



Full wwPDB EM Validation Report ⓘ

May 7, 2024 – 10:38 AM JST

PDB ID : 7Y41
EMDB ID : EMD-33599
Title : Mycobacterium smegmatis 50S ribosomal subunit from Log Phase of growth
Authors : Sengupta, J.; Baid, P.
Deposited on : 2022-06-13
Resolution : 4.10 Å(reported)
Based on initial model : 5O60

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

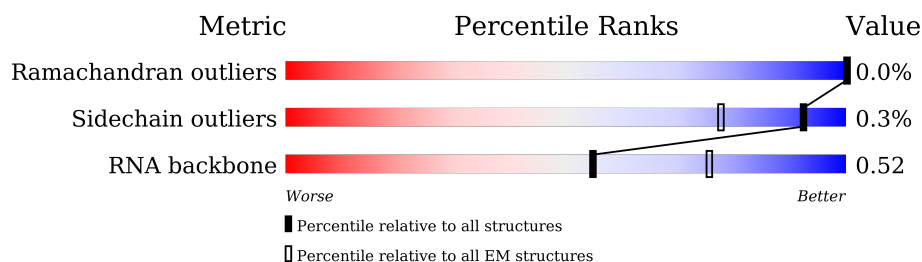
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)
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 ≥ 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	3	24	<div> <div>33%</div> <div>96%</div> <div>.</div> </div>
2	A	3120	<div> <div>76%</div> <div>24%</div> <div>.</div> </div>
3	B	118	<div> <div>81%</div> <div>19%</div> <div>.</div> </div>
4	C	278	<div> <div>99%</div> <div>.</div> </div>
5	D	217	<div> <div>99%</div> <div>.</div> </div>
6	E	215	<div> <div>97%</div> <div>.</div> </div>
7	F	187	<div> <div>96%</div> <div>..</div> </div>
8	G	179	<div> <div>98%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	175	
10	J	142	
11	K	147	
12	L	122	
13	M	147	
14	N	138	
15	O	199	
16	P	127	
17	Q	113	
18	R	129	
19	S	103	
20	T	153	
21	U	100	
22	V	105	
23	W	215	
24	X	88	
25	Y	64	
26	Z	77	
27	a	61	
28	b	57	
29	c	55	
30	d	47	
31	e	64	
32	f	37	
33	g	75	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 97056 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 protein called 50S ribosomal subunit bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	274	Total	C	N	O	S	0	0
			2105	1295	437	369	4		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	126	Total	C	N	O		0	0
			956	586	199	171			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	124	Total	C	N	O		0	0
			988	613	203	172			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	100	Total	C	N	O		0	0
			754	478	137	139			

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	114	Total	C	N	O		0	0
			873	543	171	159			

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 29 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	63	Total	C	N	O		0	0
			502	302	115	85			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
34	A	386	Total	Mg	0
			386	386	
34	B	9	Total	Mg	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
34	C	5	Total 5	Mg 5	0
34	E	1	Total 1	Mg 1	0
34	F	1	Total 1	Mg 1	0
34	M	1	Total 1	Mg 1	0
34	N	2	Total 2	Mg 2	0
34	T	1	Total 1	Mg 1	0
34	e	1	Total 1	Mg 1	0

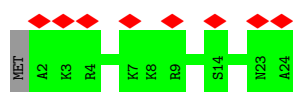
- Molecule 35 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	Y	1	Total 1	Zn 1	0
35	c	1	Total 1	Zn 1	0
35	f	1	Total 1	Zn 1	0
35	g	1	Total 1	Zn 1	0

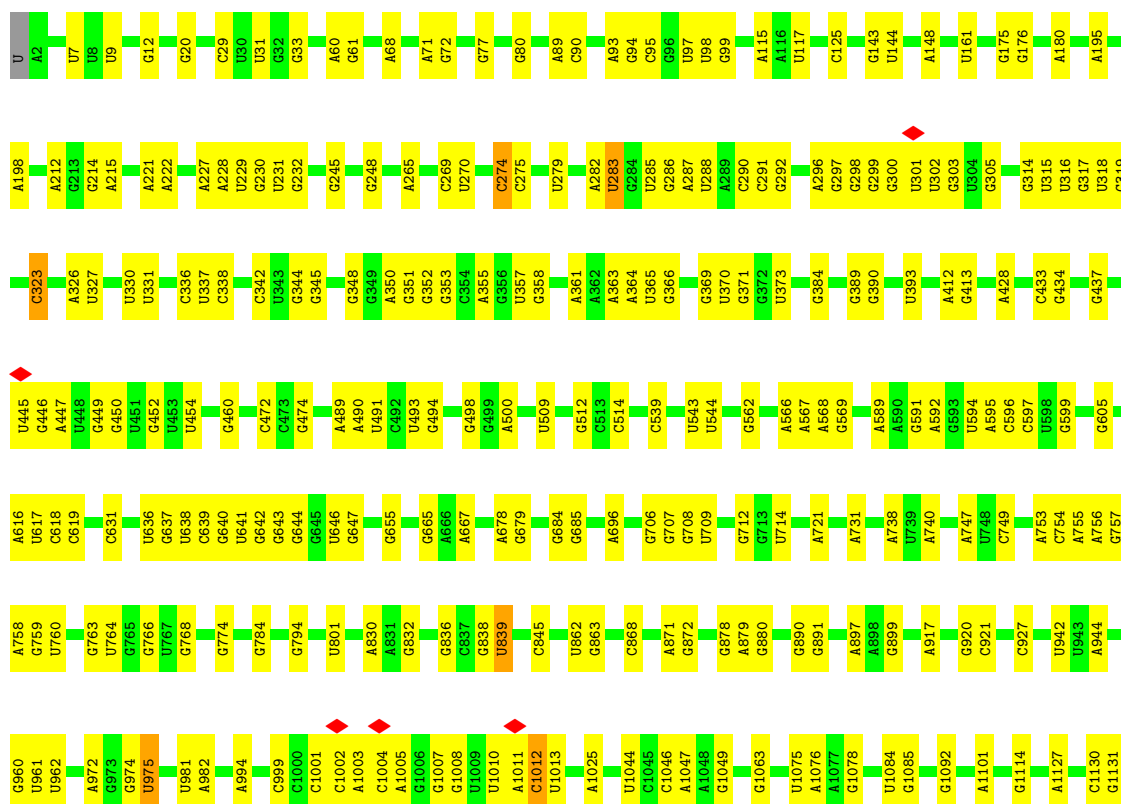
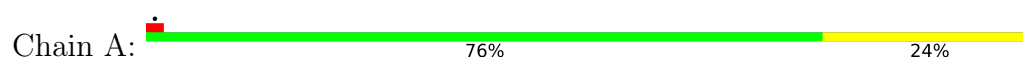
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal subunit bL37




- Molecule 2: 23S ribosomal RNA



C3120	G2968	G2408	A2342	C2191	G2075	U1798	A1648	C1568	U1444	G1230	U1141
A2972	G2975	G2413	G2343	A2194	C2085	G1802	C1649	G1574	C1448	U1231	G1143
G2975	A2609	A2421	G2346	G2196	U2086	A1828	G1654	A1575	G1456	A1233	A1144
U2980	A2609	A2422	A2349	U2215	C2087	U1828	G1674	C1577	G1462	U1237	U1151
A2981	C2627	G2427	G2350	U2216	C2088	A1844	U1675	G1578	G1462	U1238	U1158
A2982	G2797	G2640	C2352	U2217	C2089	G1845	G1677	A1580	C1465	C1239	G1161
G2985	G2640	A2434	G2353	A2221	U2091	A1848	U1678	C1581	U1466	G1240	C1162
A2989	U2647	U2436	G2354	A2227	U2092	A1852	A1679	C1582	U1467	U1245	A1163
A2989	C2648	U2437	G2355	A2227	G2093	A1852	A1680	U1583	A1480	U1246	A1164
U2809	A2649	C2438	G2356	A2227	G2094	A1852	U1681	U1584	A1480	G1173	G1174
A3002	G2446	G2446	A2357	C2243	G2095	U1864	G1688	U1585	U1494	U1248	A1175
U3009	G2653	A2449	G2358	C2243	G2096	A1865	U1697	U1586	A1499	G1250	G1174
A3014	A2654	G2462	G2359	C2244	A2106	A1865	U1697	C1586	G1507	U1251	A1178
C3015	U2855	G2463	C2360	U2246	G2107	C1866	G1703	U1587	G1507	C1253	U1178
C3016	U2833	A2449	U2361	A2247	G2107	G1869	A1710	G1588	A1508	G1253	U1178
A3021	U2837	G2462	C2362	G2251	U2111	U1870	G1711	G1589	U1509	C1260	G1181
G3022	U2855	G2503	A2364	A2255	U2112	A1872	G1712	U1590	A1510	A1261	C1182
U3029	A2856	C2507	C2366	A2257	C2117	G1892	U1713	U1591	U1511	G1283	U1184
A3042	A2857	C2507	C2367	G2263	G2130	C1900	A1716	U1592	U1512	G1293	A1184
C3046	G2858	A2511	C2368	C2267	G2131	C1900	U1717	C1596	A1518	G1298	A1185
U3054	G2865	A2529	C2369	G2268	U2132	G1933	U1721	U1599	G1522	U1325	A1186
A3056	G2877	A2530	C2371	A2276	U2135	U1946	G1724	G1601	C1531	G1335	A1187
U3057	U2878	G2532	G2372	C2279	A2136	U1947	G1725	U1602	G1532	A1344	A1188
G3070	A2877	C2532	G2373	G2279	A2137	A1948	U1728	G1603	C1533	G1345	C1190
U3082	G2909	A2534	U2701	A2286	A2138	C1949	A1730	G1604	C1534	G1351	A1191
C3088	A2912	U2536	G2380	A2286	A2140	G1950	A1730	G1605	A1536	C1351	G1192
A3093	U2913	G2544	A2381	A2284	U2141	C1973	A1731	A1611	G1541	C1352	C1193
A3094	C2915	G2545	G2382	G2285	A2142	A1974	U1732	G1614	A1546	G1353	C1194
C3095	A2926	U2548	C2383	C2320	A2143	A1975	U1732	G1615	G1547	G1359	C1195
G3098	C2936	C2568	U2387	A2324	C2144	U1981	G1737	A1616	C1548	U1371	C1196
C3099	U2937	A2569	G2388	U2325	C2144	U1981	G1738	A1616	G1549	U1380	U1199
C3101	G2938	A2560	U2389	U2328	C2144	U1981	G1738	A1616	G1549	A1380	U1200
C3105	C2948	C2571	U2390	U2332	A2151	A1990	G1746	A1616	G1549	U1551	A1202
C3106	A2949	G2574	G2391	G2333	A2152	C1991	C1752	A1616	G1549	C1553	A1203
A3112	C2950	A2578	A2392	U2334	G2153	C2017	G1754	A1616	G1549	U1554	A1204
A3113	U2953	A2578	A2393	U2335	G2154	C2017	A1755	A1555	U1554	C1385	G1205
A3114	G2956	G2581	A2394	U2336	U2155	G2018	G1756	A1556	U1554	A1387	A1206
A3115	A2957	G2753	A2399	U2337	U2162	G2024	U1757	C1557	C1557	U1388	G1207
		G2759	C2400	U2338	U2163	A2026	U1757	U1560	U1560	A1415	G1209
			C2401	G2339	U2164	A2026	U1757	C1561	C1562	A1416	U1212
			C2402	U2401	U2168	A2046	G1780	C1561	C1562	A1563	A1213
			U2403	U2401	U2187	A2064	G1783	C1561	C1562	A1564	A1214
			G2404	U2401	G2188	A2065	G1783	C1561	C1562	A1565	U1215
			A2405	U2401	C2189	A2065	A1789	C1561	C1562	A1566	U1219
			C2407	U2401	C2190	G2066		C1561	C1562	C1567	U1226

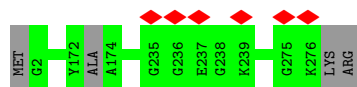
- Molecule 3: 5S ribosomal RNA

Chain B:  81% 19%



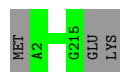
- Molecule 4: 50S ribosomal protein L2

Chain C:  99%



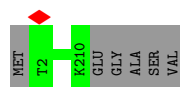
- Molecule 5: 50S ribosomal protein L3

Chain D:  99%



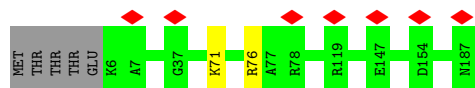
- Molecule 6: 50S ribosomal protein L4

Chain E:  97%



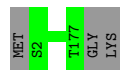
- Molecule 7: 50S ribosomal protein L5

Chain F:  96%



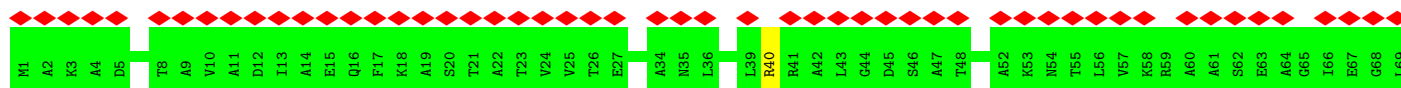
- Molecule 8: 50S ribosomal protein L6

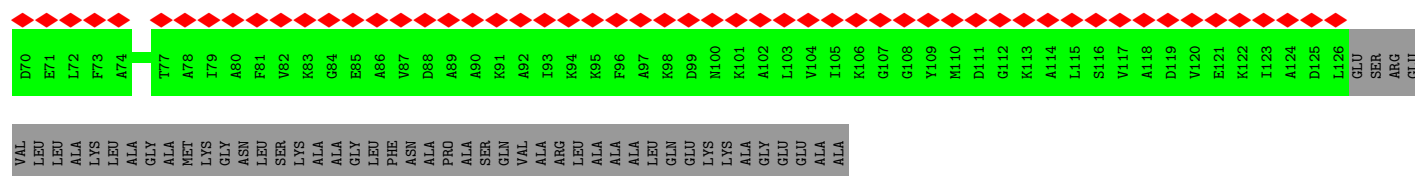
Chain G:  98%



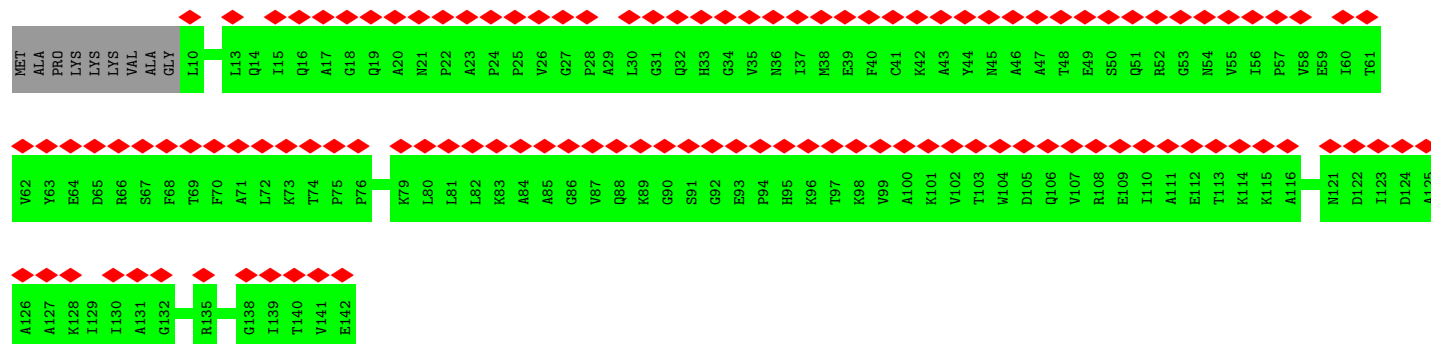
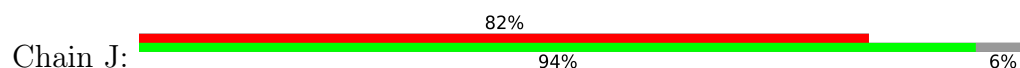
- Molecule 9: 50S ribosomal protein L10

Chain I:  62% 71% 28%





- Molecule 10: 50S ribosomal protein L11



- Molecule 11: 50S ribosomal protein L13

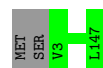


- Molecule 12: 50S ribosomal protein L14

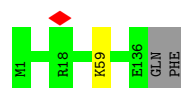


There are no outlier residues recorded for this chain.

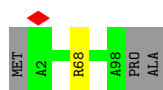
- Molecule 13: 50S ribosomal protein L15



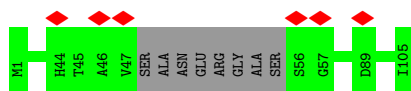
- Molecule 14: 50S ribosomal protein L16



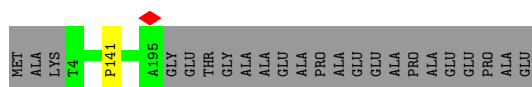
- Molecule 15: 50S ribosomal protein L17



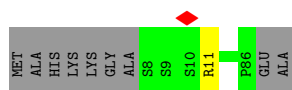
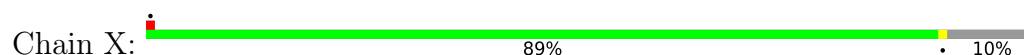
- Molecule 22: 50S ribosomal protein L24



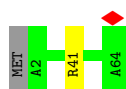
- Molecule 23: 50S ribosomal protein L25



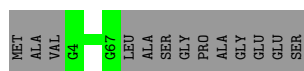
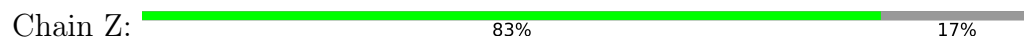
- Molecule 24: 50S ribosomal protein L27



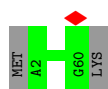
- Molecule 25: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L29

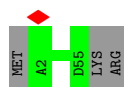


- Molecule 27: 50S ribosomal protein L30




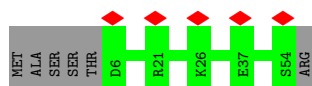
- Molecule 28: 50S ribosomal protein L32

Chain b:  95% 5%



- Molecule 29: 50S ribosomal protein L33 1

Chain c:  9% 89% 11%

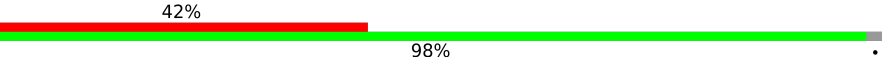


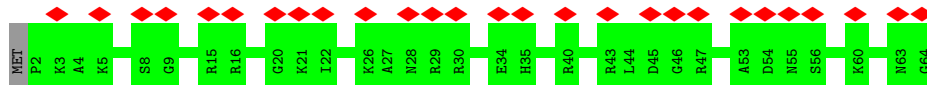
- Molecule 30: 50S ribosomal protein L34

Chain d:  98%



- Molecule 31: 50S ribosomal protein L35

Chain e:  42% 98%



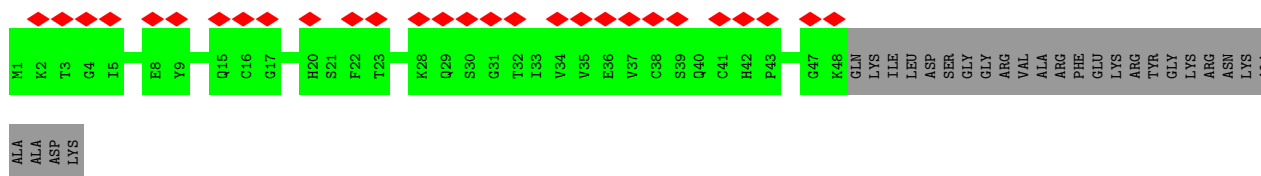
- Molecule 32: 50S ribosomal protein L36

Chain f:  97%



- Molecule 33: 50S ribosomal protein L31

Chain g:  37% 64% 36%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	483.0, 483.0, 483.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	3	0.24	0/191	0.62	0/247
2	A	0.50	0/75001	0.82	29/117027 (0.0%)
3	B	0.45	0/2821	0.81	4/4396 (0.1%)
4	C	0.31	0/2147	0.59	0/2885
5	D	0.33	0/1609	0.59	0/2165
6	E	0.31	0/1592	0.52	0/2153
7	F	0.30	0/1467	0.60	0/1973
8	G	0.31	0/1369	0.56	0/1848
9	I	0.28	0/925	0.54	0/1246
10	J	0.26	0/1006	0.55	0/1364
11	K	0.36	0/1157	0.55	0/1567
12	L	0.32	0/946	0.60	0/1268
13	M	0.33	0/1091	0.57	0/1457
14	N	0.32	0/1118	0.59	0/1506
15	O	0.33	0/945	0.57	0/1267
16	P	0.29	0/966	0.59	0/1298
17	Q	0.32	0/921	0.58	0/1236
18	R	0.32	0/1000	0.57	0/1341
19	S	0.32	0/764	0.52	0/1030
20	T	0.32	0/887	0.59	0/1204
21	U	0.32	0/766	0.57	0/1030
22	V	0.30	0/738	0.55	0/987
23	W	0.30	0/1443	0.57	1/1970 (0.1%)
24	X	0.33	0/595	0.60	0/798
25	Y	0.33	0/478	0.59	0/641
26	Z	0.35	0/534	0.70	0/713
27	a	0.30	0/477	0.62	0/640
28	b	0.28	0/427	0.64	0/572
29	c	0.32	0/413	0.61	0/553
30	d	0.28	0/380	0.68	0/500
31	e	0.24	0/507	0.60	0/672
32	f	0.31	0/303	0.60	0/401

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.28	0/372	0.53	0/503
All	All	0.46	0/105356	0.77	34/158458 (0.0%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	88	C	N1-C2-O2	7.86	123.61	118.90
3	B	88	C	C2-N1-C1'	7.36	126.89	118.80
2	A	323	C	N1-C2-O2	6.71	122.93	118.90
2	A	323	C	C2-N1-C1'	6.70	126.17	118.80
2	A	2245	C	N1-C2-O2	6.52	122.81	118.90
2	A	274	C	C2-N1-C1'	6.43	125.87	118.80
2	A	1614	G	C5-C6-O6	6.30	132.38	128.60
2	A	1428	U	C2-N1-C1'	6.28	125.24	117.70
2	A	1992	U	C5-C4-O4	-6.25	122.15	125.90
2	A	1568	C	N3-C2-O2	-6.21	117.56	121.90
2	A	2245	C	C2-N1-C1'	6.19	125.61	118.80
3	B	88	C	N3-C2-O2	-6.02	117.68	121.90
2	A	2521	C	C2-N1-C1'	6.02	125.42	118.80
2	A	3046	C	C2-N1-C1'	5.91	125.30	118.80
2	A	1557	C	N1-C2-O2	5.86	122.42	118.90
2	A	1621	C	N3-C2-O2	-5.82	117.83	121.90
2	A	1991	C	N3-C2-O2	-5.78	117.85	121.90
2	A	2117	C	N3-C2-O2	-5.76	117.86	121.90
23	W	141	PRO	CA-N-CD	-5.73	103.48	111.50
2	A	1012	C	C2-N1-C1'	5.72	125.09	118.80
2	A	283	U	C2-N1-C1'	5.55	124.36	117.70
3	B	88	C	C6-N1-C1'	-5.50	114.19	120.80
2	A	2245	C	N3-C2-O2	-5.48	118.06	121.90
2	A	2243	C	C2-N1-C1'	5.44	124.78	118.80
2	A	975	U	C2-N1-C1'	5.41	124.19	117.70
2	A	1992	U	N3-C4-O4	5.41	123.19	119.40
2	A	962	U	C2-N1-C1'	5.31	124.07	117.70
2	A	839	U	C2-N1-C1'	5.26	124.02	117.70
2	A	323	C	C6-N1-C1'	-5.16	114.61	120.80
2	A	2094	G	OP1-P-O3'	5.13	116.49	105.20
2	A	1557	C	N3-C2-O2	-5.10	118.33	121.90
2	A	2689	C	C2-N1-C1'	5.09	124.40	118.80
2	A	1557	C	N3-C4-N4	-5.09	114.44	118.00
2	A	1614	G	N1-C6-O6	-5.01	116.89	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	
1	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
4	C	270/278 (97%)	258 (96%)	12 (4%)	0	100	100
5	D	212/217 (98%)	199 (94%)	13 (6%)	0	100	100
6	E	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
7	F	180/187 (96%)	169 (94%)	11 (6%)	0	100	100
8	G	174/179 (97%)	168 (97%)	6 (3%)	0	100	100
9	I	124/175 (71%)	115 (93%)	9 (7%)	0	100	100
10	J	131/142 (92%)	121 (92%)	10 (8%)	0	100	100
11	K	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
12	L	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
13	M	143/147 (97%)	130 (91%)	13 (9%)	0	100	100
14	N	134/138 (97%)	129 (96%)	4 (3%)	1 (1%)	22	60
15	O	116/199 (58%)	110 (95%)	6 (5%)	0	100	100
16	P	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
17	Q	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
18	R	122/129 (95%)	117 (96%)	5 (4%)	0	100	100
19	S	98/103 (95%)	92 (94%)	6 (6%)	0	100	100
20	T	112/153 (73%)	111 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	95/100 (95%)	92 (97%)	3 (3%)	0	100	100
22	V	93/105 (89%)	92 (99%)	1 (1%)	0	100	100
23	W	190/215 (88%)	183 (96%)	7 (4%)	0	100	100
24	X	77/88 (88%)	72 (94%)	5 (6%)	0	100	100
25	Y	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
26	Z	62/77 (80%)	59 (95%)	3 (5%)	0	100	100
27	a	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
28	b	52/57 (91%)	52 (100%)	0	0	100	100
29	c	47/55 (86%)	44 (94%)	3 (6%)	0	100	100
30	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
31	e	61/64 (95%)	61 (100%)	0	0	100	100
32	f	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	g	46/75 (61%)	43 (94%)	3 (6%)	0	100	100
All	All	3463/3840 (90%)	3310 (96%)	152 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	N	59	LYS

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	
1	3	18/19 (95%)	18 (100%)	0	100	100
4	C	215/218 (99%)	215 (100%)	0	100	100
5	D	160/163 (98%)	160 (100%)	0	100	100
6	E	169/173 (98%)	169 (100%)	0	100	100
7	F	151/156 (97%)	149 (99%)	2 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	148/150 (99%)	148 (100%)	0	100	100
9	I	89/120 (74%)	88 (99%)	1 (1%)	73	84
10	J	102/108 (94%)	102 (100%)	0	100	100
11	K	119/120 (99%)	119 (100%)	0	100	100
12	L	100/100 (100%)	100 (100%)	0	100	100
13	M	112/114 (98%)	112 (100%)	0	100	100
14	N	114/116 (98%)	114 (100%)	0	100	100
15	O	97/158 (61%)	97 (100%)	0	100	100
16	P	93/94 (99%)	93 (100%)	0	100	100
17	Q	100/100 (100%)	98 (98%)	2 (2%)	55	73
18	R	97/99 (98%)	97 (100%)	0	100	100
19	S	81/83 (98%)	81 (100%)	0	100	100
20	T	90/117 (77%)	90 (100%)	0	100	100
21	U	83/85 (98%)	82 (99%)	1 (1%)	71	83
22	V	81/86 (94%)	81 (100%)	0	100	100
23	W	155/168 (92%)	155 (100%)	0	100	100
24	X	58/63 (92%)	57 (98%)	1 (2%)	60	78
25	Y	50/51 (98%)	49 (98%)	1 (2%)	55	73
26	Z	58/66 (88%)	58 (100%)	0	100	100
27	a	52/54 (96%)	52 (100%)	0	100	100
28	b	43/46 (94%)	43 (100%)	0	100	100
29	c	47/52 (90%)	47 (100%)	0	100	100
30	d	35/36 (97%)	35 (100%)	0	100	100
31	e	53/54 (98%)	53 (100%)	0	100	100
32	f	35/35 (100%)	34 (97%)	1 (3%)	42	64
33	g	43/63 (68%)	43 (100%)	0	100	100
All	All	2848/3067 (93%)	2839 (100%)	9 (0%)	92	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	F	71	LYS
7	F	76	ARG

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Mol	Chain	Res	Type
9	I	40	ARG
17	Q	50	GLN
17	Q	79	ASN
21	U	68	ARG
24	X	11	ARG
25	Y	41	ARG
32	f	36	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	143	HIS
4	C	227	ASN
10	J	33	HIS
13	M	58	HIS
16	P	9	ASN
17	Q	82	HIS
18	R	27	GLN
20	T	67	ASN
23	W	86	HIS
23	W	93	GLN
23	W	101	GLN
23	W	126	GLN
25	Y	34	GLN
29	c	31	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3118/3120 (99%)	721 (23%)	28 (0%)
3	B	117/118 (99%)	22 (18%)	1 (0%)
All	All	3235/3238 (99%)	743 (22%)	29 (0%)

All (743) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	9	U
2	A	12	G
2	A	20	G

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Mol	Chain	Res	Type
2	A	29	C
2	A	31	U
2	A	33	G
2	A	60	A
2	A	61	G
2	A	68	A
2	A	71	A
2	A	72	G
2	A	77	G
2	A	80	G
2	A	90	C
2	A	93	A
2	A	94	G
2	A	95	C
2	A	98	U
2	A	99	G
2	A	115	A
2	A	117	U
2	A	125	C
2	A	143	G
2	A	144	U
2	A	148	A
2	A	161	U
2	A	175	G
2	A	176	G
2	A	180	A
2	A	195	A
2	A	198	A
2	A	212	A
2	A	214	G
2	A	215	A
2	A	221	A
2	A	222	A
2	A	227	A
2	A	228	A
2	A	229	U
2	A	230	G
2	A	231	U
2	A	232	G
2	A	245	G
2	A	248	G
2	A	265	A

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Mol	Chain	Res	Type
2	A	269	C
2	A	270	U
2	A	274	C
2	A	275	C
2	A	279	U
2	A	282	A
2	A	283	U
2	A	285	U
2	A	286	G
2	A	287	A
2	A	288	U
2	A	290	C
2	A	291	C
2	A	292	G
2	A	296	A
2	A	297	G
2	A	298	G
2	A	299	G
2	A	300	G
2	A	301	U
2	A	302	U
2	A	303	G
2	A	305	G
2	A	314	G
2	A	315	U
2	A	317	G
2	A	318	U
2	A	319	G
2	A	323	C
2	A	326	A
2	A	327	U
2	A	330	U
2	A	331	U
2	A	336	C
2	A	337	U
2	A	338	C
2	A	342	C
2	A	344	G
2	A	345	G
2	A	348	G
2	A	350	A
2	A	351	G

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Mol	Chain	Res	Type
2	A	352	G
2	A	353	G
2	A	355	A
2	A	357	U
2	A	358	G
2	A	361	A
2	A	363	A
2	A	364	A
2	A	365	U
2	A	366	G
2	A	369	G
2	A	370	U
2	A	371	G
2	A	373	U
2	A	384	G
2	A	389	G
2	A	390	G
2	A	393	U
2	A	412	A
2	A	413	G
2	A	428	A
2	A	433	C
2	A	434	G
2	A	437	G
2	A	445	U
2	A	446	G
2	A	447	A
2	A	449	G
2	A	450	G
2	A	452	G
2	A	454	U
2	A	460	G
2	A	472	C
2	A	474	G
2	A	489	A
2	A	490	A
2	A	491	U
2	A	493	U
2	A	494	G
2	A	498	G
2	A	500	A
2	A	509	U

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Mol	Chain	Res	Type
2	A	512	G
2	A	514	C
2	A	539	C
2	A	543	U
2	A	544	U
2	A	562	G
2	A	566	A
2	A	568	A
2	A	569	G
2	A	589	A
2	A	591	G
2	A	592	A
2	A	594	U
2	A	595	A
2	A	596	C
2	A	597	C
2	A	599	G
2	A	605	G
2	A	616	A
2	A	617	U
2	A	618	C
2	A	619	C
2	A	631	C
2	A	636	U
2	A	637	G
2	A	638	U
2	A	639	C
2	A	640	G
2	A	641	U
2	A	642	G
2	A	643	G
2	A	644	G
2	A	646	U
2	A	647	G
2	A	655	G
2	A	665	G
2	A	667	A
2	A	678	A
2	A	679	G
2	A	684	G
2	A	685	G
2	A	696	A

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Mol	Chain	Res	Type
2	A	706	G
2	A	707	G
2	A	708	G
2	A	709	U
2	A	712	G
2	A	714	U
2	A	721	A
2	A	731	A
2	A	738	A
2	A	740	A
2	A	747	A
2	A	749	C
2	A	753	A
2	A	754	C
2	A	755	A
2	A	756	A
2	A	757	G
2	A	758	A
2	A	759	G
2	A	760	U
2	A	763	G
2	A	764	U
2	A	766	G
2	A	768	G
2	A	774	G
2	A	784	G
2	A	794	G
2	A	801	U
2	A	830	A
2	A	832	G
2	A	836	G
2	A	838	G
2	A	839	U
2	A	845	C
2	A	862	U
2	A	863	G
2	A	868	C
2	A	871	A
2	A	872	G
2	A	878	G
2	A	879	A
2	A	880	G

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Mol	Chain	Res	Type
2	A	890	G
2	A	891	G
2	A	897	A
2	A	899	G
2	A	917	A
2	A	920	G
2	A	921	C
2	A	927	C
2	A	942	U
2	A	944	A
2	A	960	G
2	A	961	U
2	A	972	A
2	A	974	G
2	A	975	U
2	A	981	U
2	A	982	A
2	A	994	A
2	A	999	C
2	A	1001	C
2	A	1002	C
2	A	1003	A
2	A	1004	C
2	A	1005	A
2	A	1007	G
2	A	1008	G
2	A	1010	U
2	A	1011	A
2	A	1012	C
2	A	1013	U
2	A	1025	A
2	A	1044	U
2	A	1046	C
2	A	1047	A
2	A	1049	G
2	A	1063	G
2	A	1075	U
2	A	1076	A
2	A	1078	G
2	A	1084	U
2	A	1085	G
2	A	1092	G

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Mol	Chain	Res	Type
2	A	1101	A
2	A	1114	G
2	A	1127	A
2	A	1130	C
2	A	1131	G
2	A	1141	U
2	A	1143	G
2	A	1144	A
2	A	1151	U
2	A	1158	U
2	A	1161	C
2	A	1163	A
2	A	1164	A
2	A	1165	G
2	A	1173	G
2	A	1174	G
2	A	1175	A
2	A	1178	U
2	A	1181	G
2	A	1184	U
2	A	1185	A
2	A	1186	G
2	A	1187	A
2	A	1188	A
2	A	1189	G
2	A	1191	A
2	A	1192	G
2	A	1197	C
2	A	1199	U
2	A	1200	U
2	A	1201	G
2	A	1202	A
2	A	1203	A
2	A	1205	G
2	A	1206	A
2	A	1207	G
2	A	1209	G
2	A	1212	U
2	A	1213	A
2	A	1214	A
2	A	1215	U
2	A	1219	U

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Mol	Chain	Res	Type
2	A	1226	U
2	A	1230	G
2	A	1232	G
2	A	1233	A
2	A	1234	U
2	A	1237	U
2	A	1238	G
2	A	1240	G
2	A	1245	U
2	A	1246	A
2	A	1248	U
2	A	1250	U
2	A	1251	A
2	A	1253	C
2	A	1254	G
2	A	1260	C
2	A	1261	A
2	A	1293	G
2	A	1298	C
2	A	1325	U
2	A	1335	G
2	A	1344	A
2	A	1345	G
2	A	1351	G
2	A	1353	G
2	A	1359	G
2	A	1371	G
2	A	1380	A
2	A	1384	G
2	A	1386	G
2	A	1387	A
2	A	1389	U
2	A	1415	A
2	A	1416	A
2	A	1436	C
2	A	1444	U
2	A	1448	C
2	A	1456	G
2	A	1462	G
2	A	1465	C
2	A	1467	U
2	A	1480	A

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Mol	Chain	Res	Type
2	A	1493	A
2	A	1494	U
2	A	1499	A
2	A	1507	G
2	A	1508	A
2	A	1510	A
2	A	1512	U
2	A	1518	A
2	A	1522	G
2	A	1531	C
2	A	1532	G
2	A	1533	U
2	A	1534	C
2	A	1536	A
2	A	1541	G
2	A	1546	A
2	A	1548	C
2	A	1550	G
2	A	1551	U
2	A	1552	A
2	A	1553	C
2	A	1554	U
2	A	1555	A
2	A	1556	A
2	A	1560	U
2	A	1562	C
2	A	1563	A
2	A	1564	A
2	A	1565	A
2	A	1566	A
2	A	1567	C
2	A	1574	G
2	A	1575	A
2	A	1576	C
2	A	1578	G
2	A	1580	A
2	A	1582	C
2	A	1584	U
2	A	1585	U
2	A	1588	G
2	A	1589	G
2	A	1591	U

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Mol	Chain	Res	Type
2	A	1596	C
2	A	1599	U
2	A	1601	G
2	A	1604	G
2	A	1605	G
2	A	1606	G
2	A	1611	A
2	A	1615	G
2	A	1617	C
2	A	1618	C
2	A	1624	U
2	A	1627	U
2	A	1628	A
2	A	1629	G
2	A	1630	U
2	A	1631	A
2	A	1632	G
2	A	1636	A
2	A	1638	C
2	A	1639	G
2	A	1640	A
2	A	1641	U
2	A	1648	A
2	A	1649	C
2	A	1654	G
2	A	1674	G
2	A	1676	G
2	A	1678	U
2	A	1679	A
2	A	1680	A
2	A	1681	U
2	A	1688	G
2	A	1697	U
2	A	1703	G
2	A	1710	A
2	A	1711	G
2	A	1713	U
2	A	1716	A
2	A	1717	U
2	A	1721	U
2	A	1724	G
2	A	1725	G

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Mol	Chain	Res	Type
2	A	1728	U
2	A	1730	U
2	A	1731	A
2	A	1732	U
2	A	1737	A
2	A	1738	G
2	A	1746	G
2	A	1752	C
2	A	1754	G
2	A	1755	A
2	A	1756	G
2	A	1757	U
2	A	1768	C
2	A	1780	G
2	A	1783	G
2	A	1786	G
2	A	1789	A
2	A	1798	U
2	A	1802	G
2	A	1828	A
2	A	1844	A
2	A	1845	G
2	A	1848	A
2	A	1852	A
2	A	1864	U
2	A	1866	C
2	A	1869	G
2	A	1870	U
2	A	1871	G
2	A	1872	A
2	A	1892	G
2	A	1893	C
2	A	1900	C
2	A	1933	G
2	A	1946	U
2	A	1947	U
2	A	1949	C
2	A	1950	G
2	A	1973	C
2	A	1975	A
2	A	1981	U
2	A	1990	A

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Mol	Chain	Res	Type
2	A	2017	C
2	A	2018	G
2	A	2024	G
2	A	2026	A
2	A	2033	U
2	A	2046	A
2	A	2064	A
2	A	2066	G
2	A	2075	G
2	A	2085	C
2	A	2086	U
2	A	2088	C
2	A	2089	C
2	A	2090	U
2	A	2091	U
2	A	2092	U
2	A	2093	G
2	A	2094	G
2	A	2095	G
2	A	2096	G
2	A	2106	A
2	A	2107	G
2	A	2111	U
2	A	2112	U
2	A	2130	G
2	A	2131	G
2	A	2133	G
2	A	2134	G
2	A	2136	A
2	A	2138	C
2	A	2140	A
2	A	2141	U
2	A	2142	A
2	A	2143	A
2	A	2144	C
2	A	2148	C
2	A	2151	A
2	A	2153	G
2	A	2154	G
2	A	2155	U
2	A	2162	A
2	A	2163	U

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Mol	Chain	Res	Type
2	A	2164	U
2	A	2168	U
2	A	2179	U
2	A	2187	U
2	A	2188	G
2	A	2190	A
2	A	2191	C
2	A	2194	A
2	A	2195	U
2	A	2196	G
2	A	2215	U
2	A	2216	G
2	A	2217	U
2	A	2221	A
2	A	2227	A
2	A	2247	A
2	A	2251	G
2	A	2255	A
2	A	2256	G
2	A	2257	A
2	A	2263	G
2	A	2267	C
2	A	2268	G
2	A	2276	G
2	A	2279	C
2	A	2280	G
2	A	2284	A
2	A	2285	G
2	A	2286	A
2	A	2316	G
2	A	2319	G
2	A	2320	C
2	A	2324	A
2	A	2325	U
2	A	2328	G
2	A	2332	U
2	A	2334	U
2	A	2335	G
2	A	2336	U
2	A	2338	G
2	A	2339	G
2	A	2340	A

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Mol	Chain	Res	Type
2	A	2341	U
2	A	2342	A
2	A	2343	G
2	A	2346	G
2	A	2349	A
2	A	2351	A
2	A	2352	C
2	A	2353	U
2	A	2354	G
2	A	2355	U
2	A	2356	G
2	A	2357	A
2	A	2359	G
2	A	2360	C
2	A	2362	C
2	A	2363	A
2	A	2367	G
2	A	2368	C
2	A	2370	A
2	A	2372	U
2	A	2374	U
2	A	2380	G
2	A	2381	A
2	A	2382	G
2	A	2384	C
2	A	2385	G
2	A	2386	U
2	A	2387	U
2	A	2388	G
2	A	2390	U
2	A	2392	A
2	A	2393	A
2	A	2394	A
2	A	2399	A
2	A	2401	U
2	A	2402	C
2	A	2404	G
2	A	2405	A
2	A	2407	C
2	A	2408	G
2	A	2413	G
2	A	2421	A

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Mol	Chain	Res	Type
2	A	2422	A
2	A	2427	G
2	A	2434	A
2	A	2436	A
2	A	2438	C
2	A	2446	G
2	A	2449	A
2	A	2462	G
2	A	2463	G
2	A	2467	U
2	A	2503	G
2	A	2507	C
2	A	2511	A
2	A	2529	A
2	A	2530	C
2	A	2532	G
2	A	2534	A
2	A	2536	U
2	A	2544	U
2	A	2545	G
2	A	2548	U
2	A	2549	G
2	A	2558	C
2	A	2559	A
2	A	2560	A
2	A	2571	C
2	A	2574	C
2	A	2578	A
2	A	2581	G
2	A	2585	U
2	A	2596	G
2	A	2607	G
2	A	2609	A
2	A	2627	C
2	A	2640	G
2	A	2647	U
2	A	2649	A
2	A	2653	G
2	A	2654	A
2	A	2655	U
2	A	2659	A
2	A	2665	C

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Mol	Chain	Res	Type
2	A	2671	G
2	A	2672	A
2	A	2677	A
2	A	2688	C
2	A	2689	C
2	A	2693	A
2	A	2694	G
2	A	2697	U
2	A	2699	C
2	A	2700	A
2	A	2702	A
2	A	2705	G
2	A	2715	U
2	A	2718	G
2	A	2726	G
2	A	2729	G
2	A	2742	A
2	A	2744	C
2	A	2749	G
2	A	2753	G
2	A	2759	G
2	A	2778	U
2	A	2786	U
2	A	2790	A
2	A	2791	G
2	A	2796	A
2	A	2797	C
2	A	2806	G
2	A	2809	U
2	A	2826	A
2	A	2827	G
2	A	2833	U
2	A	2837	U
2	A	2852	U
2	A	2853	C
2	A	2854	A
2	A	2856	A
2	A	2858	G
2	A	2862	G
2	A	2865	G
2	A	2876	C
2	A	2878	A

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Mol	Chain	Res	Type
2	A	2909	G
2	A	2912	A
2	A	2913	U
2	A	2915	C
2	A	2926	A
2	A	2936	C
2	A	2938	G
2	A	2948	C
2	A	2950	C
2	A	2953	U
2	A	2956	G
2	A	2957	A
2	A	2968	G
2	A	2972	A
2	A	2975	G
2	A	2981	A
2	A	2982	A
2	A	2985	G
2	A	2989	A
2	A	3002	A
2	A	3009	U
2	A	3013	C
2	A	3014	A
2	A	3015	C
2	A	3016	C
2	A	3021	A
2	A	3022	G
2	A	3029	U
2	A	3042	A
2	A	3054	U
2	A	3056	A
2	A	3057	U
2	A	3070	G
2	A	3082	U
2	A	3088	C
2	A	3093	A
2	A	3095	C
2	A	3098	G
2	A	3100	A
2	A	3101	C
2	A	3105	C
2	A	3106	C

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Mol	Chain	Res	Type
2	A	3112	A
2	A	3114	A
2	A	3115	A
3	B	3	U
3	B	4	A
3	B	9	G
3	B	11	U
3	B	12	C
3	B	13	C
3	B	26	A
3	B	30	G
3	B	35	G
3	B	42	C
3	B	45	G
3	B	57	U
3	B	58	A
3	B	85	C
3	B	87	U
3	B	88	C
3	B	89	C
3	B	90	G
3	B	103	G
3	B	107	A
3	B	114	A
3	B	115	A

All (29) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	89	A
2	A	97	U
2	A	299	G
2	A	316	U
2	A	336	C
2	A	357	U
2	A	445	U
2	A	567	A
2	A	974	G
2	A	981	U
2	A	1002	C
2	A	1004	C
2	A	1010	U

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Mol	Chain	Res	Type
2	A	1046	C
2	A	1084	U
2	A	1186	G
2	A	1253	C
2	A	1603	G
2	A	1635	A
2	A	1730	U
2	A	2088	C
2	A	2094	G
2	A	2139	U
2	A	2141	U
2	A	2350	G
2	A	2381	A
2	A	2698	C
2	A	2980	U
3	B	10	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](#)

Of 411 ligands modelled in this entry, 411 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

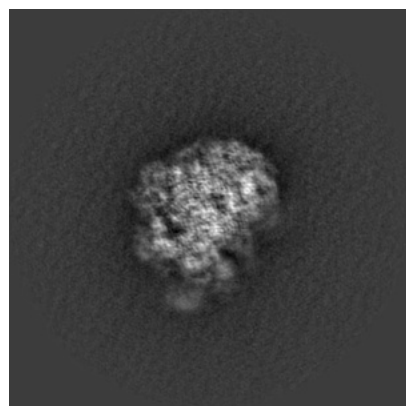
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33599. These allow visual inspection of the internal detail of the map and identification of artifacts.

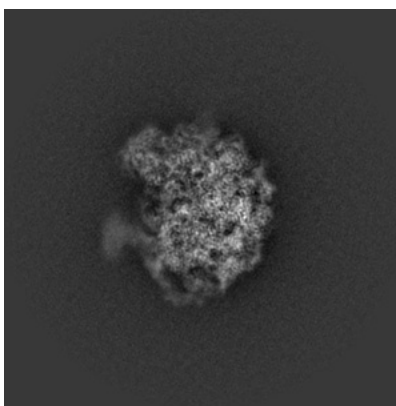
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

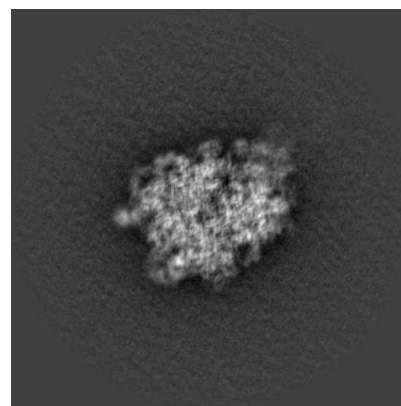
6.1.1 Primary map



X

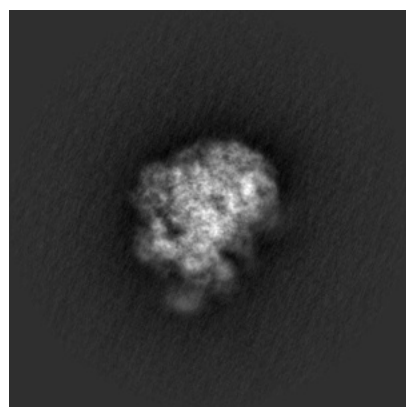


Y

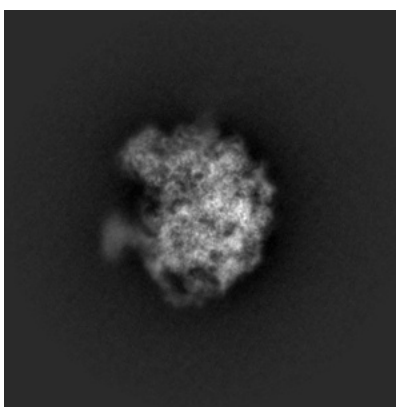


Z

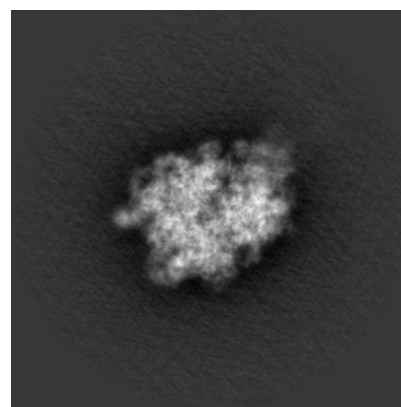
6.1.2 Raw map



X



Y

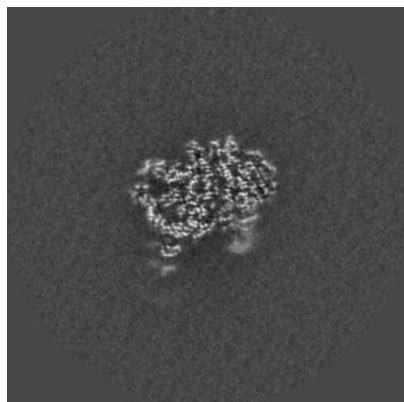


Z

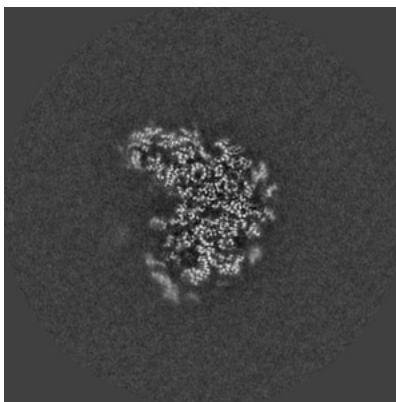
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

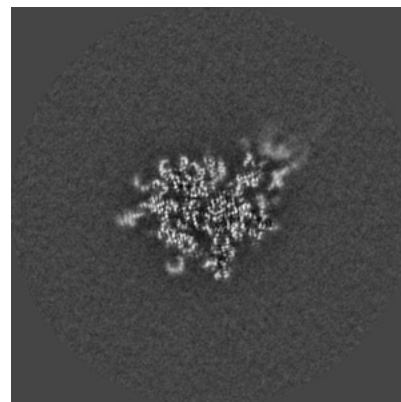
6.2.1 Primary map



X Index: 175

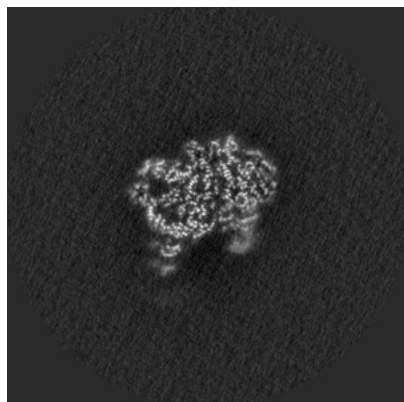


Y Index: 175

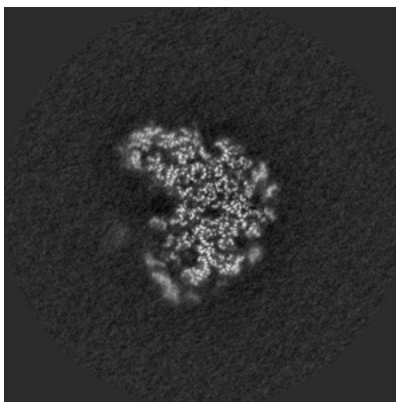


Z Index: 175

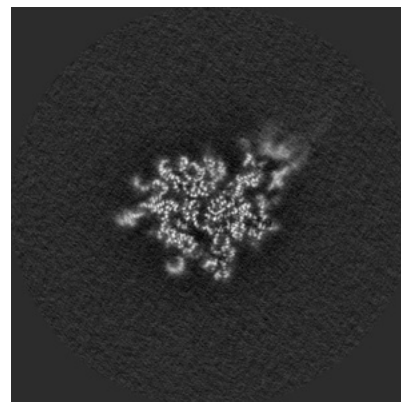
6.2.2 Raw map



X Index: 175



Y Index: 175

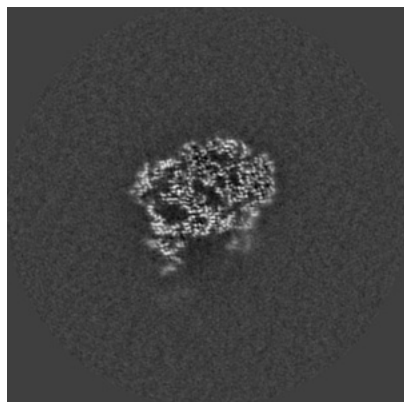


Z Index: 175

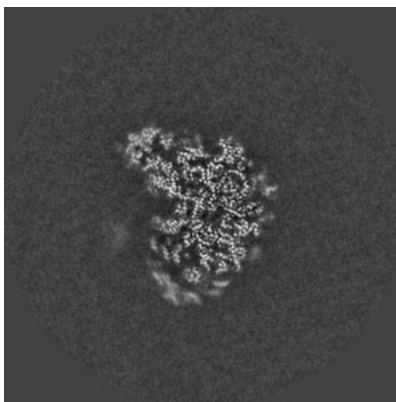
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

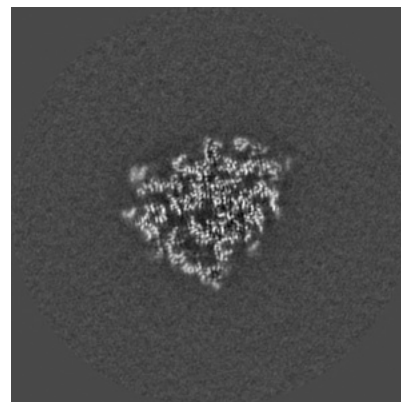
6.3.1 Primary map



X Index: 172

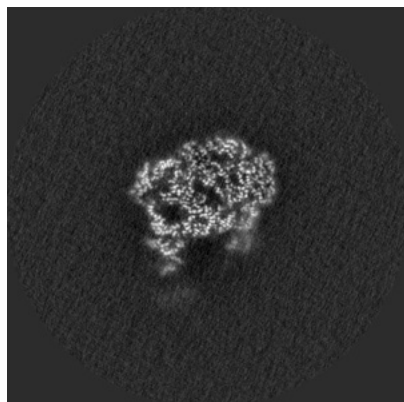


Y Index: 172

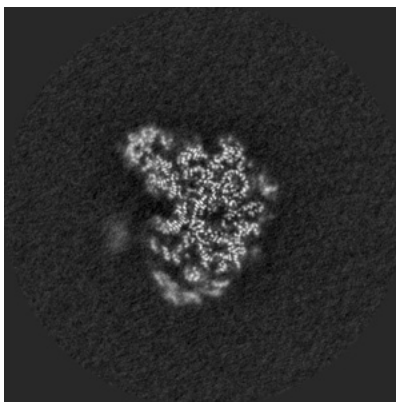


Z Index: 189

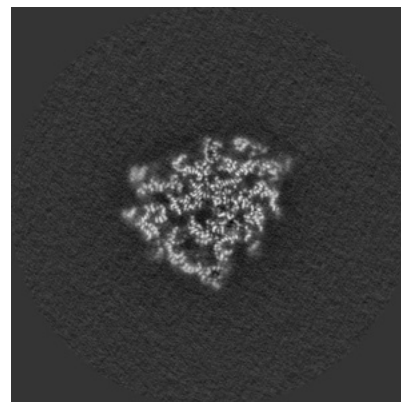
6.3.2 Raw map



X Index: 172



Y Index: 171

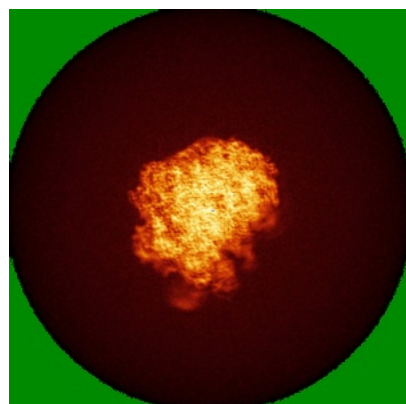


Z Index: 189

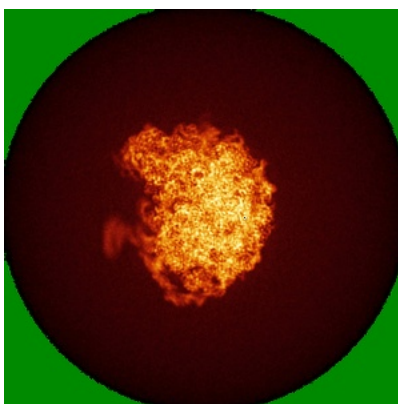
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

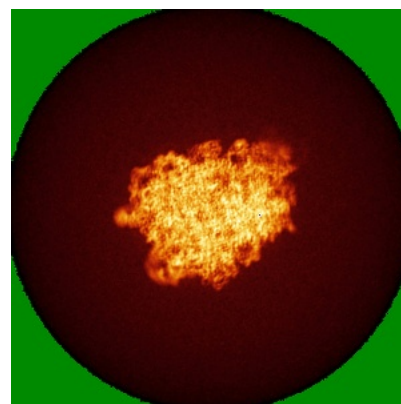
6.4.1 Primary map



X

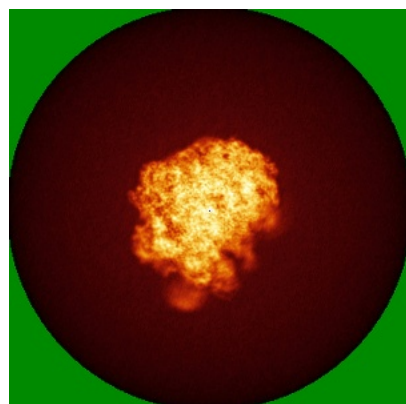


Y

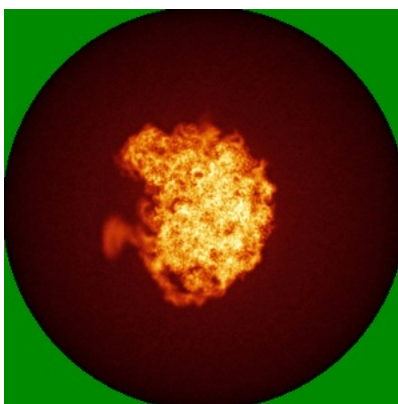


Z

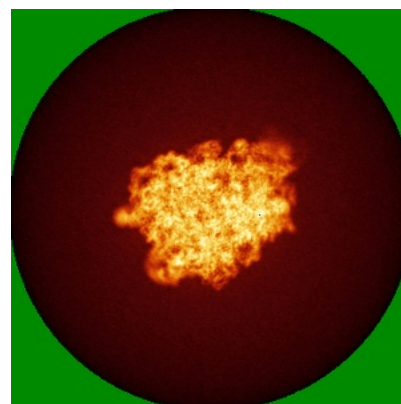
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

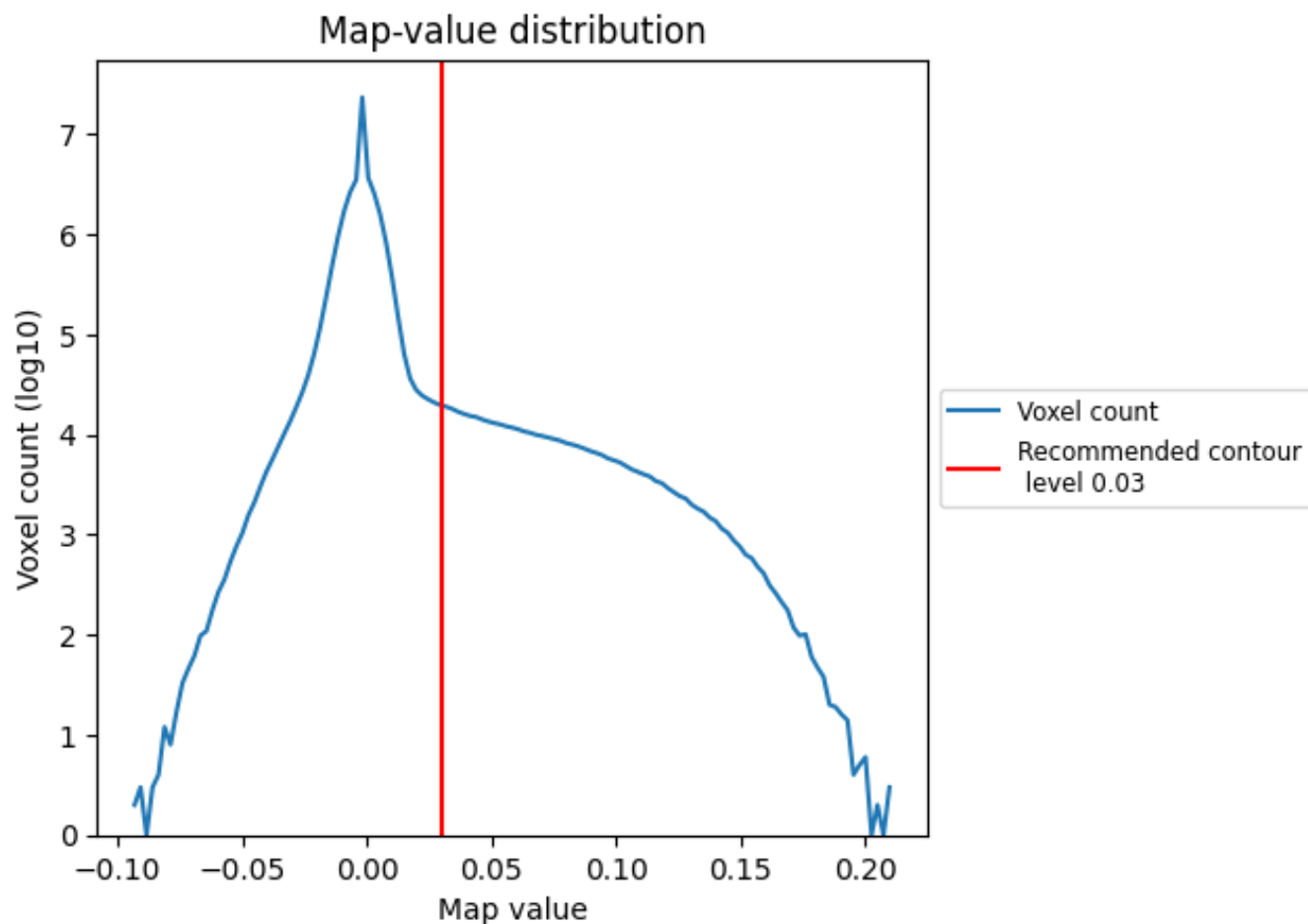
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

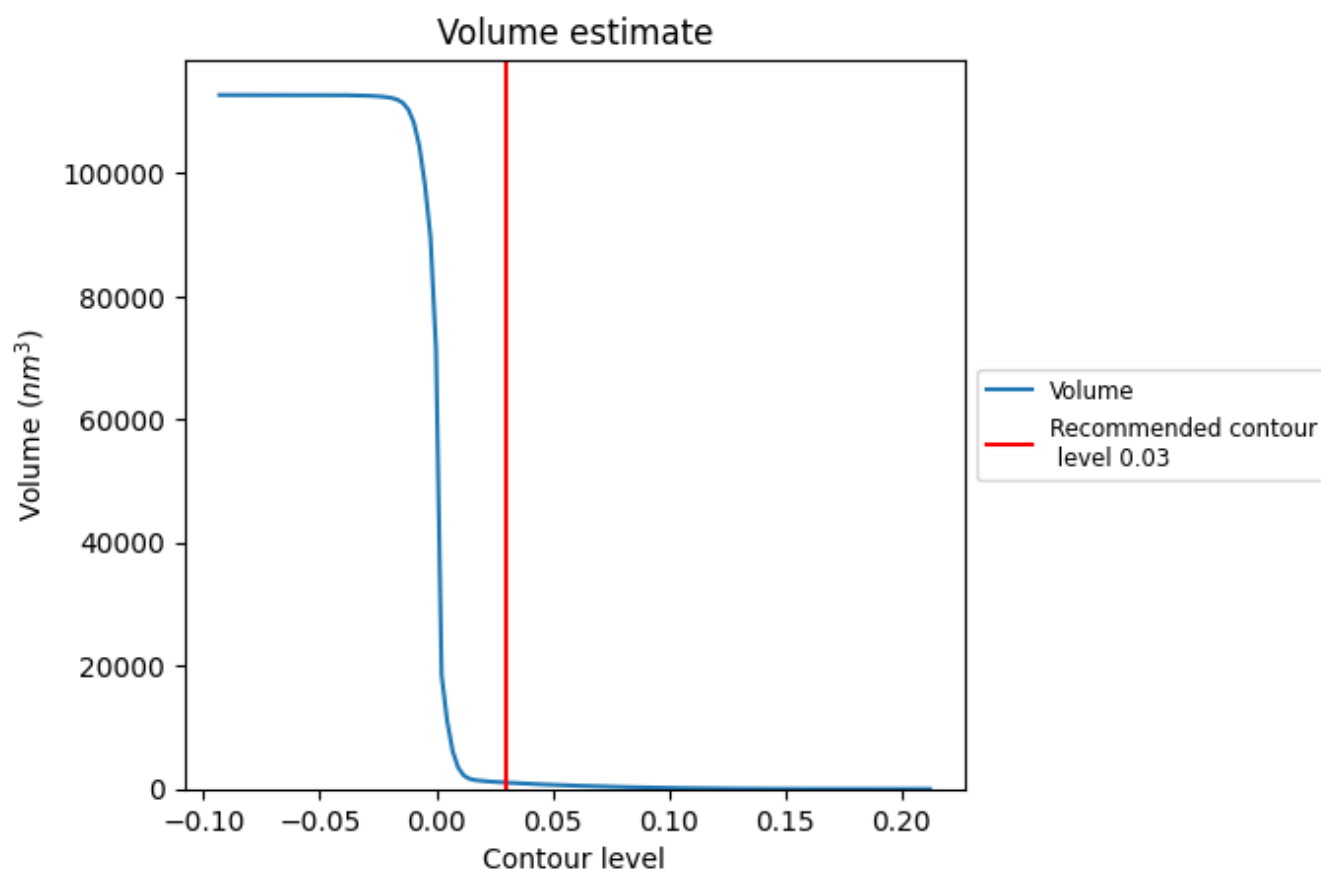
This section contains the results of statistical analysis of the map.

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.

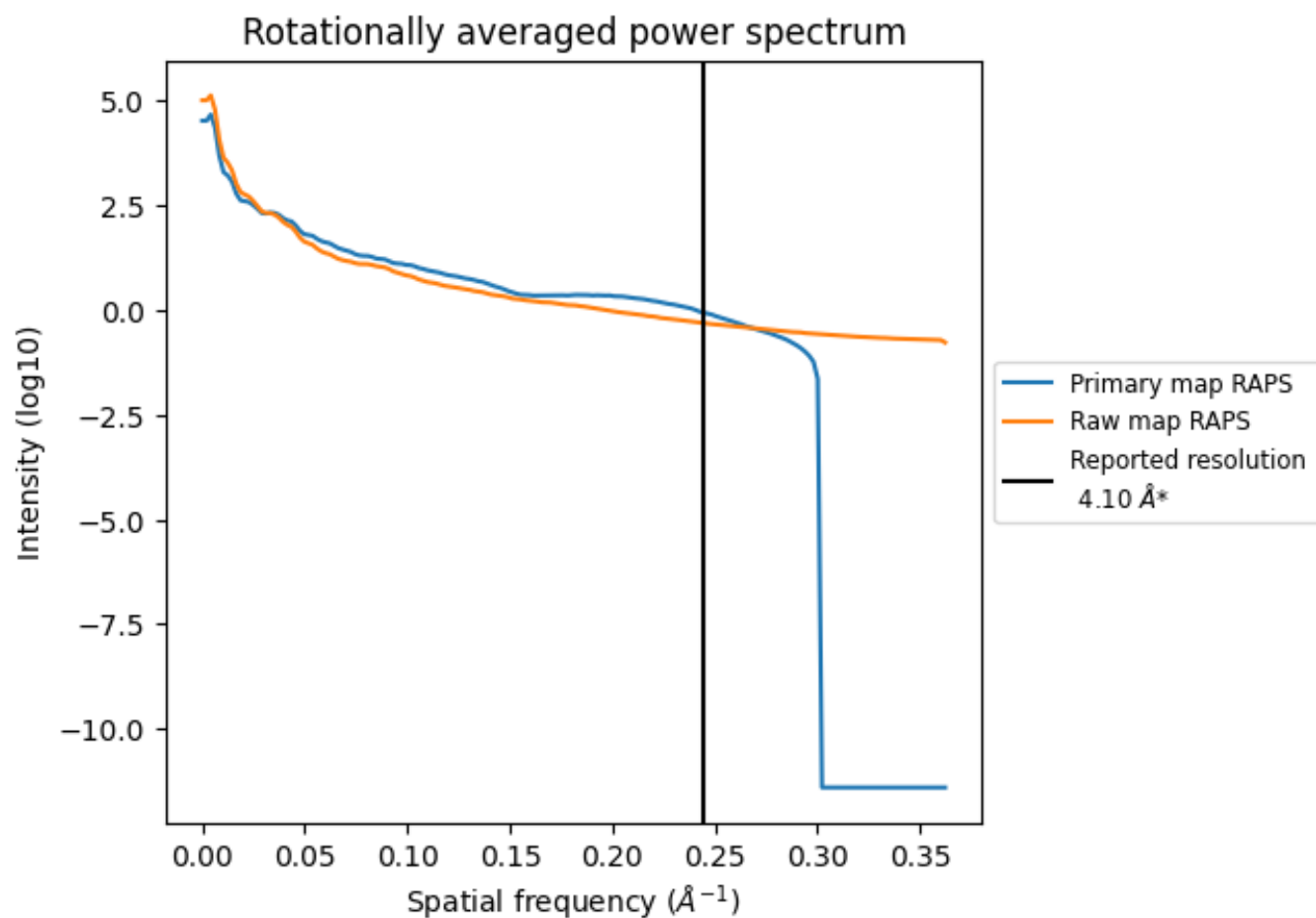
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1034 nm^3 ; this corresponds to an approximate mass of 934 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 ⓘ

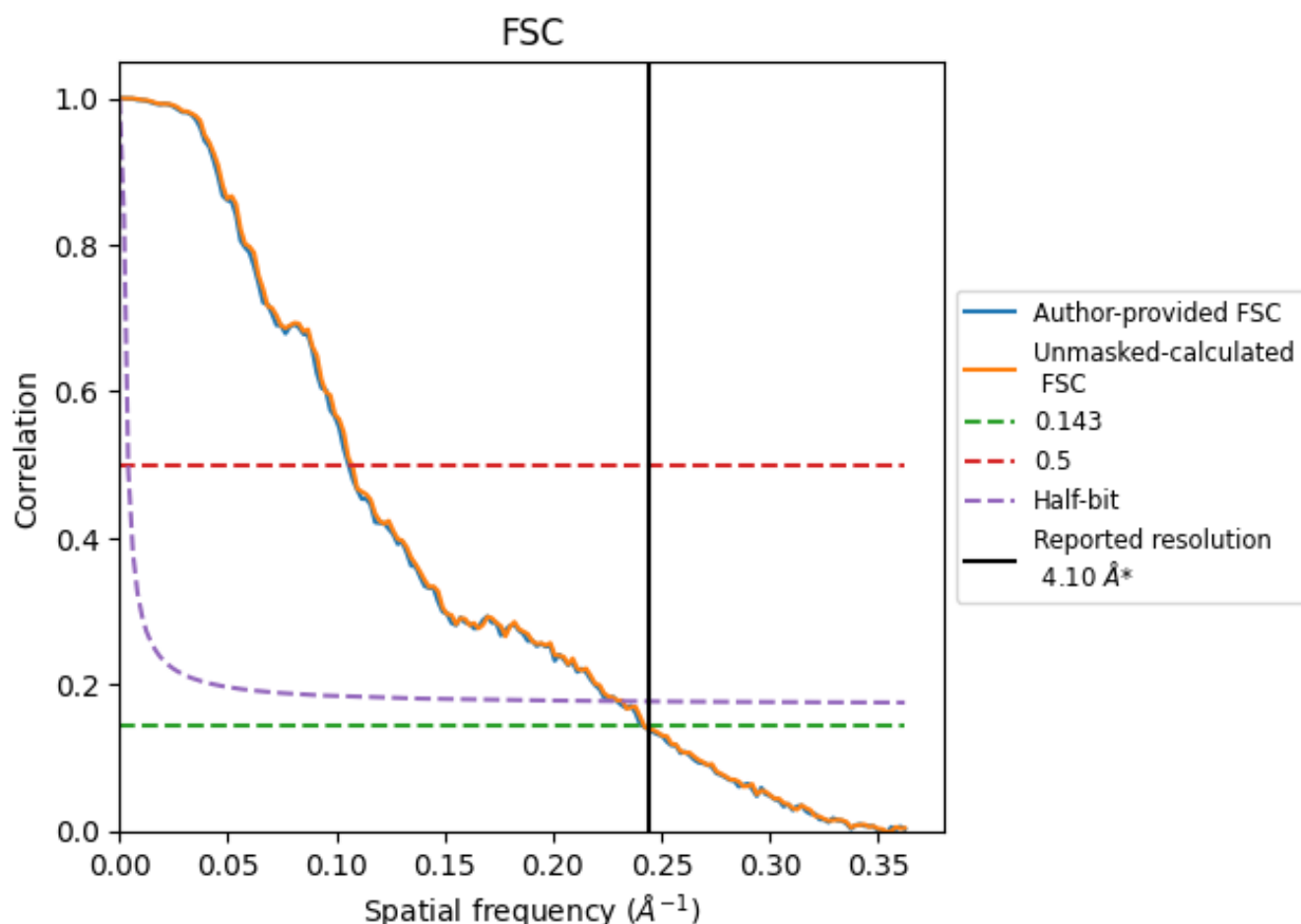


*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

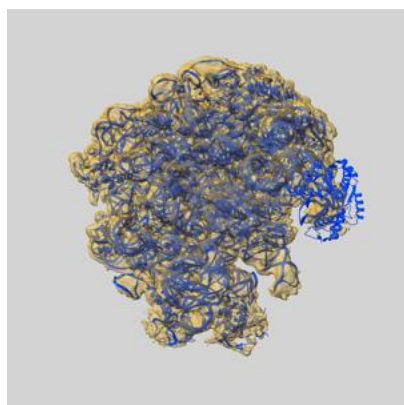
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	9.47	4.36
Unmasked-calculated*	4.13	9.35	4.31

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

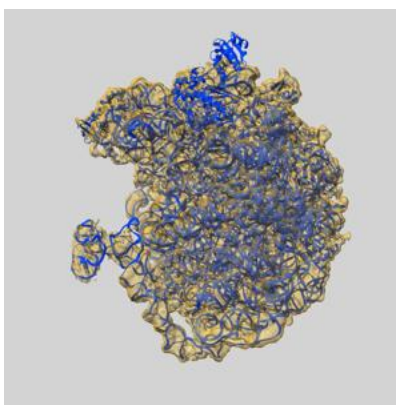
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33599 and PDB model 7Y41. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

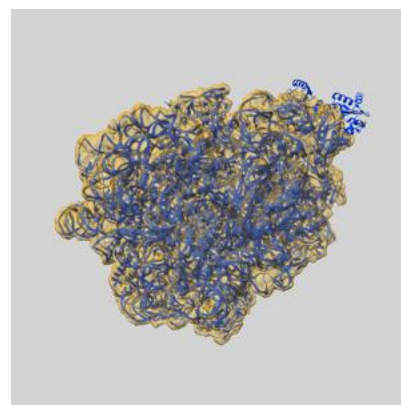
9.1 Map-model overlay [i](#)



X



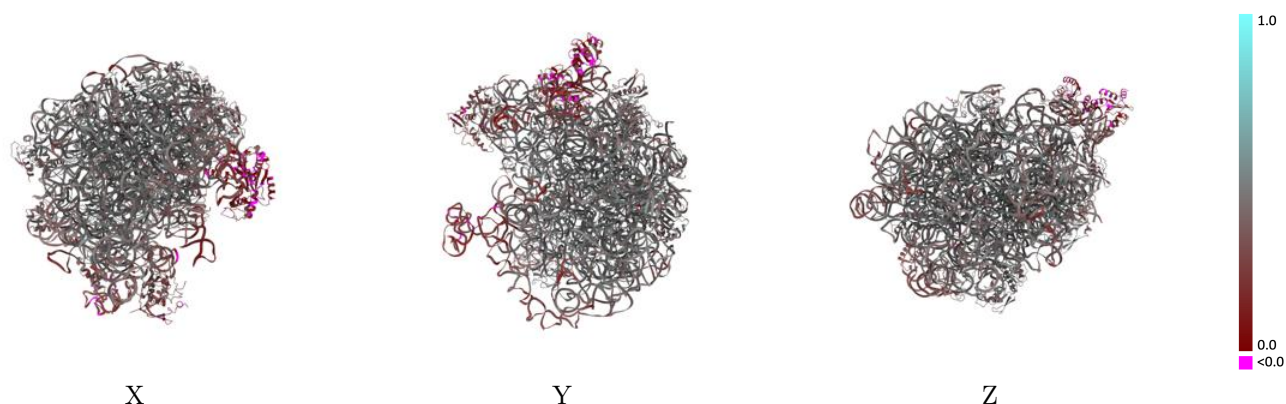
Y



Z

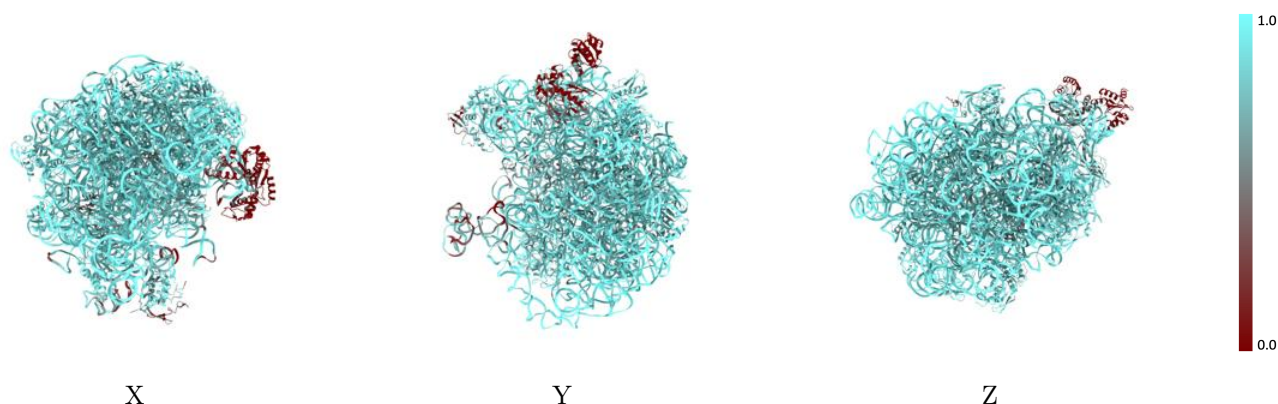
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



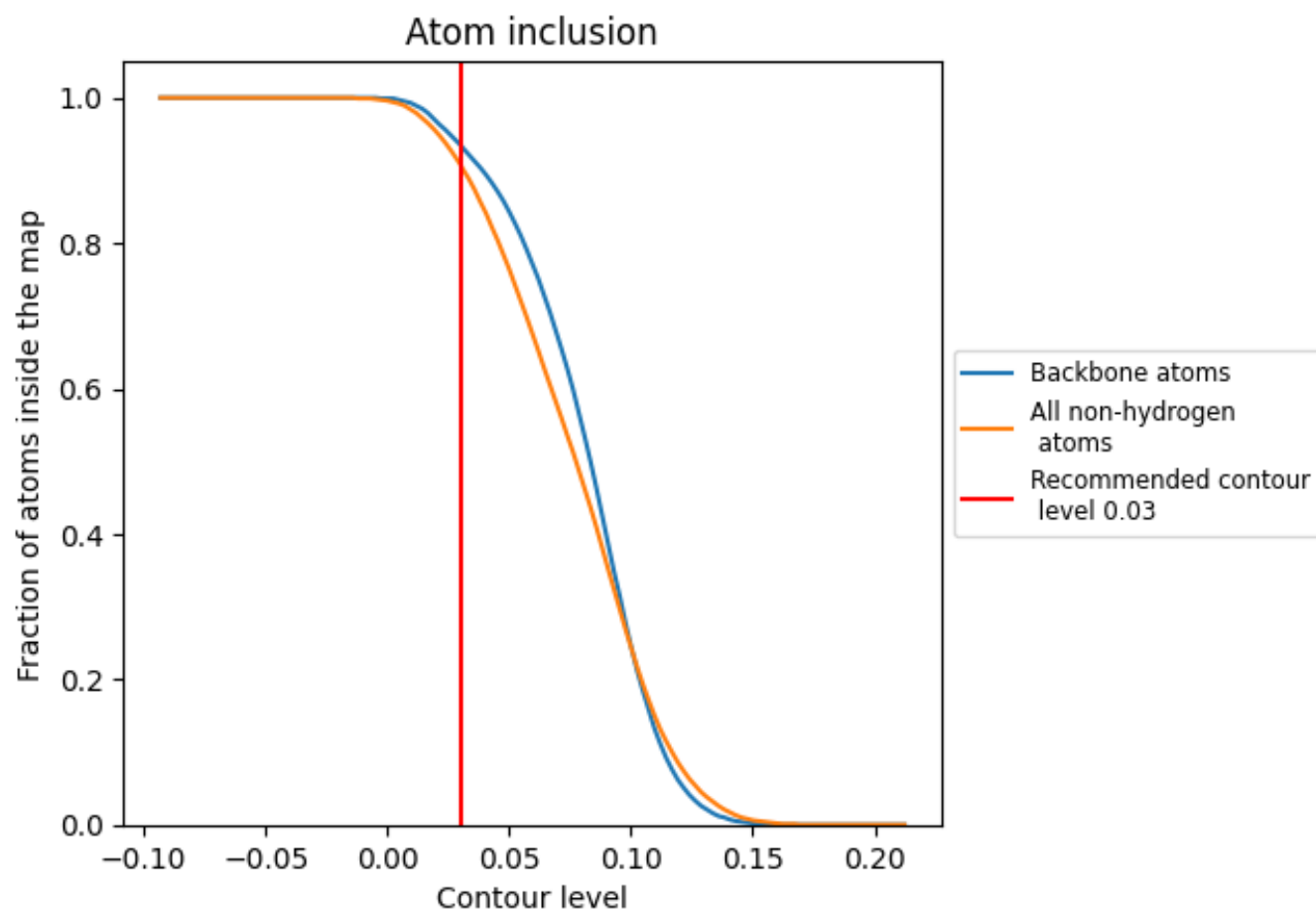
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9080	 0.4220
3	 0.5870	 0.4360
A	 0.9550	 0.4270
B	 0.9820	 0.4200
C	 0.8560	 0.4650
D	 0.8800	 0.4600
E	 0.8760	 0.4470
F	 0.7710	 0.3090
G	 0.8940	 0.3970
I	 0.1230	 0.1180
J	 0.1240	 0.1420
K	 0.8820	 0.4650
L	 0.8360	 0.4370
M	 0.8460	 0.4490
N	 0.8430	 0.4520
O	 0.8630	 0.4590
P	 0.8750	 0.4080
Q	 0.8280	 0.4130
R	 0.8670	 0.4600
S	 0.8990	 0.4750
T	 0.8600	 0.4610
U	 0.8150	 0.4410
V	 0.8360	 0.4020
W	 0.8000	 0.4020
X	 0.8730	 0.4700
Y	 0.8790	 0.4670
Z	 0.8800	 0.3930
a	 0.8630	 0.4460
b	 0.8660	 0.4700
c	 0.6810	 0.4250
d	 0.8200	 0.4770
e	 0.4370	 0.4400
f	 0.8120	 0.4700
g	 0.3300	 0.1850

