wwPDB EM Validation Summary Report

Nov 20, 2022 – 05:07 AM EST

PDB ID	:	7TTU
EMDB ID	:	EMD-26124
Title	:	50S ribosomal subunit from Staphylococcus aureus (Strain ATCC43300)
Authors	:	Belousoff, M.J.; Piper, S.; Johnson, R.
Deposited on	:	2022-02-01
Resolution	:	3.00 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

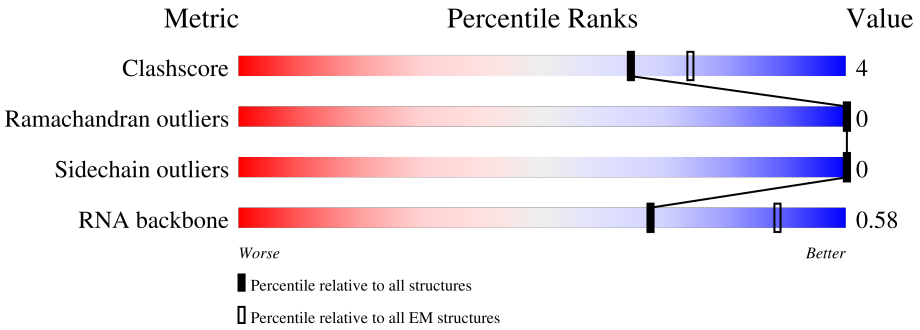
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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
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 <=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	116	90% 8%
2	B	277	85% 14%
3	C	118	93% 5%
4	D	102	7% 88% 10%
5	E	117	80% 15% 5%
6	F	87	92% 8%
7	G	105	72% 13% 14%

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Mol	Chain	Length	Quality of chain
8	H	217	6% 41% 57%
9	I	94	74% 9% 17%
10	J	61	85% 11%
11	K	73	74% 10% 16%
12	L	220	92% 6%
13	M	59	83% 12% 5%
14	N	57	75% 12% 12%
15	O	49	71% 24%
16	P	45	87% 11%
17	Q	65	95%
18	R	37	89% 11%
19	S	207	84% 9% 7%
20	V	145	88% 11%
21	W	122	81% 18%
22	X	146	88% 11%
23	Y	144	83% 12% 6%
24	Z	122	86% 13%
25	a	119	5% 92% 8%
26	1	2923	63% 25% 8%
27	2	115	59% 28% 10%

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 80724 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 protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	113	915	576	184	155	0	0

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	273	2085	1297	413	370	5	0	0

- Molecule 3 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	116	943	593	189	157	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	100	785	499	139	146	1	0	0

- Molecule 5 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	111	853	532	163	155	3	0	0

- Molecule 6 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	87	711	447	128	132	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	87	ASP	ILE	conflict	UNP W8TUB4

- Molecule 7 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	90	Total	C	N	O	S	0	0
			698	442	128	127	1		

- Molecule 8 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	93	Total	C	N	O	S	0	0
			727	465	129	132	1		

- Molecule 9 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	78	Total	C	N	O	0	0
			597	367	116	114		

- Molecule 10 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	59	Total	C	N	O	S	0	0
			463	287	99	76	1		

- Molecule 11 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	61	Total	C	N	O	S	0	0
			503	310	95	97	1		

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	215	Total	C	N	O	S	0	0
			1628	1018	299	306	5		

- Molecule 13 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	56	Total 432	C 269	N 82	O 81	0	0

- Molecule 14 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	50	Total 397	C 241	N 83	O 68	S 5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	47	Total 390	C 233	N 79	O 73	S 5	0	0

- Molecule 16 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	44	Total 372	C 228	N 90	O 53	S 1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	64	Total 521	C 324	N 113	O 82	S 2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	37	Total 296	C 186	N 60	O 45	S 5	0	0

- Molecule 19 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	192	Total 1472	C 924	N 271	O 275	S 2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	143	Total	C	N	O	S	0	0
			1138	710	209	217	2		

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	121	Total	C	N	O	S	0	0
			911	566	173	168	4		

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	144	Total	C	N	O	0	0
			1082	669	213	200		

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	121	Total	C	N	O	S	0	0
			955	586	183	185	1		

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	110	Total	C	N	O	0	0
			857	536	165	156		

- Molecule 26 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2684	Total	C	N	O	P	0	0
			57543	25704	10562	18603	2674		

- Molecule 27 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	111	Total	C	N	O	P	0	0
			2361	1057	423	771	110		

3 Residue-property plots (i)

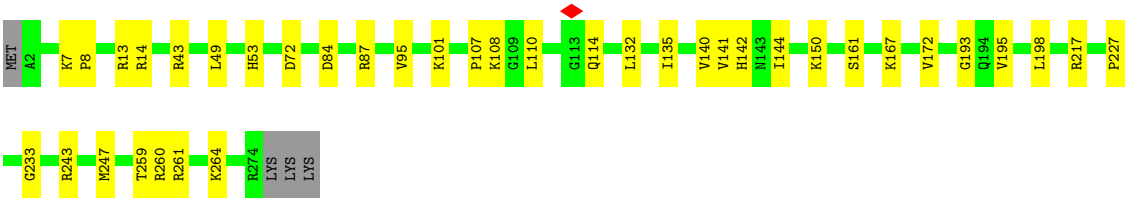
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 protein L19

Chain A:

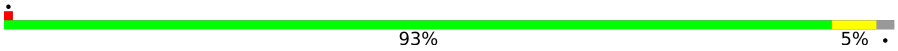
• Molecule 2: 50S ribosomal protein L2

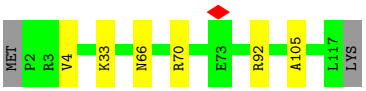
Chain B:



• Molecule 3: 50S ribosomal protein L20

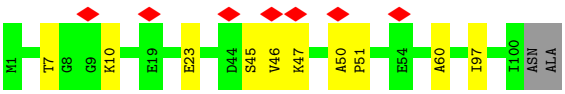
Chain C:





• Molecule 4: 50S ribosomal protein L21

Chain D:

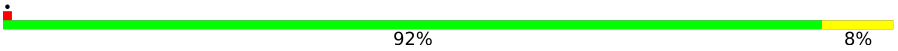


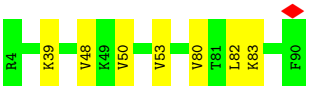
• Molecule 5: 50S ribosomal protein L22

Chain E:

• Molecule 6: 50S ribosomal protein L23

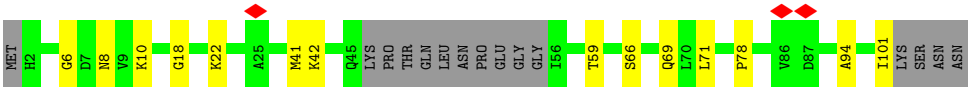
Chain F:





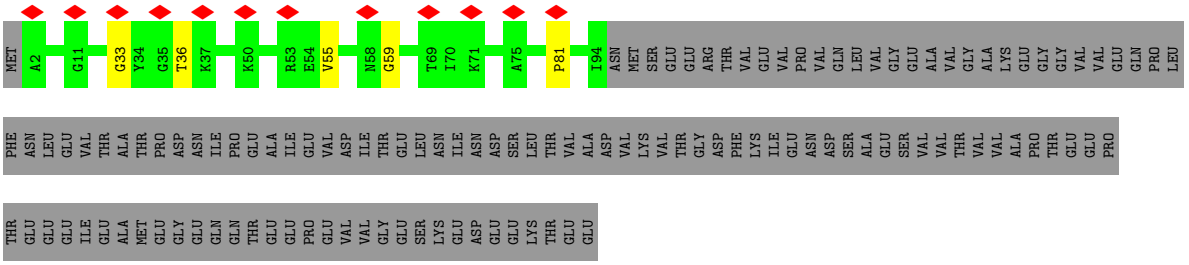
• Molecule 7: 50S ribosomal protein L24

Chain G:



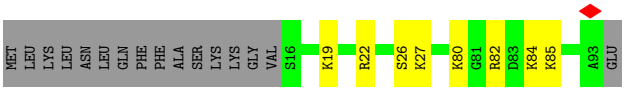
• Molecule 8: 50S ribosomal protein L25

Chain H:



• Molecule 9: 50S ribosomal protein L27

Chain I:

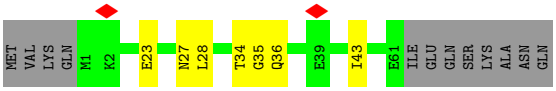


• Molecule 10: 50S ribosomal protein L28

Chain J:

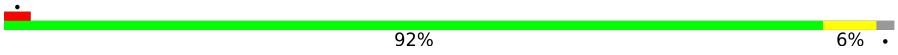
• Molecule 11: 50S ribosomal protein L29

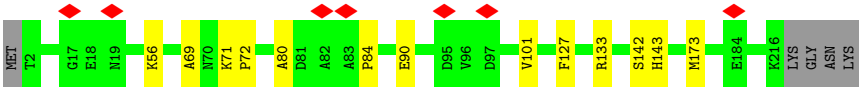
Chain K:



• Molecule 12: 50S ribosomal protein L3

Chain L:





• Molecule 13: 50S ribosomal protein L30

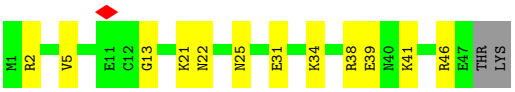
Chain M:

• Molecule 14: 50S ribosomal protein L32

Chain N:

• Molecule 15: 50S ribosomal protein L33

Chain O:

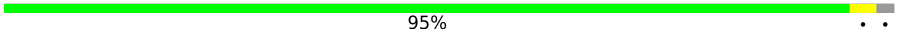


• Molecule 16: 50S ribosomal protein L34

Chain P:

• Molecule 17: 50S ribosomal protein L35

Chain Q:

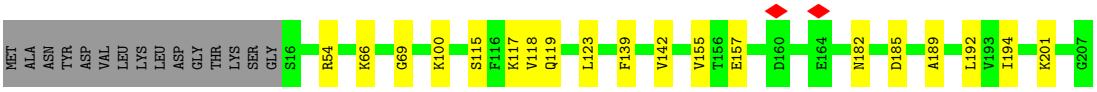


• Molecule 18: 50S ribosomal protein L36

Chain R:

• Molecule 19: 50S ribosomal protein L4

Chain S:

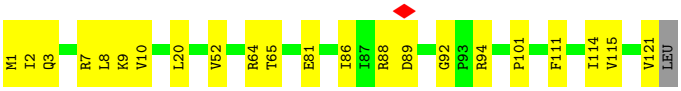


• Molecule 20: 50S ribosomal protein L13

Chain V:

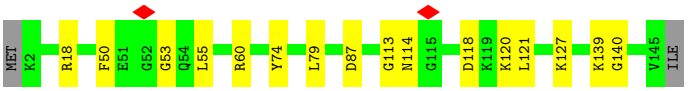
• Molecule 21: 50S ribosomal protein L14

Chain W:



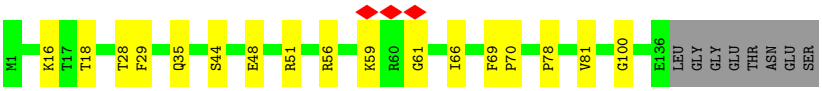
• Molecule 22: 50S ribosomal protein L15

Chain X:



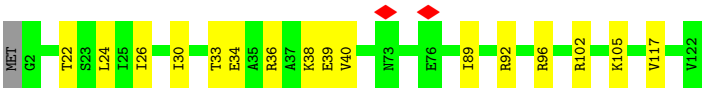
• Molecule 23: 50S ribosomal protein L16

Chain Y:



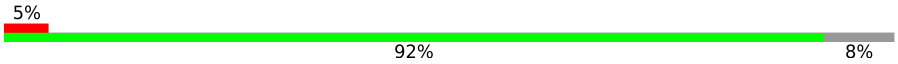
• Molecule 24: 50S ribosomal protein L17

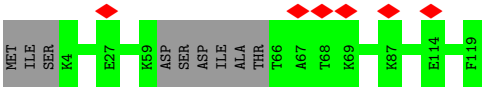
Chain Z:



• Molecule 25: 50S ribosomal protein L18

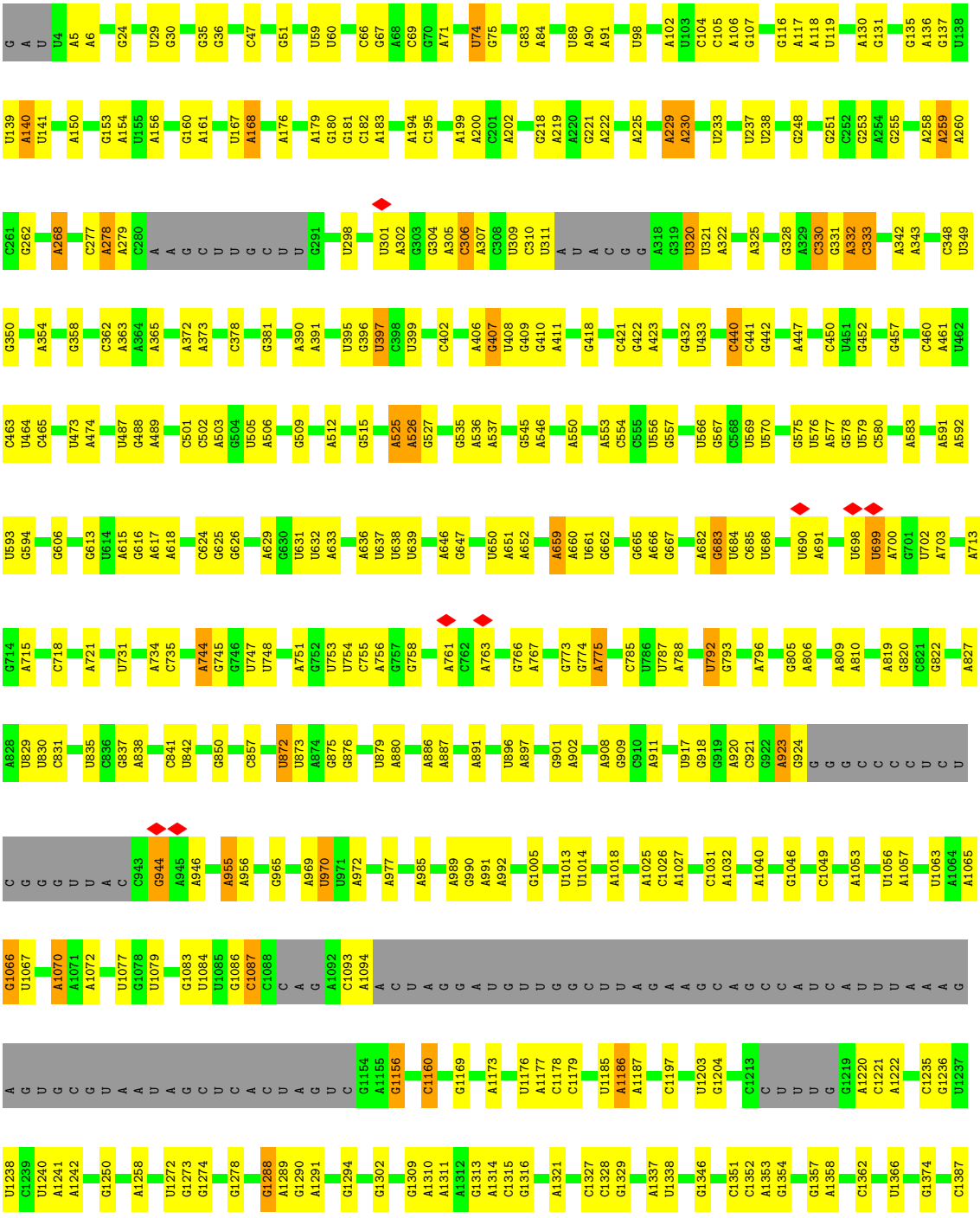
Chain a:

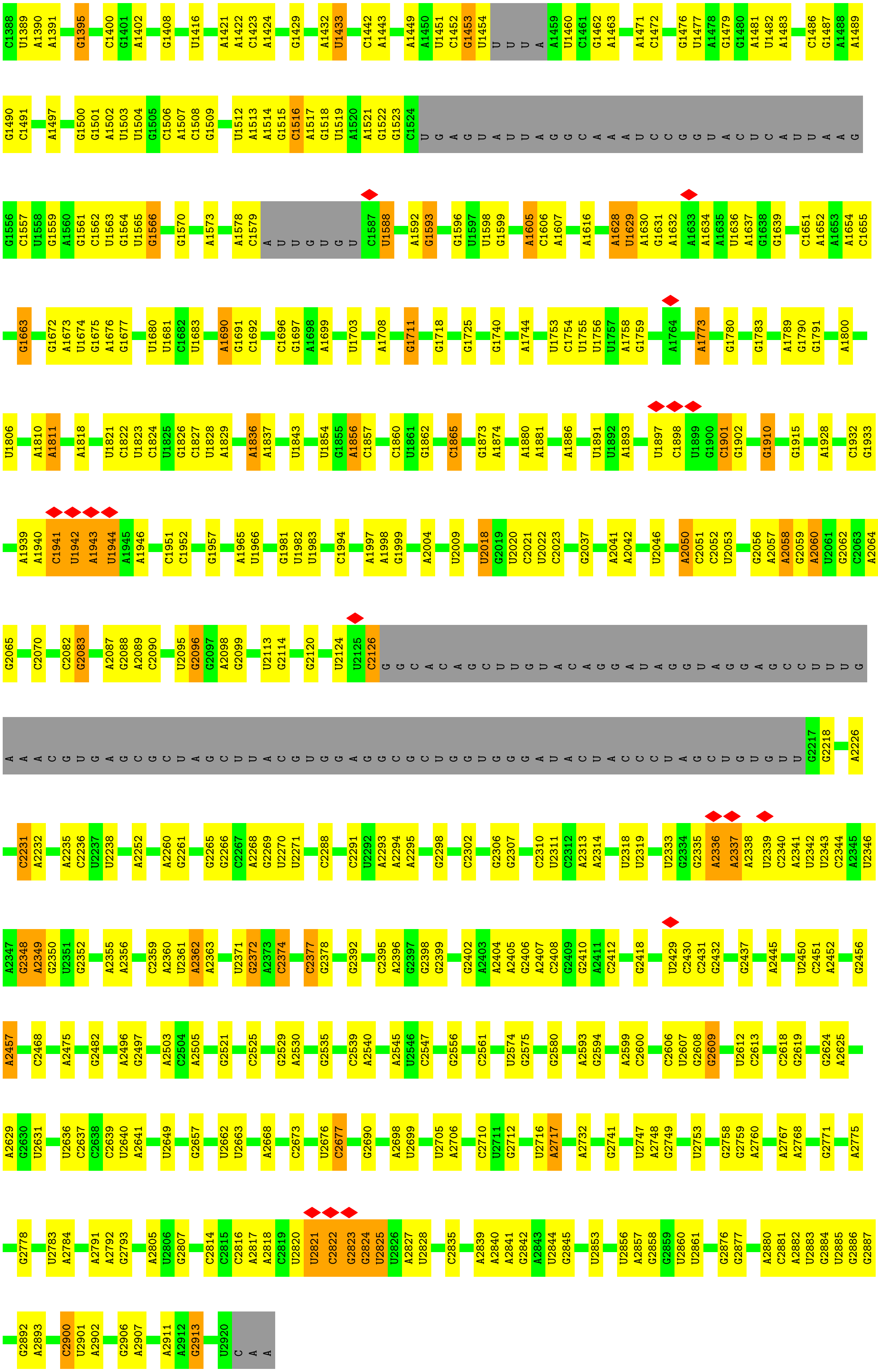




• Molecule 26: 23S rRNA

Chain 1:




C1388 U1389 A1390 A1391 G1395 C1400 G1401 A1402 G1408 U1416 A1421 A1422 C1423 A1424 G1429 A1432 U1433 C1442 A1443 A1449 A1450 U1451 C1452 G1453 U1454 U U U A A1459 U1460 C1461 G1462 A1463 A1471 C1472 G1476 U1477 A1478 G1479 G1480 A1481 U1482 A1483 C1486 G1487 A1488 A1489
G1490 C1491 A1497 G1500 G1501 A1502 U1503 U1504 G1505 C1506 A1507 C1508 G1509 U1512 A1513 A1514 G1515 C1516 A1517 G1518 U1519 A1520 A1521 G1522 G1523 C1524 U G A G U A U U A G G C A A A U C C G G U A C U C A U U A A G
G1556 C1557 U1558 G1559 A1560 G1561 C1562 U1563 G1564 U1565 G1566 G1570 A1573 A1578 C1579 A U U G U G U C1587 U1588 A1592 G1593 G1596 U1597 U1598 G1599 A1605 C1606 A1607 A1616 A1628 U1629 A1630 G1631 A1632 A1633 A1634 A1635 U1636 A1637 G1638 G1639 C1651 A1652 A1653 A1654 C1655
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U1806 A1810 A1811 A1818 U1821 C1822 U1823 C1824 U1825 G1826 C1827 U1828 A1829 A1836 A1837 U1843 U1854 G1855 A1856 C1857 C1860 U1861 G1862 C1865 G1873 A1874 A1880 A1881 A1886 U1891 U1892 A1893 U1897 C1898 U1899 G1900 C1901 G1902 G1910 G1915 A1928 C1932 G1933
A1939 A1940 C1941 U1942 A1943 U1944 A1945 A1946 C1951 C1952 G1957 A1965 U1966 G1981 U1982 U1983 C1994 A1997 A1998 G1999 A2004 U2009 U2018 G2019 U2020 C2021 U2022 C2023 G2037 A2041 A2042 U2046 A2050 C2051 C2052 U2053 G2056 A2057 A2058 G2059 A2060 U2061 G2062 C2063 A2064
G2065 C2070 C2082 G2083 A2087 G2088 A2089 C2090 U2095 G2096 G2097 A2098 G2099 U2113 G2114 G2120 U2124 U2125 C2126 G G C A C A G C U U G G U A C A G G A U A G G U A G G A G C C U U U G
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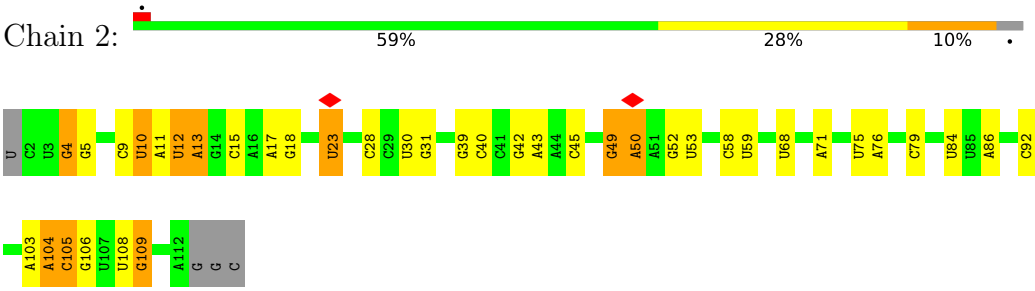
A2347 G2348 A2349 G2350 U2351 G2352 A2355 A2356 C2359 A2360 U2361 A2362 A2363 U2371 G2372 A2373 C2374 C2377 G2378 G2392 C2395 A2396 G2397 G2398 G2399 G2402 A2403 A2404 A2405 G2406 A2407 C2408 G2409 G2410 A2411 C2412 G2418 U2429 C2430 C2431 G2432 G2437 A2445 U2450 C2451 A2452 G2456
A2457 C2468 A2475 G2482 A2496 G2497 A2503 C2504 A2505 G2521 C2525 G2529 A2530 G2535 C2539 A2540 A2545 U2546 C2547 G2556 C2561 U2574 G2575 G2580 A2593 G2594 A2599 C2600 C2606 U2607 G2608 G2609 U2612 C2613 C2618 G2619 G2624 A2625
A2629 G2630 U2631 U2636 C2637 C2638 C2639 U2640 A2641 U2649 G2657 U2662 U2663 A2668 C2673 U2676 C2677 G2690 A2698 U2699 U2705 A2706 C2710 U2711 G2712 U2716 A2717 A2732 G2741 U2747 A2748 G2749 U2753 G2758 G2759 A2760 A2767 A2768 G2771 A2775
G2778 U2783 A2784 A2791 A2792 G2793 A2805 U2806 G2807 C2814 C2815 C2816 A2817 A2818 C2819 U2820 U2821 C2822 G2823 G2824 U2825 U2826 A2827 U2828 C2835 A2839 A2840 A2841 G2842 A2843 U2844 G2845 U2853 U2856 A2857 G2858 G2859 U2860 U2861 G2876 G2877 A2880 C2881 A2882 U2883 G2884 U2885 G2886 G2887
G2892 A2893 C2900 U2901 A2902 G2906 A2907 A2911 A2912 G2913 U2920 C A A

• Molecule 27: 5S rRNA

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	47.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.353	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	400.96, 400.96, 400.96	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.895, 0.895, 0.895	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.23	0/927	0.57	0/1239
2	B	0.24	0/2120	0.53	0/2847
3	C	0.23	0/955	0.49	0/1265
4	D	0.24	0/795	0.51	0/1062
5	E	0.23	0/861	0.53	0/1159
6	F	0.24	0/719	0.50	0/959
7	G	0.23	0/704	0.48	0/938
8	H	0.24	0/735	0.47	0/986
9	I	0.25	0/603	0.55	0/801
10	J	0.23	0/469	0.54	0/625
11	K	0.22	0/504	0.53	0/670
12	L	0.25	0/1652	0.50	0/2216
13	M	0.22	0/434	0.51	0/585
14	N	0.24	0/404	0.54	0/537
15	O	0.23	0/393	0.57	0/523
16	P	0.26	0/376	0.59	0/491
17	Q	0.24	0/526	0.55	0/690
18	R	0.22	0/299	0.51	0/393
19	S	0.26	0/1494	0.51	0/2018
20	V	0.23	0/1160	0.48	0/1563
21	W	0.24	0/918	0.56	0/1232
22	X	0.24	0/1096	0.51	0/1461
23	Y	0.24	0/1113	0.53	0/1493
24	Z	0.23	0/959	0.54	0/1282
25	a	0.24	0/865	0.52	0/1154
26	1	0.21	0/64448	0.76	9/100506 (0.0%)
27	2	0.18	0/2640	0.79	3/4112 (0.1%)
All	All	0.21	0/88169	0.71	12/132807 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	1	1865	C	C2-N1-C1'	7.37	126.91	118.80
26	1	1865	C	N1-C2-O2	7.17	123.20	118.90
26	1	1865	C	N3-C2-O2	-5.72	117.89	121.90
27	2	79	C	C2-N1-C1'	5.50	124.85	118.80
26	1	2825	U	N3-C2-O2	-5.45	118.39	122.20

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	915	0	987	7	0
2	B	2085	0	2192	26	0
3	C	943	0	1014	6	0
4	D	785	0	825	6	0
5	E	853	0	914	11	0
6	F	711	0	743	4	0
7	G	698	0	756	9	0
8	H	727	0	777	3	0
9	I	597	0	607	6	0
10	J	463	0	501	4	0
11	K	503	0	536	4	0
12	L	1628	0	1667	10	0
13	M	432	0	472	5	0
14	N	397	0	407	5	0
15	O	390	0	396	7	0
16	P	372	0	420	4	0
17	Q	521	0	586	2	0
18	R	296	0	340	2	0
19	S	1472	0	1520	11	0
20	V	1138	0	1130	10	0
21	W	911	0	970	15	0
22	X	1082	0	1119	10	0
23	Y	1089	0	1155	12	0
24	Z	955	0	1002	10	0
25	a	857	0	903	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	1	57543	0	28959	376	0
27	2	2361	0	1197	19	0
All	All	80724	0	52095	533	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 4.

The worst 5 of 533 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)
9:I:85:LYS:NZ	26:1:902:A:OP1	2.17	0.76
27:2:5:G:H1	27:2:108:U:H3	1.30	0.76
26:1:1862:G:H1	26:1:1932:C:H5	1.33	0.74
2:B:107:PRO:HD2	2:B:110:LEU:HD22	1.70	0.73
27:2:4:G:H22	27:2:109:G:H1	1.35	0.72

There are no symmetry-related clashes.

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	A	111/116 (96%)	106 (96%)	5 (4%)	0	100	100
2	B	271/277 (98%)	264 (97%)	7 (3%)	0	100	100
3	C	114/118 (97%)	114 (100%)	0	0	100	100
4	D	98/102 (96%)	93 (95%)	5 (5%)	0	100	100
5	E	109/117 (93%)	107 (98%)	2 (2%)	0	100	100
6	F	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
7	G	86/105 (82%)	79 (92%)	7 (8%)	0	100	100
8	H	91/217 (42%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	76/94 (81%)	71 (93%)	5 (7%)	0	100	100
10	J	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
11	K	59/73 (81%)	56 (95%)	3 (5%)	0	100	100
12	L	213/220 (97%)	205 (96%)	8 (4%)	0	100	100
13	M	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
14	N	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
15	O	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
16	P	42/45 (93%)	42 (100%)	0	0	100	100
17	Q	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
18	R	35/37 (95%)	35 (100%)	0	0	100	100
19	S	190/207 (92%)	180 (95%)	10 (5%)	0	100	100
20	V	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
21	W	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
22	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
23	Y	134/144 (93%)	132 (98%)	2 (2%)	0	100	100
24	Z	119/122 (98%)	115 (97%)	4 (3%)	0	100	100
25	a	106/119 (89%)	102 (96%)	4 (4%)	0	100	100
All	All	2607/2904 (90%)	2513 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	A	99/102 (97%)	99 (100%)	0	100	100
2	B	220/224 (98%)	220 (100%)	0	100	100
3	C	96/98 (98%)	96 (100%)	0	100	100
4	D	85/86 (99%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	90/94 (96%)	90 (100%)	0	100	100
6	F	79/79 (100%)	79 (100%)	0	100	100
7	G	77/90 (86%)	77 (100%)	0	100	100
8	H	81/190 (43%)	81 (100%)	0	100	100
9	I	61/75 (81%)	61 (100%)	0	100	100
10	J	49/51 (96%)	49 (100%)	0	100	100
11	K	55/66 (83%)	55 (100%)	0	100	100
12	L	173/177 (98%)	173 (100%)	0	100	100
13	M	50/53 (94%)	50 (100%)	0	100	100
14	N	45/50 (90%)	45 (100%)	0	100	100
15	O	45/47 (96%)	45 (100%)	0	100	100
16	P	39/40 (98%)	39 (100%)	0	100	100
17	Q	55/56 (98%)	55 (100%)	0	100	100
18	R	35/35 (100%)	35 (100%)	0	100	100
19	S	158/170 (93%)	158 (100%)	0	100	100
20	V	122/123 (99%)	122 (100%)	0	100	100
21	W	99/100 (99%)	99 (100%)	0	100	100
22	X	110/112 (98%)	110 (100%)	0	100	100
23	Y	113/119 (95%)	113 (100%)	0	100	100
24	Z	101/102 (99%)	101 (100%)	0	100	100
25	a	87/95 (92%)	87 (100%)	0	100	100
All	All	2224/2434 (91%)	2224 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2673/2923 (91%)	388 (14%)	5 (0%)
27	2	110/115 (95%)	21 (19%)	1 (0%)
All	All	2783/3038 (91%)	409 (14%)	6 (0%)

5 of 409 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	35	G
26	1	36	G
26	1	51	G
26	1	60	U
26	1	69	C

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	2783	U
26	1	2827	A
27	2	49	G
26	1	525	A
26	1	229	A

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

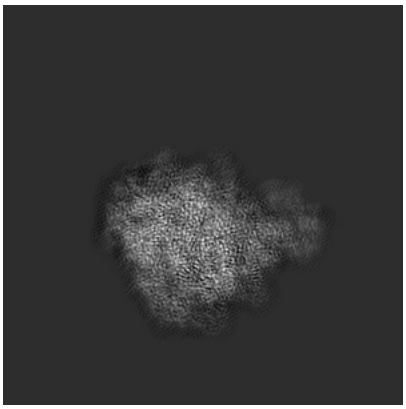
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26124. These allow visual inspection of the internal detail of the map and identification of artifacts.

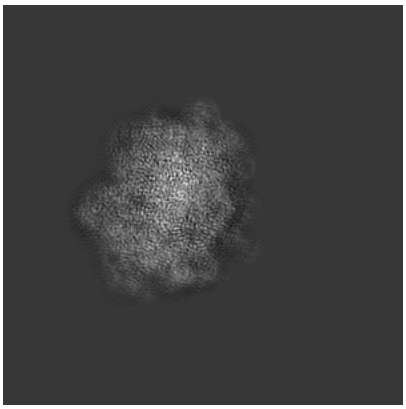
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

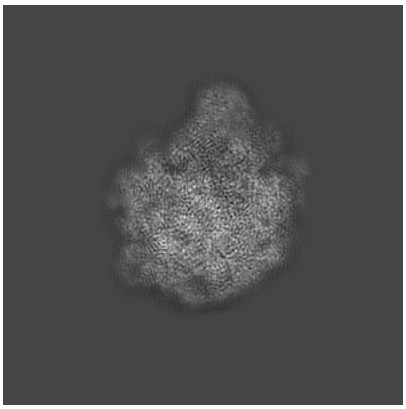
6.1.1 Primary map



X

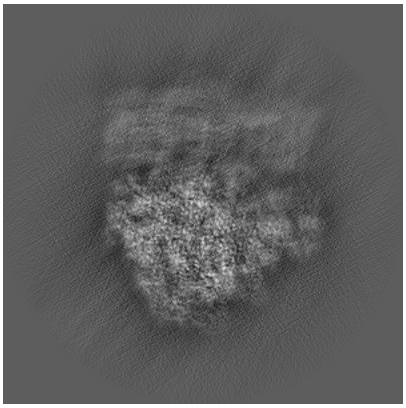


Y

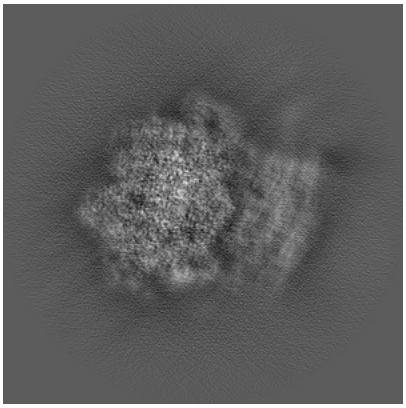


Z

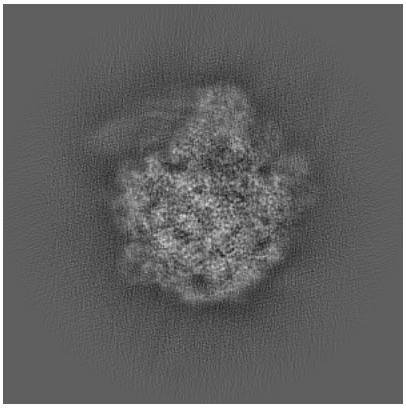
6.1.2 Raw map



X



Y

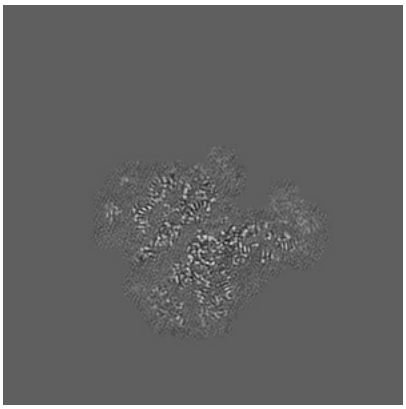


Z

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

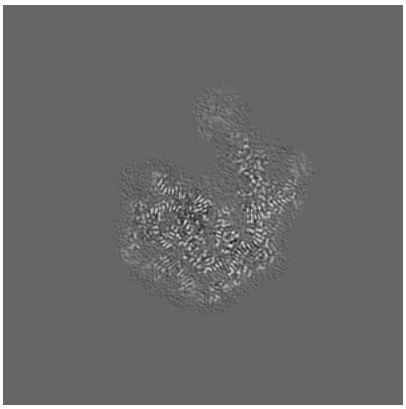
6.2 Central slices (i)

6.2.1 Primary map



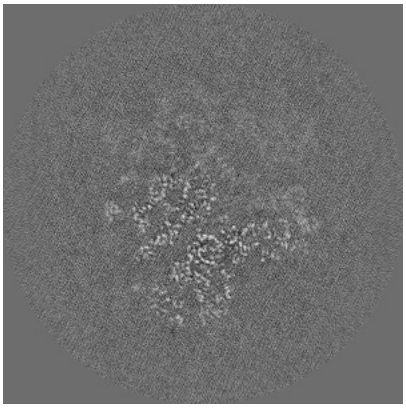
X Index: 224

Y Index: 224

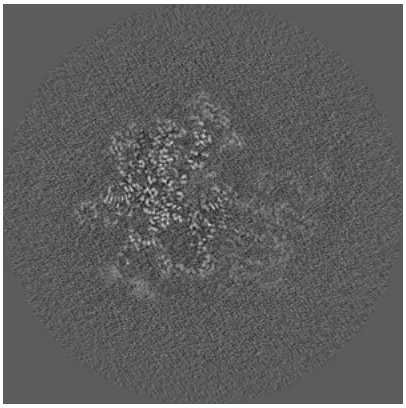


Z Index: 224

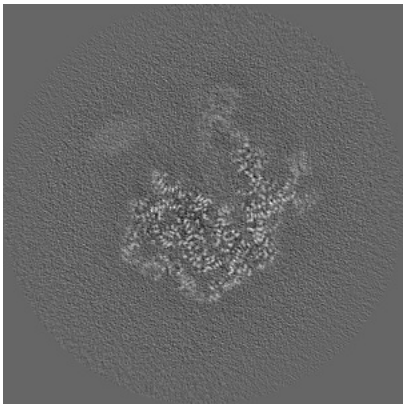
6.2.2 Raw map



X Index: 224



Y Index: 224

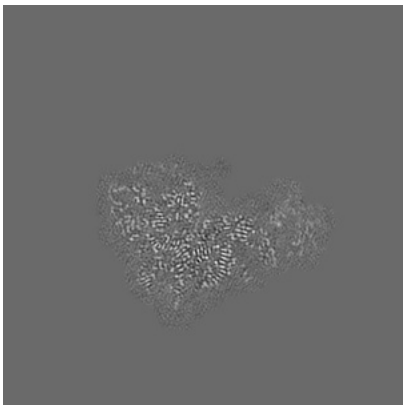


Z Index: 224

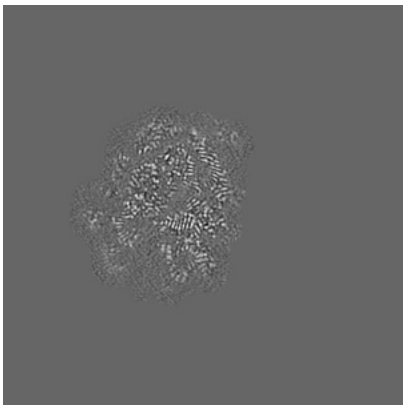
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

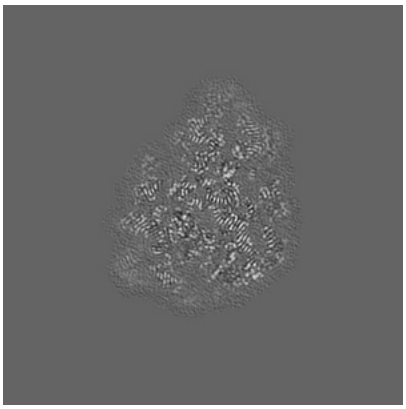
6.3.1 Primary map



X Index: 247

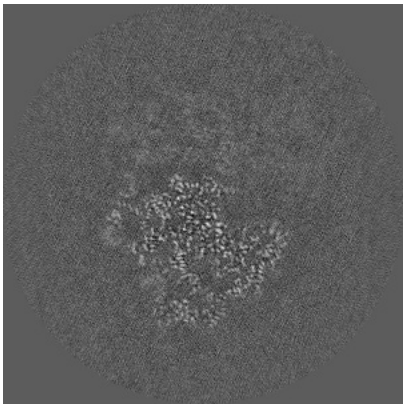


Y Index: 210

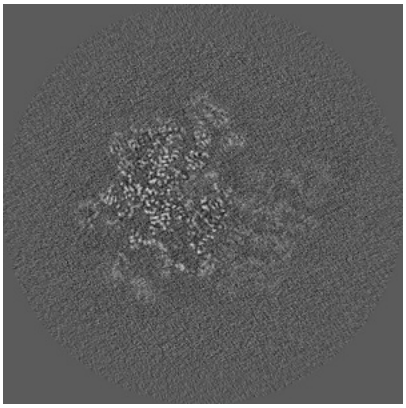


Z Index: 191

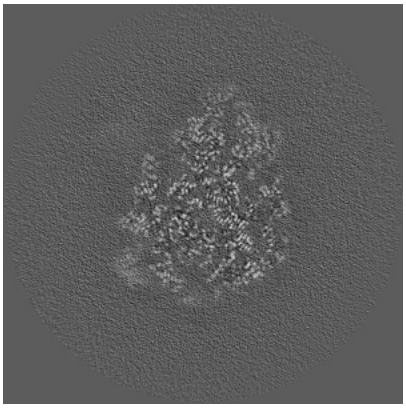
6.3.2 Raw map



X Index: 209



Y Index: 223

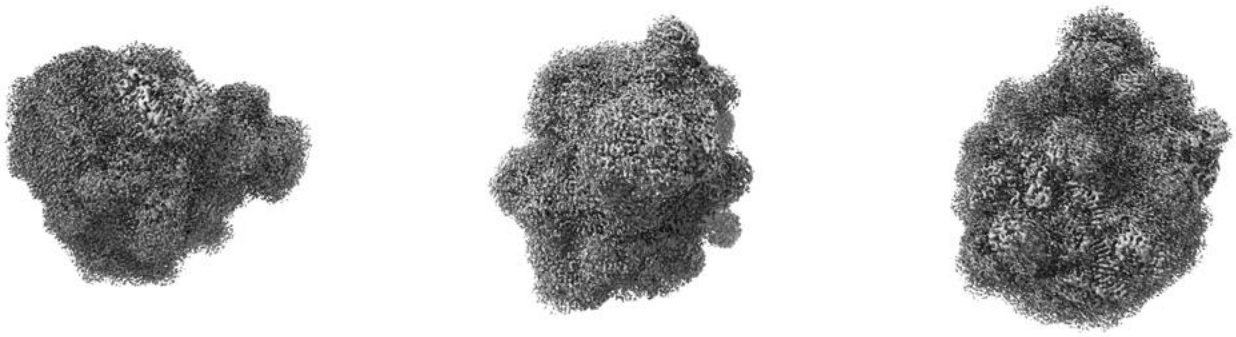


Z Index: 191

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

6.4 Orthogonal surface views (i)

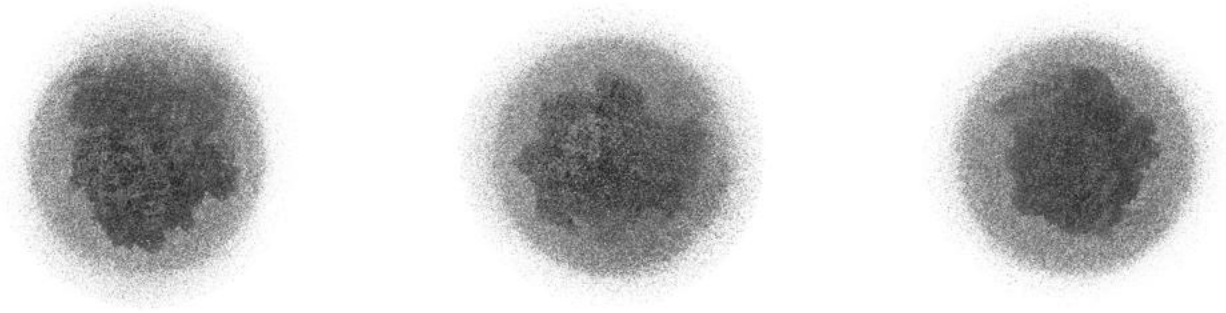
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

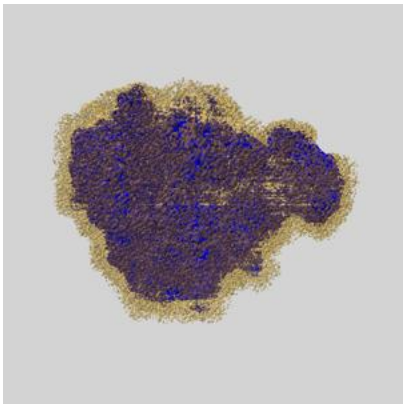
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

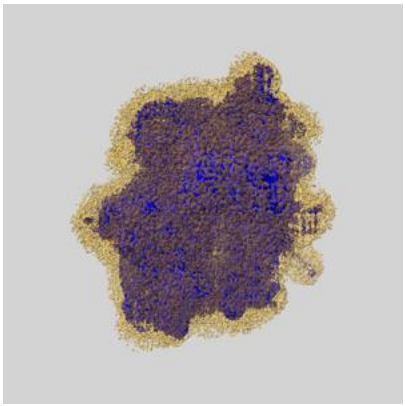
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

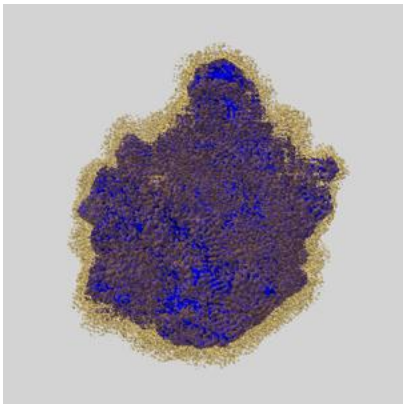
6.5.1 emd_26124_msk_1.map (i)



X



Y

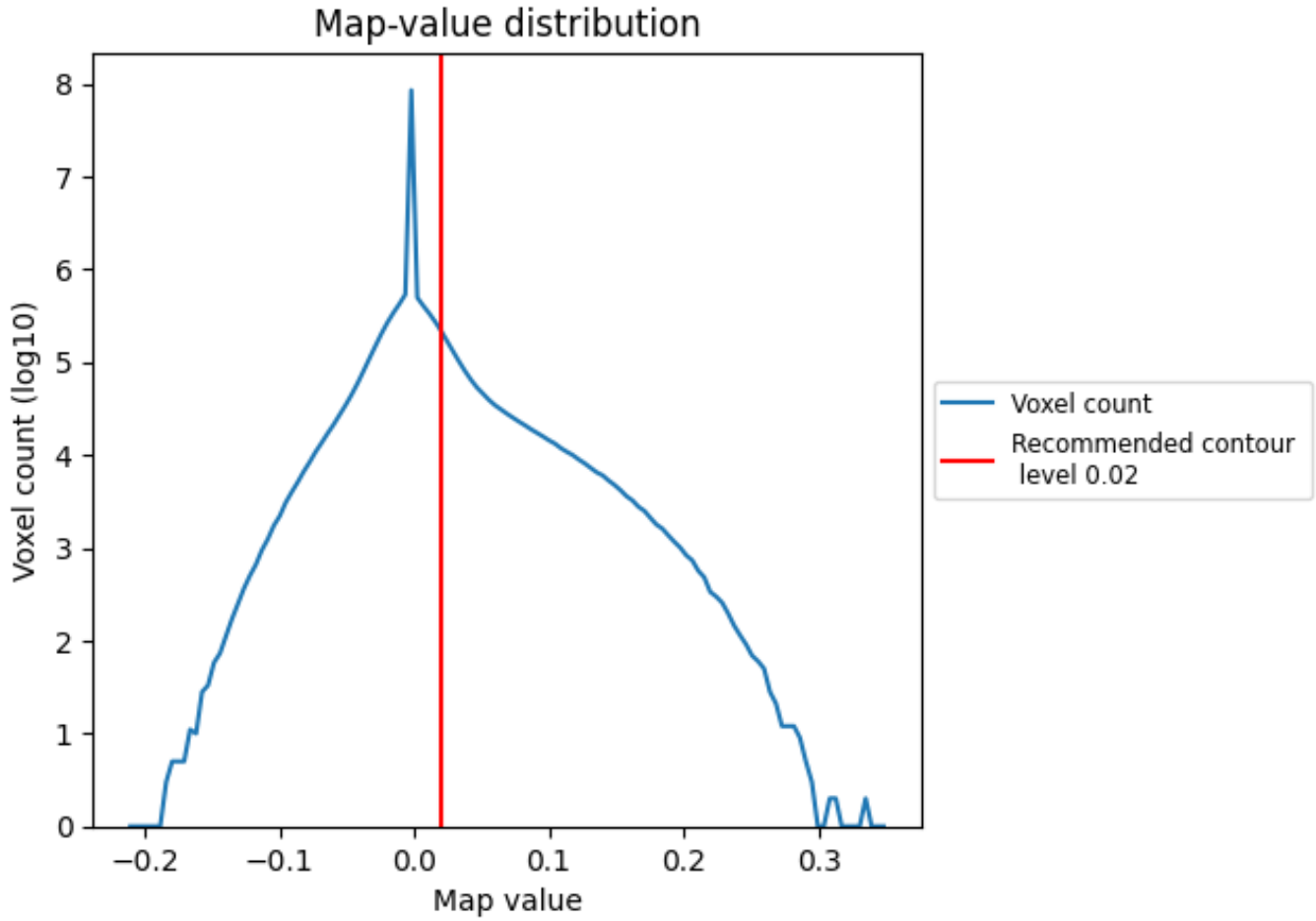


Z

7 Map analysis

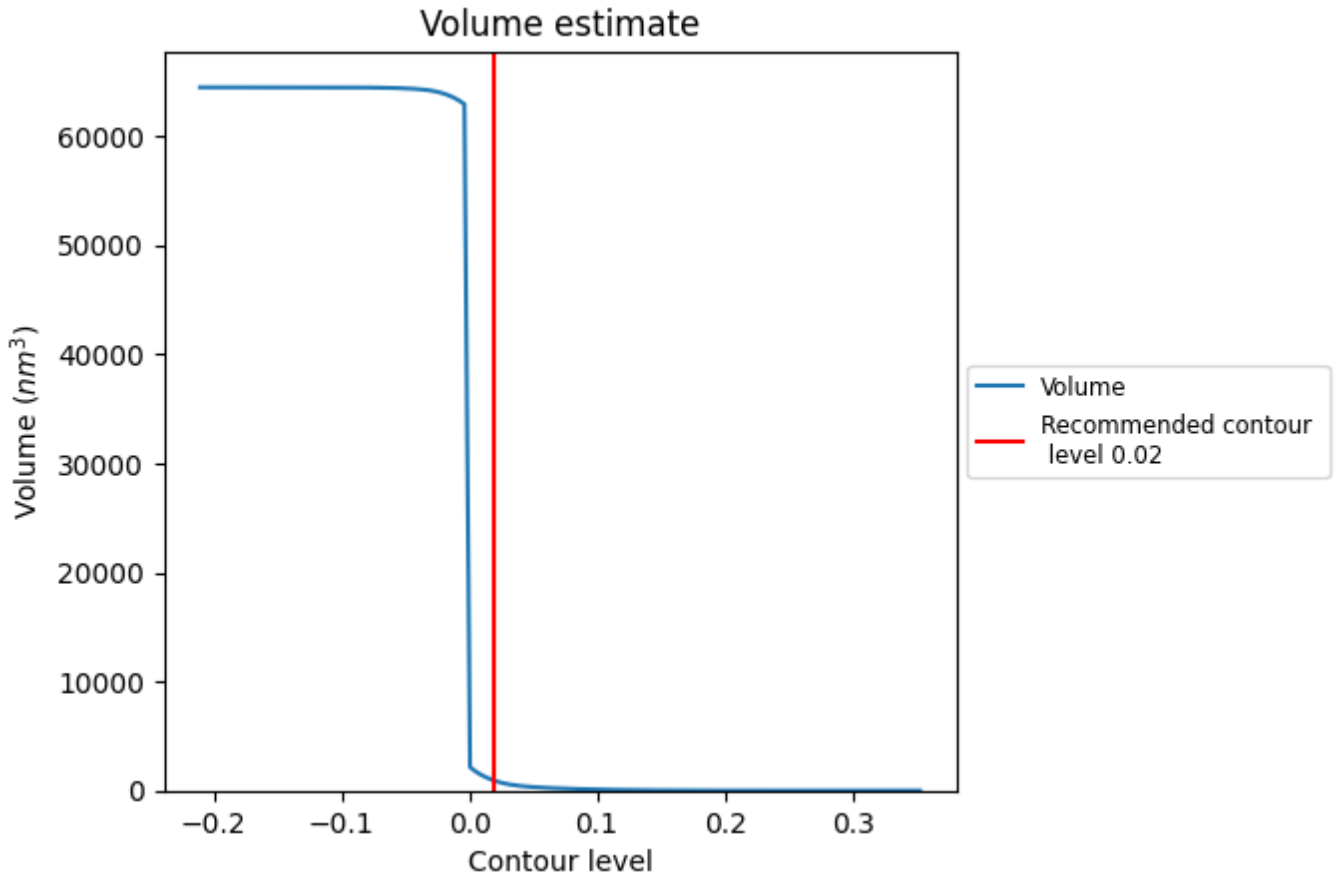
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

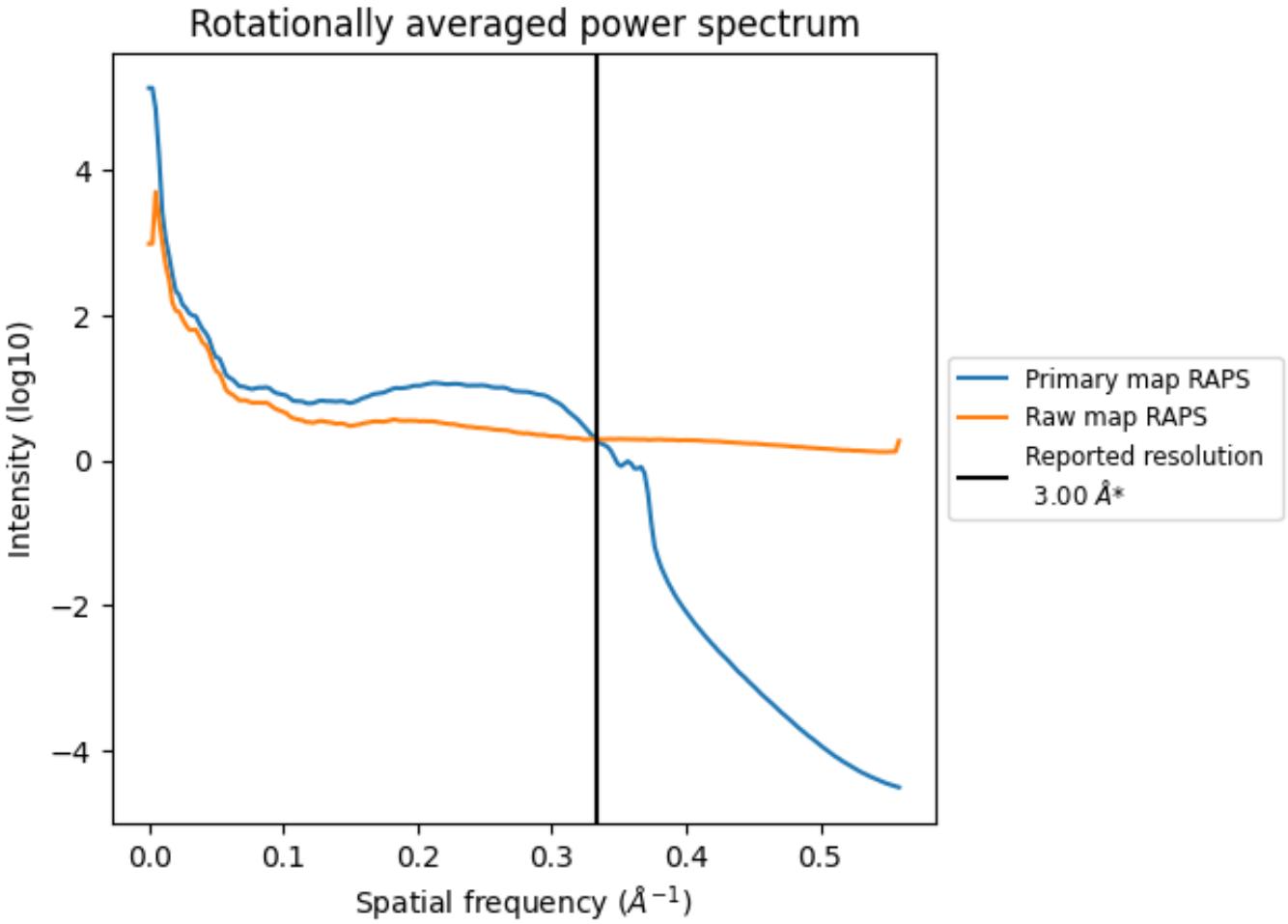
7.2 Volume estimate (i)



The volume at the recommended contour level is 903 nm^3; this corresponds to an approximate mass of 816 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)

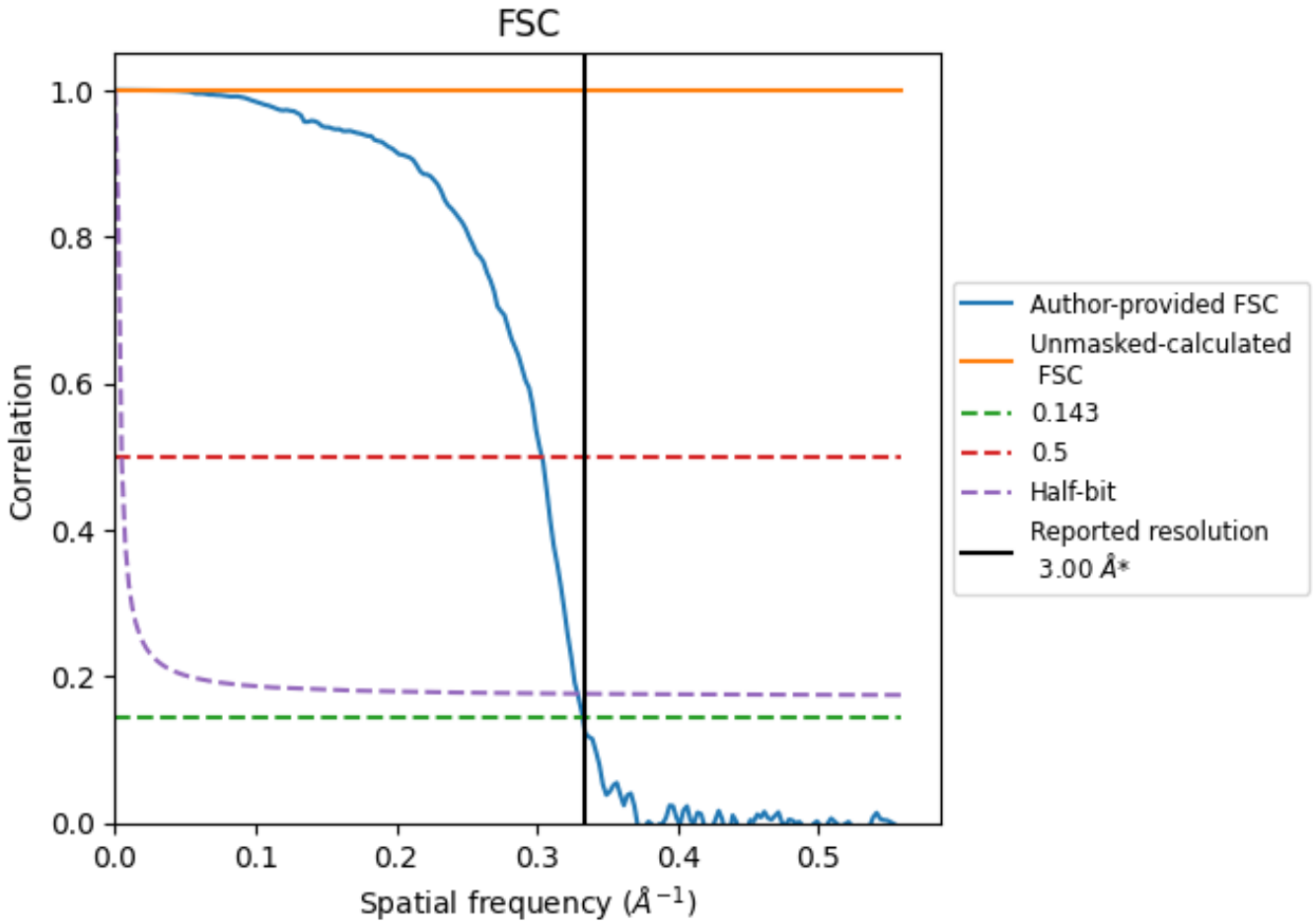


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

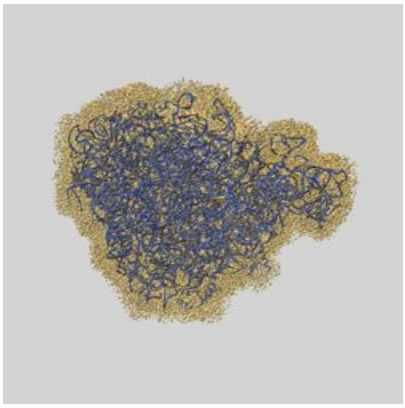
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.30	3.04
Unmasked-calculated*	-	-	-

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

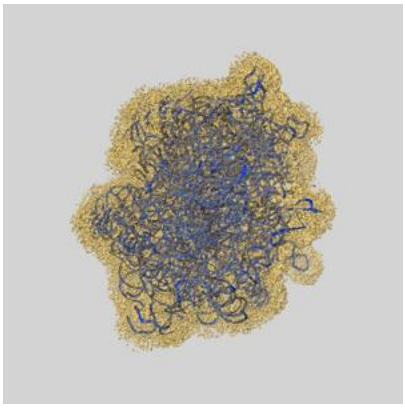
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26124 and PDB model 7TTU. Per-residue inclusion information can be found in section 3 on page 9.

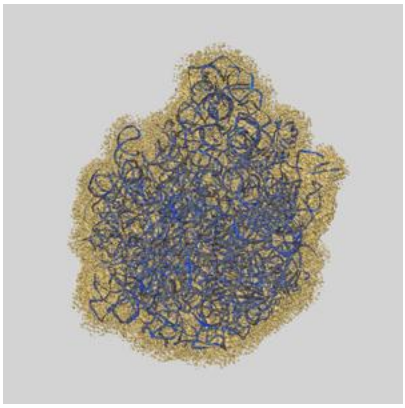
9.1 Map-model overlay



X



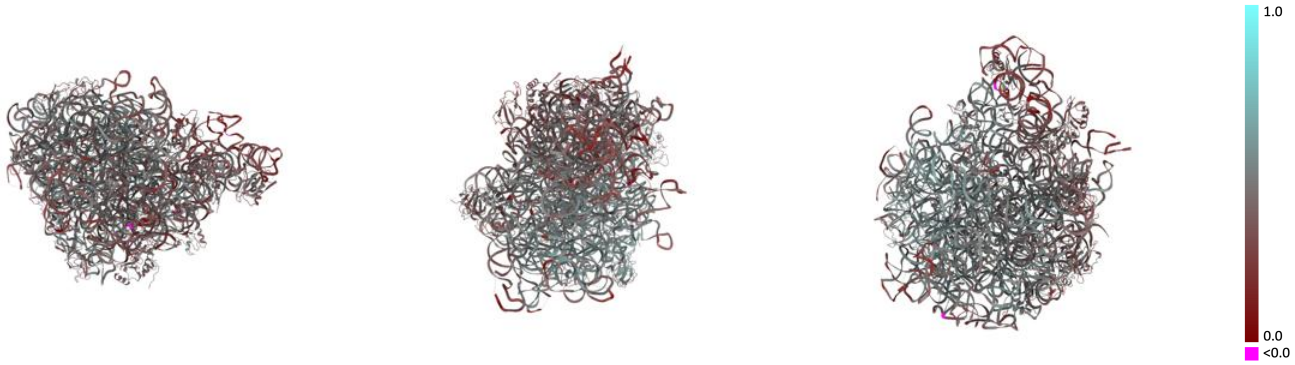
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

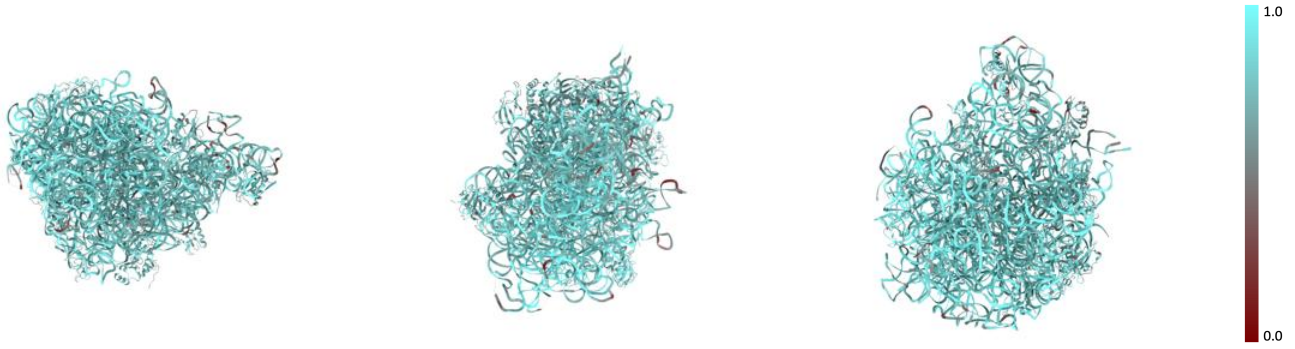
9.2 Q-score mapped to coordinate model



X Y Z

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.

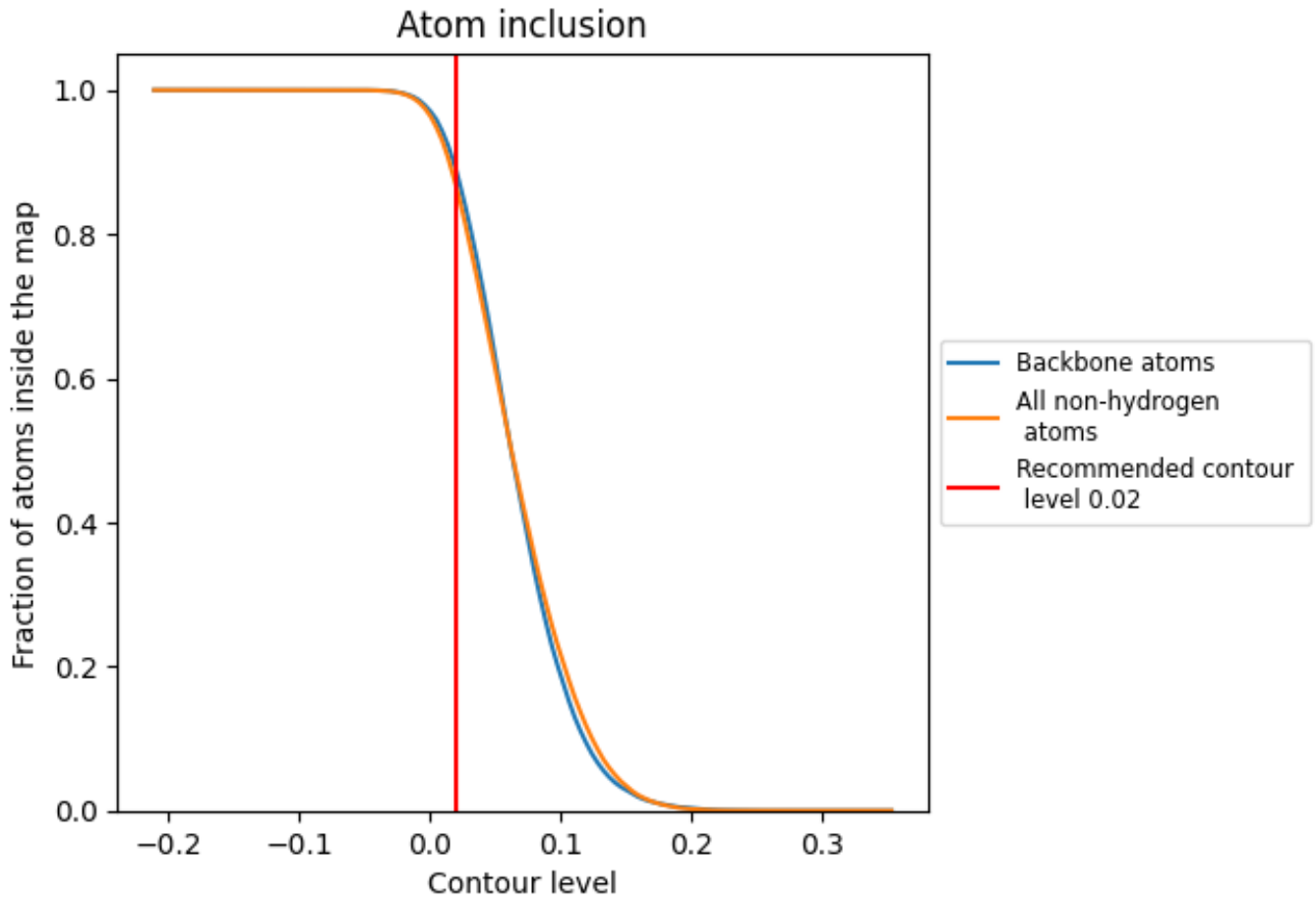
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8678	0.4470
1	0.8873	0.4580
2	0.7759	0.3340
A	0.8077	0.4420
B	0.8945	0.5270
C	0.8231	0.3960
D	0.7568	0.3500
E	0.8652	0.4600
F	0.8672	0.4760
G	0.7612	0.3820
H	0.6443	0.3270
I	0.8114	0.4230
J	0.8837	0.4930
K	0.8501	0.4090
L	0.8335	0.4280
M	0.7877	0.3850
N	0.8956	0.4520
O	0.7905	0.4180
P	0.9544	0.5620
Q	0.8884	0.5010
R	0.7655	0.3730
S	0.8315	0.4380
V	0.8027	0.3880
W	0.8041	0.4160
X	0.8347	0.4430
Y	0.7913	0.4120
Z	0.8644	0.4690
a	0.7305	0.3610