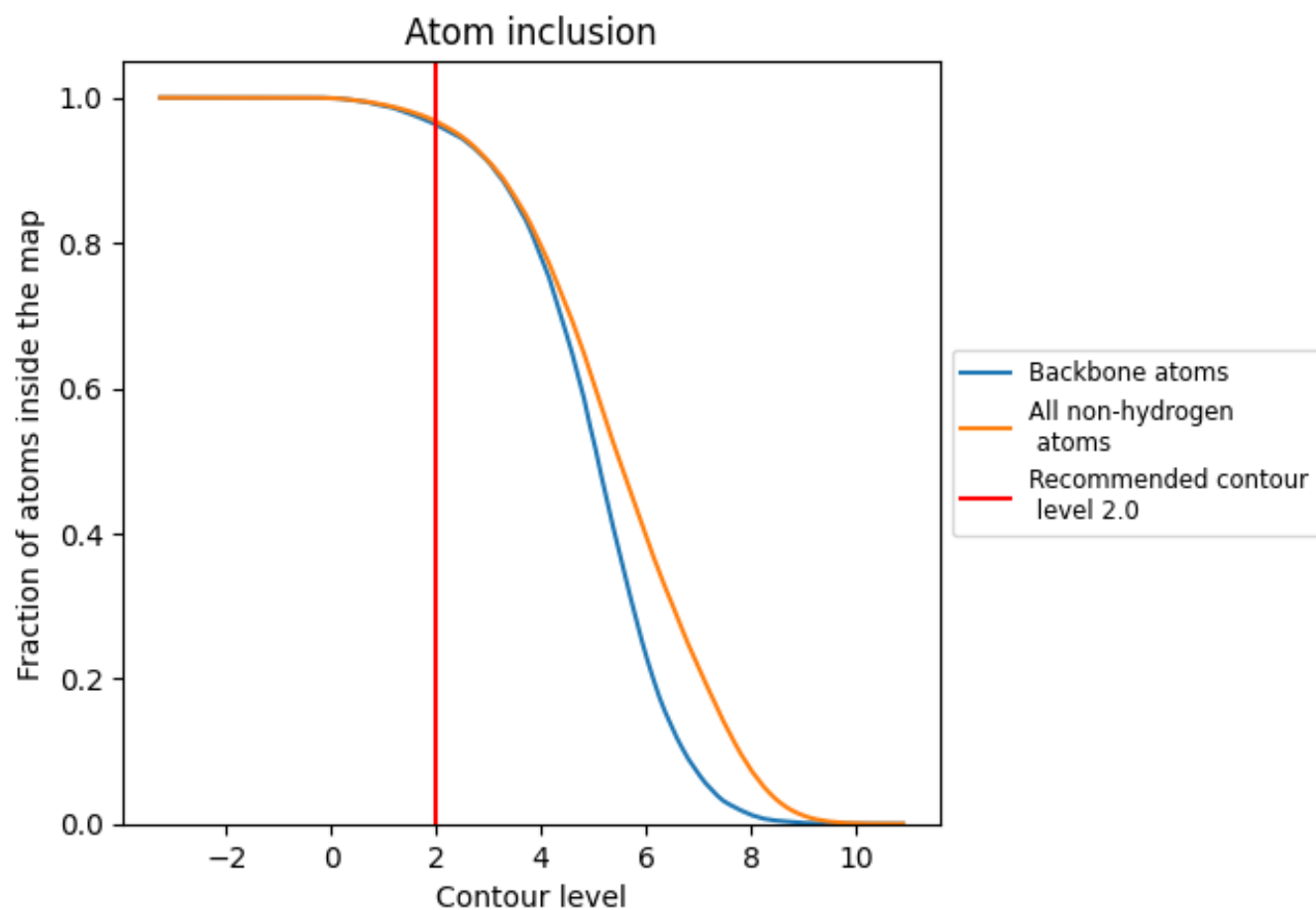
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.0).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9673	 0.1190
0	 0.9952	 0.0450
2	 0.9942	 0.0670
5	 0.9411	 0.0570
6	 0.3722	 0.0390
A	 0.9734	 0.1310
C	 0.9744	 0.0650
D	 0.9890	 0.0800
E	 0.9765	 0.0850
G	 0.9852	 0.1250
J	 0.9937	 0.0970
K	 0.9955	 0.1000
L	 0.9473	 0.0560
N	 0.9935	 0.0700
P	 0.9886	 0.1030
Q	 0.9923	 0.0770
R	 0.9962	 0.0960
S	 0.9787	 0.0910
T	 0.9839	 0.0830
U	 0.9987	 0.0700
X	 0.9980	 0.1520

