



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 02:55 PM EST

PDB ID : 6WQN
EMDB ID : EMD-21872
Title : Structure of the 50S subunit of the ribosome from Methicillin Resistant Staphylococcus aureus in complex with the antibiotic, contezolid
Authors : Belousoff, M.J.
Deposited on : 2020-04-29
Resolution : 2.90 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 ⓘ 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:

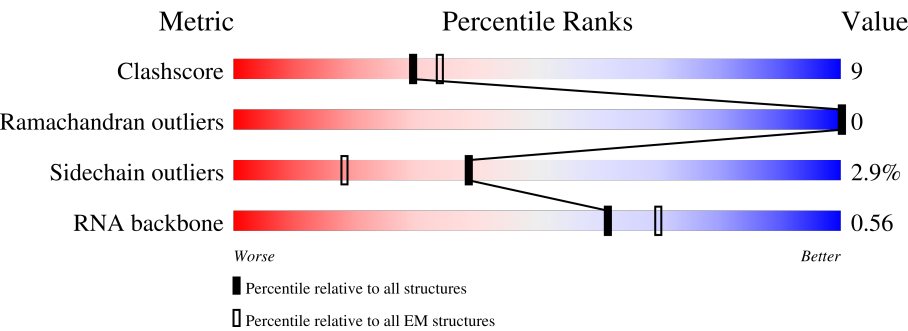
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.90 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.




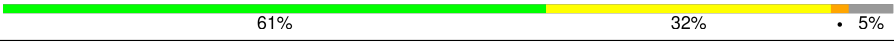
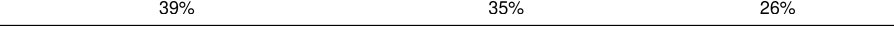
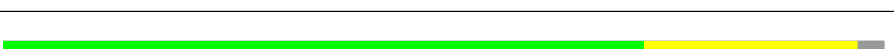



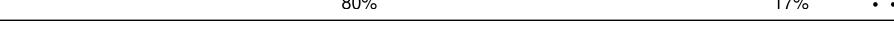



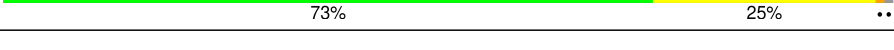

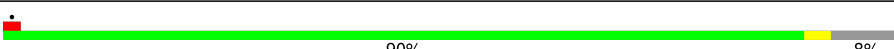


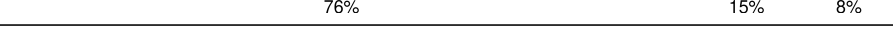



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	116	<div><div></div><div>72%23%..</div></div>
2	B	277	<div><div></div><div>75%23%. .</div></div>
3	C	118	<div><div></div><div>80%18%..</div></div>
4	D	105	<div><div></div><div>70%25%. 5%</div></div>
5	E	117	<div><div></div><div>70%24%6%</div></div>
6	F	91	<div><div></div><div>54%34%. 11%</div></div>
7	G	105	<div><div></div><div>60%27%13%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	107	
9	J	62	
10	K	72	
11	L	217	
12	M	58	
13	N	57	
14	O	49	
15	P	50	
16	Q	65	
17	R	37	
18	S	207	
19	V	145	
20	W	122	
21	X	146	
22	Y	144	
23	Z	122	
24	a	119	
25	1	2923	
26	2	115	
27	I	85	

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 80715 atoms, of which 15 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
1	A	112	Total	C	N	O	0	0
			907	572	182	153		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	110	Total	C	N	O	S	0	0
			845	527	162	154	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	ALA	GLY	variant	UNP A0A077UKF9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	81	Total	C	N	O	S	0	0
			654	410	116	125	3		

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	91	Total	C	N	O	S	0	0
			702	444	129	128	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	54	SER	GLY	variant	UNP W8TRD5

- 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 L28.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	62	ALA	-	insertion	UNP A0A077URJ8

- Molecule 10 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	53	Total	C	N	O	0	0
			436	269	82	85		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	215	Total	C	N	O	S	0	0
			1621	1015	299	303	4		

- Molecule 12 is a protein called 50S ribosomal protein L30.

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

- Molecule 13 is a protein called 50S ribosomal protein L32.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	54	ALA	VAL	variant	UNP A0A077UWR7

- Molecule 14 is a protein called 50S ribosomal protein L33.

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

- Molecule 15 is a protein called 50S ribosomal protein L34.

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

- Molecule 16 is a protein called 50S ribosomal protein L35.

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

- Molecule 17 is a protein called 50S ribosomal protein L36.

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

- Molecule 18 is a protein called 50S ribosomal protein L4.

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

- Molecule 19 is a protein called 50S ribosomal protein L13.

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

- Molecule 20 is a protein called 50S ribosomal protein L14.

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

- Molecule 21 is a protein called 50S ribosomal protein L15.

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

- Molecule 22 is a protein called 50S ribosomal protein L16.

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

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	120	Total	C	N	O	S	0	0
			951	584	182	184	1		

- Molecule 24 is a protein called 50S ribosomal protein L18.

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

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	2687	Total	C	N	O	P	0	0
			57631	25735	10578	18635	2683		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1866	A	G	conflict	GB 1760383645

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	111	Total	C	N	O	P	0	0
			2358	1056	422	770	110		

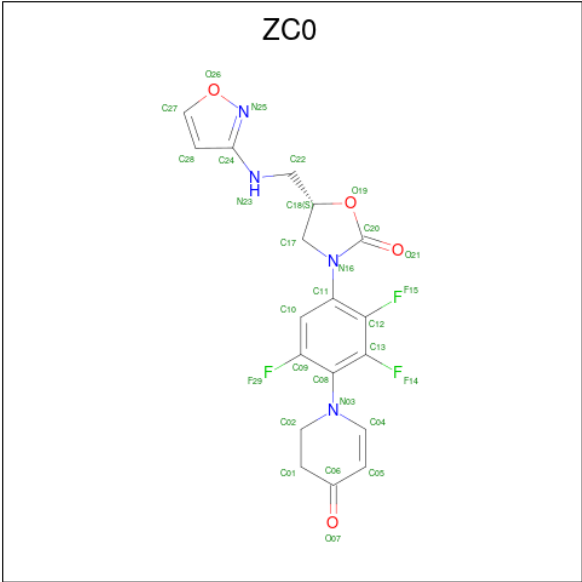
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	80	C	G	variant	GB 1750990749
2	109	C	G	variant	GB 1750990749
2	111	A	C	variant	GB 1750990749
2	112	G	A	variant	GB 1750990749

- Molecule 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is Contezolid (three-letter code: ZC0) (formula: $C_{18}H_{15}F_3N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	H	N	O	
28	1	1	44	18	3	15	4	4	0

3 Residue-property plots


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

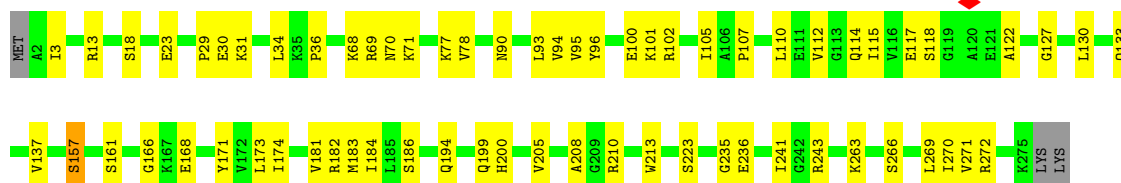
- Molecule 1: 50S ribosomal protein L19

Chain A: 




- Molecule 2: 50S ribosomal protein L2

Chain B: 



- Molecule 3: 50S ribosomal protein L20

Chain C: 



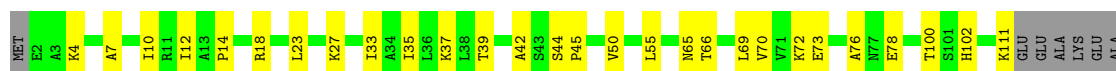
- Molecule 4: 50S ribosomal protein L21

Chain D: 



- Molecule 5: 50S ribosomal protein L22

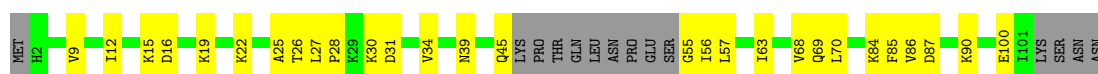
Chain E: 



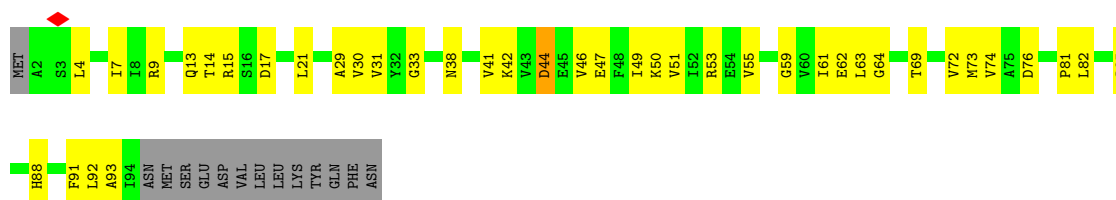
- Molecule 6: 50S ribosomal protein L23



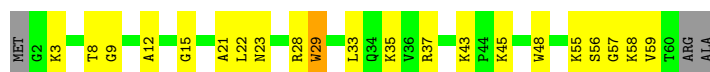
- Molecule 7: 50S ribosomal protein L24



- Molecule 8: 50S ribosomal protein L25



- Molecule 9: 50S ribosomal protein L28



- Molecule 10: 50S ribosomal protein L29



- Molecule 11: 50S ribosomal protein L3

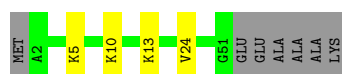
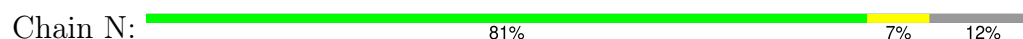




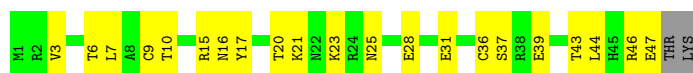
- Molecule 12: 50S ribosomal protein L30



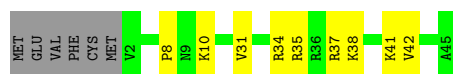
- Molecule 13: 50S ribosomal protein L32



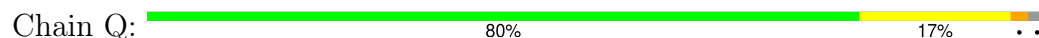
- Molecule 14: 50S ribosomal protein L33



- Molecule 15: 50S ribosomal protein L34



- Molecule 16: 50S ribosomal protein L35

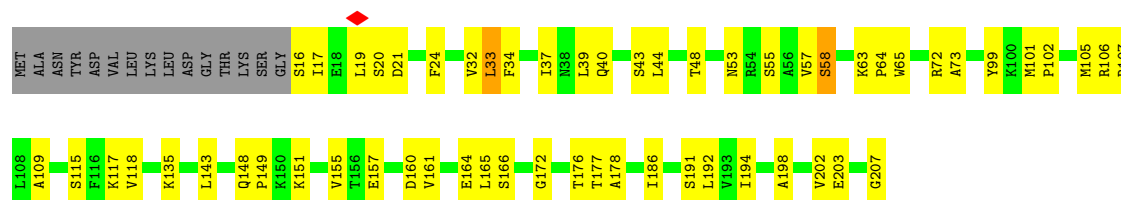


- Molecule 17: 50S ribosomal protein L36



- Molecule 18: 50S ribosomal protein L4





- Molecule 19: 50S ribosomal protein L13

Chain V: 80% 19%



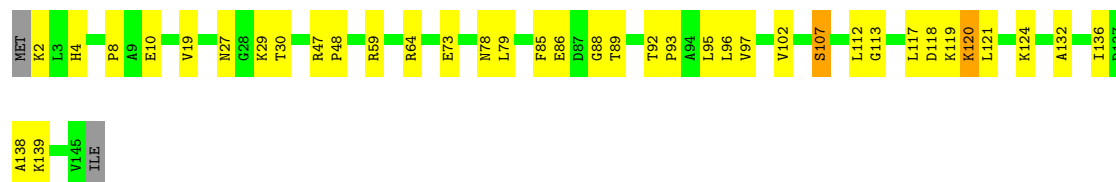
- Molecule 20: 50S ribosomal protein L14

Chain W: 81% 18%



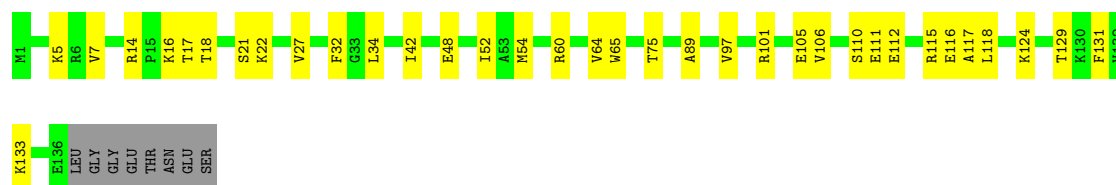
- Molecule 21: 50S ribosomal protein L15

Chain X: 73% 25%



- Molecule 22: 50S ribosomal protein L16

Chain Y: 70% 24% 6%



- Molecule 23: 50S ribosomal protein L17

Chain Z: 70% 27%



- Molecule 24: 50S ribosomal protein L18

Frequency	Percentage
Daily	90%
Weekly	8%
Other	2%



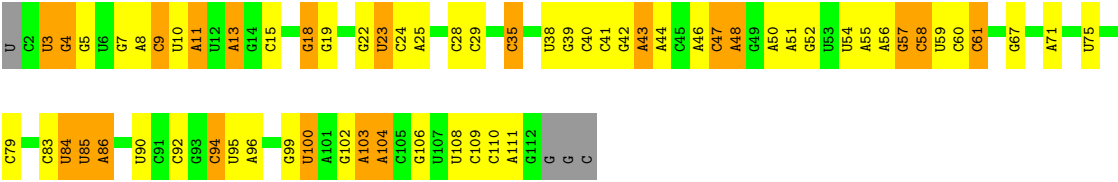
Response	Percentage
Yes, the U.S. should take action to address climate change	59%
No, the U.S. should focus on other issues	25%
It's not the U.S.'s responsibility	8%
Don't know	8%



A2784	U2649	G2556	C2449	C2344	A2226	U	G	G2079	A1955	G1849	G1709	C1587	G1523	U	U	G1309
A2791	A2856	U2557	U2450	A2347	C2229	G	A	G2080	G1956	U	G1710	U1588	G1526	U	U	A1310
A2792	G2657	U2564	C2451	G2348	A2230	A	G	A2081	G1957	U1854	G1711	C1589	A	U	U	A1311
G2793	U2663	C2565	A2452	A2349	C2231	C	A	G2083	A1965	C1864	G1718	G1591	U	A	A	A1312
U2800	U2664	C2566	C2454	G2358	C2236	G	C	A2086	C1969	C1865	U1737	G1592	G	U	G	A1313
C2801	U2665	G2567	G2455	C2359	U2237	U	U	A2087	U1978	U1872	C1738	G1593	A	U	G	A1314
A2805	G2672	A2568	G2456	U2361	A2239	A	A	G2088	U1979	G1873	G1739	U1594	U	U	U	C1315
U2806	U2673	C2569	A2465	A2362	U2240	C	G	A2089	A1980	A1874	C1754	G1595	A	U	U	G1320
U2807	U2674	U2574	U2466	A2363	U2242	U	C	G2094	G1981	A1875	U1755	U1597	G	A	G	A1321
A2817	G2682	G2580	C2467	A2368	A2252	U	U	U2095	U1982	A1881	U1756	U1598	G	C	G	G1322
A2818	U2683	U2582	C2468	G2368	C2255	A	A	G2096	U1983	U	U1757	U1599	U	U	U	A1323
U2819	A2692	U2590	A2475	C2369	A2254	C	C	U2102	C1990	A1886	U1758	A1605	A	A	A	A1471
U2820	C2693	A2591	U2476	U2370	U2257	G	G	U2103	G1991	G1887	G1759	C1606	A	A	C	C1472
U2821	C2694	A2592	A2477	U2371	G2265	U	U	A2122	C1994	U1888	G1760	U1606	U	U	U	U1330
G2823	G2695	A2593	A2478	C2372	G2266	G	G	A2123	G1995	G1889	U1761	G1613	C	U	G	G1476
G2824	G2696	G2594	U2489	A2373	U2270	A	A	A2124	A1996	G1890	A1764	A1616	C1542	U	U	G1336
U2825	G2697	C2595	C2490	C2374	U2271	G	G	C2126	A1997	U1891	A1765	A1617	U	U	U	A1337
U2826	A2698	G2596	U2491	G2377	U2272	G	G	G	A1998	A1893	U1766	U1617	A1545	U	U	G1478
A2827	U2705	G2597	A2496	C2378	A2294	C	C	U	G1999	G1894	A1771	U1625	C	U	U	G1479
U2828	U2706	U2598	U2497	A2391	A2295	G	C	A	G2007	U	G1760	A1626	U	U	U	G1480
A2840	U2711	C2600	U2500	C2391	A2296	U	U	C	A2008	U	U	U	U	U	U	G1346
A2841	U2712	G2601	U2501	G2397	C2308	U	U	A	U2009	U	G1763	U1629	C	U	U	G1347
G2842	G2715	C2602	C2502	G2398	C2309	G	G	A	U2010	C	U	A1630	G	U	U	U1348
U2845	U2716	G2603	A2503	G2399	C2310	G	G	U	G2011	U	G1783	A1631	A	U	U	U1349
U2846	U2717	A2504	C2504	U2400	C2311	U	U	C	U2012	G1900	G1790	A1632	A	U	U	U1350
U2847	A2717	U2505	U2505	C2401	U2311	G	G	U	G2013	C1901	G1791	A1633	G	U	U	C1351
G2850	C2718	G2605	U2506	C2412	C2312	G	G	U	U2014	A1904	A1800	A1634	U	U	U	A1353
G2851	U2725	U2607	G2507	G2413	C2313	G	G	U	G2015	G1905	U1806	A1635	C1556	U	U	G1354
U2852	G2726	G2608	C2508	G2414	A2314	A	A	U	U2016	U1906	U1807	A1636	C1557	U	U	G1357
U2853	U2727	G2609	A2509	G2415	U2315	U	U	A	U2017	C1907	U1808	C1558	U1558	U	U	U1492
A2854	U2728	U2610	U2511	A2411	U2316	A	A	C	C2023	U1907	A1810	A1562	C1559	U	U	G1361
U2855	G2729	U2611	C2512	C2412	C2317	U	U	G	G2037	G1910	A1811	A1563	G1561	U	U	U1497
G2885	C2730	U2612	A2513	G2416	C2322	A	A	A	U2038	A1911	A1812	C1562	C1561	U	U	U1498
G2886	U2739	C2613	G2514	U2417	U2323	C	C	U	G2039	A1912	A1813	C1563	U1563	U	U	U1499
U2892	A2740	G2618	A2530	G2418	C2324	U	U	A	A2040	U1913	A1814	C1564	U1564	U	U	G1500
A2899	G2741	U2619	U2531	A2419	A2325	C	C	G	U2049	G1915	C1817	U1565	U1565	U	U	A1396
C2900	C2742	G2622	G2532	U2420	C2326	A	A	U	G2048	U1821	U1822	C1566	G1566	U	U	U1504
U2901	U2747	A2625	G2535	C2422	A2328	C	C	A	U2053	C1922	U1823	A1661	U1567	U	U	G1505
A2902	G2753	G2626	G2536	U2429	U2329	U	U	G	G2054	G1931	C1824	A1662	U1568	U	U	A1402
U2903	U2754	U2627	U2537	C2430	G2330	G	G	A	U2055	C1932	C1827	C1669	U1569	U	U	A1405
U2904	A2760	C2628	C2538	C2431	U2332	U	U	A	G2056	G1933	U1828	A1670	C1570	U	U	U1416
U2909	U2770	A2629	A2540	C2432	U2333	G	G	C	A2057	A1939	A1829	G1675	G1574	U	U	A1421
G2910	G2771	U2630	U2541	C2433	G2334	U	U	U	U2058	A1940	G1834	A1678	G1577	U	U	A1422
G2913	U2774	U2636	G2542	A2434	G2335	C	C	G2217	G2059	C1941	U1835	A1684	C1578	U	U	U1431
U2917	A2775	C2637	A2545	G2437	A2336	U	U	G2218	A2060	U1836	A1836	A1690	A1579	U	U	A1432
A2918	U2779	G2638	U2549	A2438	A2337	A	A	U2220	U2061	A1946	U1837	A1691	G1575	U	U	A1449
U2919	C2779	C2639	U2554	A2439	U2338	G	G	U2221	G2062	G1949	U1843	C1692	A1576	U	U	A1450
U2920	U2783	C2644	G2553	A2445	U2339	A	A	U2222	C2070	U1950	U1846	G1693	G1576	G	U	U1451
C			U2555	G2448	U2343	C	C	U2223	C2077	C1951	U1847	U1520	A1577	U	U	C1452
						G	G	A2725	A2078	A1954	A1848	G1522	A1578	U	U	A1454

A
A

• Molecule 26: 5S rRNA



• Molecule 27: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	127000	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.435	Depositor
Minimum map value	-0.224	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	372.32, 372.32, 372.32	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89500004, 0.89500004, 0.89500004	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZC0

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	0.48	0/919	0.56	0/1228
2	B	0.27	0/2129	0.44	0/2858
3	C	0.22	0/955	0.34	0/1265
4	D	0.29	0/795	0.48	0/1062
5	E	0.28	0/853	0.44	0/1149
6	F	0.29	0/659	0.43	0/879
7	G	0.50	0/708	0.57	0/943
8	H	0.45	0/735	0.52	0/986
9	J	0.30	0/469	0.49	0/625
10	K	0.22	0/437	0.36	0/583
11	L	0.34	0/1645	0.51	0/2208
12	M	0.22	0/434	0.40	0/585
13	N	0.45	1/404 (0.2%)	0.54	0/537
14	O	0.22	0/393	0.44	0/523
15	P	0.37	0/376	0.47	0/491
16	Q	0.30	0/526	0.45	0/690
17	R	0.51	0/299	0.60	0/393
18	S	0.27	0/1494	0.41	0/2018
19	V	0.28	0/1160	0.41	0/1563
20	W	0.39	0/918	0.55	0/1232
21	X	0.32	0/1096	0.47	0/1461
22	Y	0.26	0/1113	0.44	0/1493
23	Z	0.22	0/955	0.41	0/1277
24	a	0.40	0/865	0.49	0/1154
25	1	0.14	0/64545	0.69	16/100652 (0.0%)
26	2	0.11	0/2636	0.64	0/4105
27	I	0.24	0/603	0.43	0/801
All	All	0.20	1/88121 (0.0%)	0.65	16/132761 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	5	LYS	C-N	5.09	1.45	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	254	A	C4'-C3'-O3'	7.94	128.88	113.00
25	1	254	A	N9-C1'-C2'	-7.69	103.54	112.00
25	1	2079	G	N9-C1'-C2'	-5.99	105.41	112.00
25	1	2078	A	C4'-C3'-O3'	-5.98	96.84	109.40
25	1	1466	G	N9-C1'-C2'	-5.84	105.57	112.00

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	907	0	981	25	0
2	B	2094	0	2205	46	0
3	C	943	0	1014	25	0
4	D	785	0	825	23	0
5	E	845	0	900	22	0
6	F	654	0	686	24	0
7	G	702	0	759	15	0
8	H	727	0	777	31	0
9	J	463	0	501	18	0
10	K	436	0	459	27	0
11	L	1621	0	1655	43	0
12	M	432	0	472	7	0
13	N	397	0	407	3	0
14	O	390	0	396	14	0
15	P	372	0	420	16	0
16	Q	521	0	586	7	0
17	R	296	0	340	9	0
18	S	1472	0	1520	46	0
19	V	1138	0	1130	21	0
20	W	911	0	970	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	X	1082	0	1119	33	0
22	Y	1089	0	1155	23	0
23	Z	951	0	999	28	0
24	a	857	0	903	0	0
25	1	57631	0	28986	613	0
26	2	2358	0	1198	50	0
27	I	597	0	607	8	0
28	1	29	15	0	0	0
All	All	80700	15	51970	1122	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 9.

The worst 5 of 1122 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)
25:1:1914:C:H2'	25:1:1915:G:H5''	1.48	0.94
25:1:1083:G:H2'	25:1:1084:U:H5''	1.53	0.91
25:1:1625:U:H2'	25:1:1626:A:H5''	1.53	0.90
15:P:41:LYS:HD2	25:1:505:U:H5''	1.52	0.89
4:D:50:ALA:HB1	4:D:51:PRO:HA	1.54	0.88

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	110/116 (95%)	103 (94%)	7 (6%)	0	100	100
2	B	272/277 (98%)	264 (97%)	8 (3%)	0	100	100
3	C	114/118 (97%)	111 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
5	E	108/117 (92%)	106 (98%)	2 (2%)	0	100	100
6	F	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
7	G	87/105 (83%)	85 (98%)	2 (2%)	0	100	100
8	H	91/107 (85%)	91 (100%)	0	0	100	100
9	J	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
10	K	51/72 (71%)	48 (94%)	3 (6%)	0	100	100
11	L	213/217 (98%)	204 (96%)	9 (4%)	0	100	100
12	M	54/58 (93%)	54 (100%)	0	0	100	100
13	N	48/57 (84%)	48 (100%)	0	0	100	100
14	O	45/49 (92%)	44 (98%)	1 (2%)	0	100	100
15	P	42/50 (84%)	42 (100%)	0	0	100	100
16	Q	62/65 (95%)	62 (100%)	0	0	100	100
17	R	35/37 (95%)	35 (100%)	0	0	100	100
18	S	190/207 (92%)	183 (96%)	7 (4%)	0	100	100
19	V	141/145 (97%)	140 (99%)	1 (1%)	0	100	100
20	W	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
21	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
22	Y	134/144 (93%)	129 (96%)	5 (4%)	0	100	100
23	Z	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
24	a	106/119 (89%)	103 (97%)	3 (3%)	0	100	100
27	I	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
All	All	2590/2793 (93%)	2515 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	98/102 (96%)	96 (98%)	2 (2%)	50	79
2	B	221/224 (99%)	214 (97%)	7 (3%)	34	69
3	C	96/98 (98%)	94 (98%)	2 (2%)	48	78
4	D	85/89 (96%)	84 (99%)	1 (1%)	67	89
5	E	89/94 (95%)	88 (99%)	1 (1%)	70	90
6	F	74/82 (90%)	71 (96%)	3 (4%)	26	60
7	G	77/91 (85%)	74 (96%)	3 (4%)	27	62
8	H	81/95 (85%)	76 (94%)	5 (6%)	15	43
9	J	49/51 (96%)	48 (98%)	1 (2%)	50	79
10	K	48/65 (74%)	48 (100%)	0	100	100
11	L	170/175 (97%)	161 (95%)	9 (5%)	19	49
12	M	50/52 (96%)	49 (98%)	1 (2%)	50	79
13	N	45/49 (92%)	45 (100%)	0	100	100
14	O	45/47 (96%)	44 (98%)	1 (2%)	47	78
15	P	39/45 (87%)	39 (100%)	0	100	100
16	Q	55/56 (98%)	52 (94%)	3 (6%)	18	48
17	R	35/35 (100%)	33 (94%)	2 (6%)	17	47
18	S	158/170 (93%)	155 (98%)	3 (2%)	52	81
19	V	122/123 (99%)	121 (99%)	1 (1%)	79	93
20	W	99/100 (99%)	97 (98%)	2 (2%)	50	79
21	X	110/112 (98%)	106 (96%)	4 (4%)	30	65
22	Y	113/119 (95%)	109 (96%)	4 (4%)	31	66
23	Z	101/102 (99%)	98 (97%)	3 (3%)	36	71
24	a	87/95 (92%)	84 (97%)	3 (3%)	32	67
27	I	61/66 (92%)	59 (97%)	2 (3%)	33	68
All	All	2208/2337 (94%)	2145 (97%)	63 (3%)	39	72

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	114	ASP
23	Z	3	TYR
14	O	28	GLU
22	Y	116	GLU

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Mol	Chain	Res	Type
24	a	71	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
21	X	78	ASN
27	I	86	GLN
13	N	45	ASN
15	P	13	HIS
15	P	27	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	1	2675/2923 (91%)	441 (16%)	48 (1%)
26	2	110/115 (95%)	30 (27%)	4 (3%)
All	All	2785/3038 (91%)	471 (16%)	52 (1%)

5 of 471 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
25	1	5	A
25	1	13	A
25	1	28	A
25	1	35	G
25	1	42	G

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	1	1568	U
25	1	2337	A
26	2	57	G
25	1	1864	C
25	1	2320	C

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	ZC0	1	3001	-	27,32,32	3.28	10 (37%)	34,46,46	2.82	15 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	ZC0	1	3001	-	-	6/11/35/35	0/4/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	3001	ZC0	C20-N16	8.99	1.46	1.36
28	1	3001	ZC0	C04-C05	7.34	1.52	1.35
28	1	3001	ZC0	O19-C20	6.64	1.44	1.35
28	1	3001	ZC0	C24-N23	6.07	1.45	1.36
28	1	3001	ZC0	C04-N03	4.91	1.50	1.36

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	3001	ZC0	C17-C18-C22	-6.27	106.26	113.38
28	1	3001	ZC0	C17-N16-C20	-5.95	106.77	111.17
28	1	3001	ZC0	C18-C17-N16	5.38	106.93	101.85
28	1	3001	ZC0	C04-C05-C06	-4.83	117.53	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	3001	ZC0	C09-C08-C13	4.36	119.93	115.25

There are no chirality outliers.

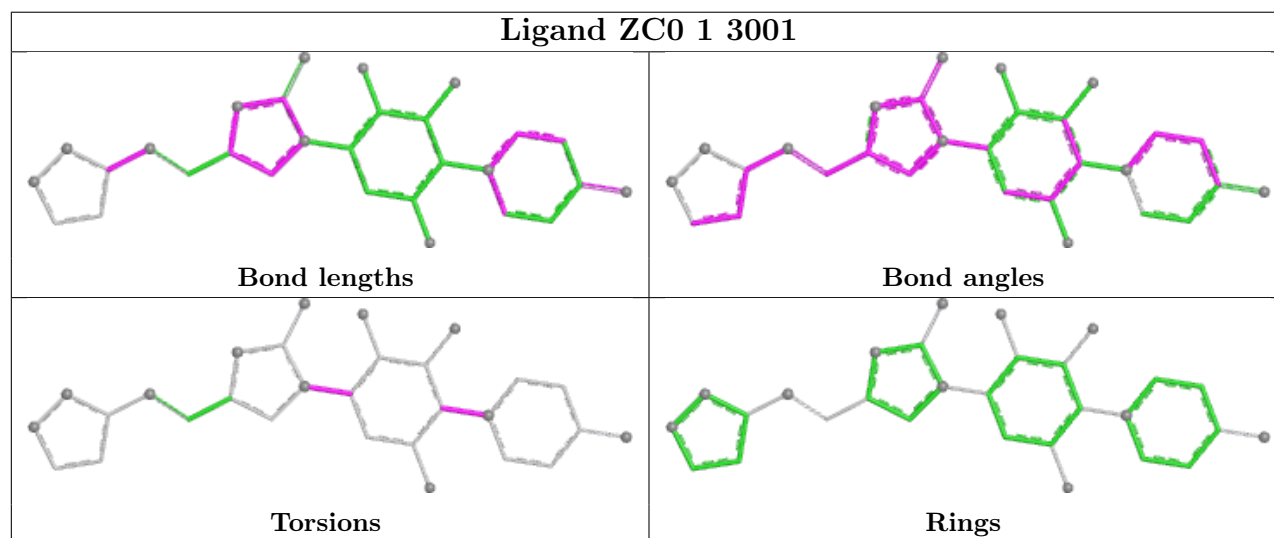
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	1	3001	ZC0	C09-C08-N03-C02
28	1	3001	ZC0	C13-C08-N03-C02
28	1	3001	ZC0	C10-C11-N16-C20
28	1	3001	ZC0	C12-C11-N16-C17
28	1	3001	ZC0	C12-C11-N16-C20

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

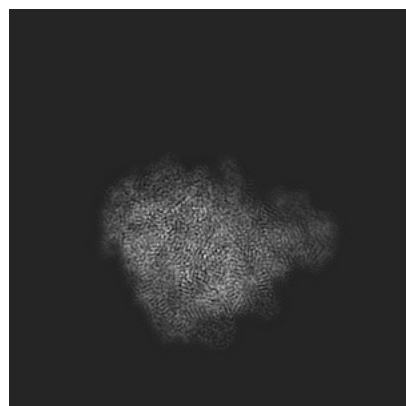
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21872. These allow visual inspection of the internal detail of the map and identification of artifacts.

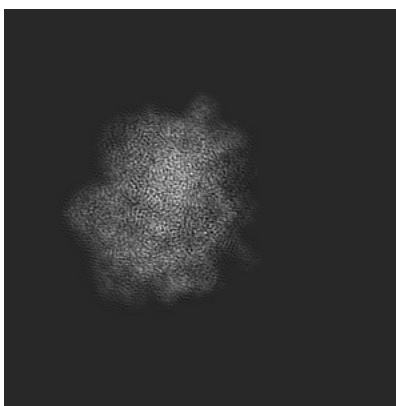
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

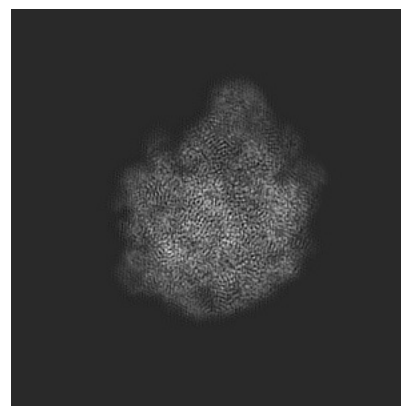
6.1.1 Primary map



X

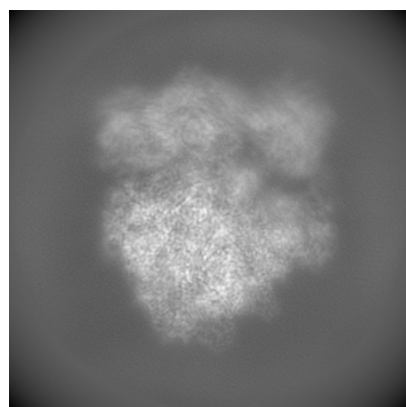


Y

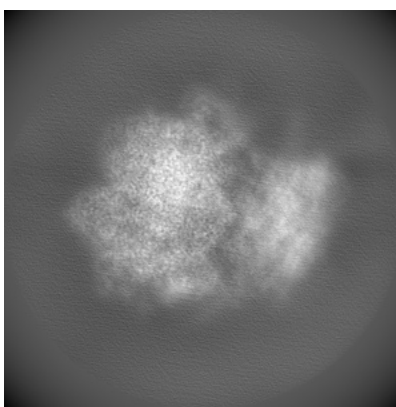


Z

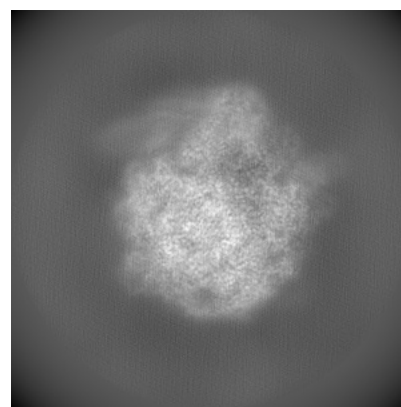
6.1.2 Raw map



X



Y

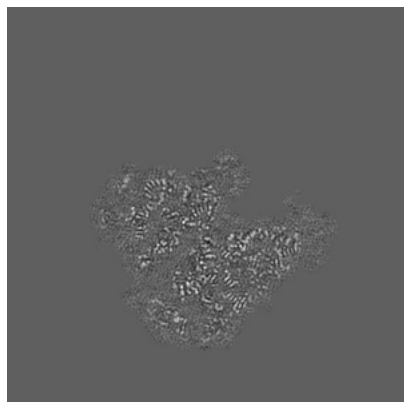


Z

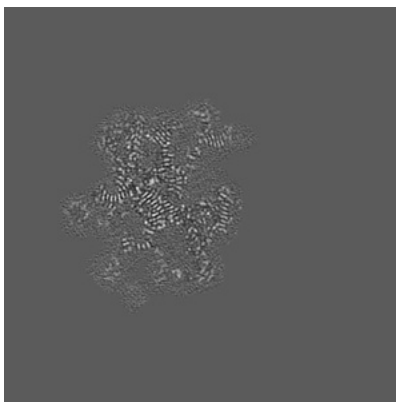
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

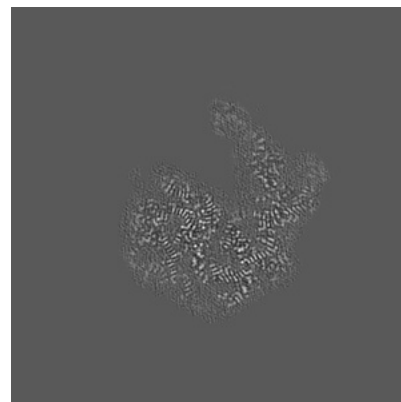
6.2.1 Primary map



X Index: 208

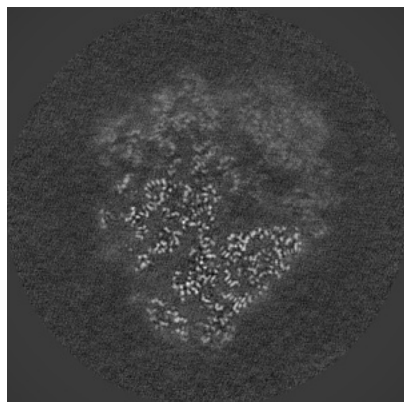


Y Index: 208

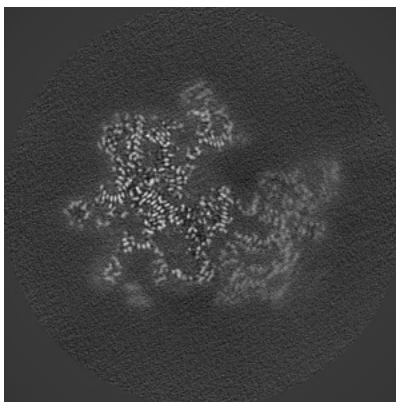


Z Index: 208

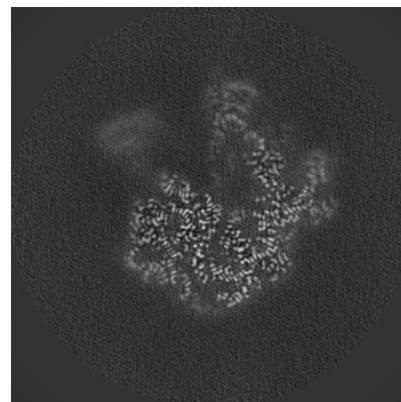
6.2.2 Raw map



X Index: 208



Y Index: 208

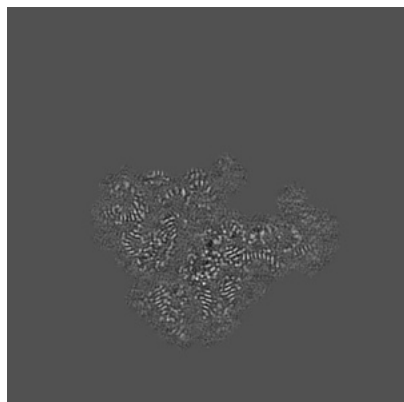


Z Index: 208

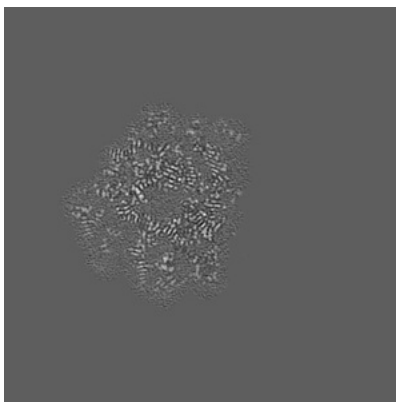
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

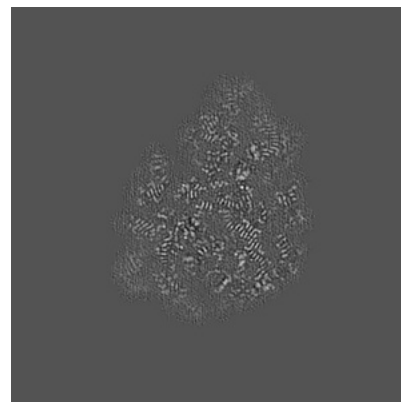
6.3.1 Primary map



X Index: 216

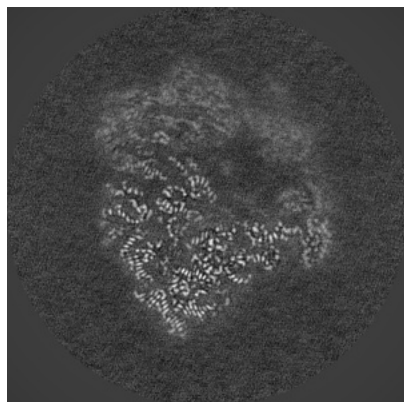


Y Index: 186

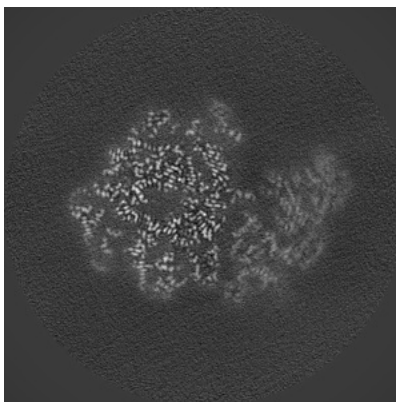


Z Index: 174

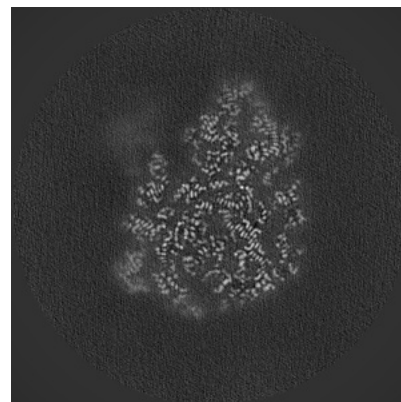
6.3.2 Raw map



X Index: 223



Y Index: 186

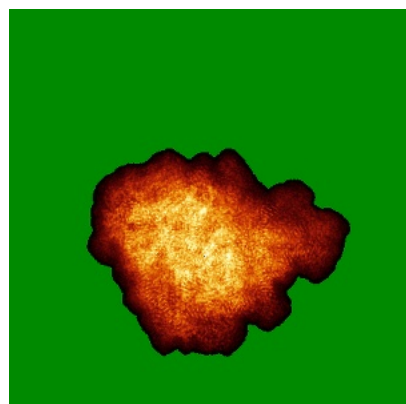


Z Index: 174

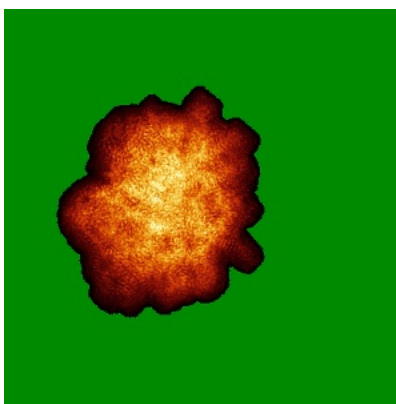
The images above show the largest variance slices of the map in three orthogonal directions.

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

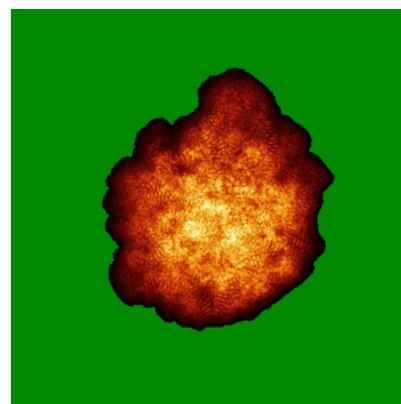
6.4.1 Primary map



X

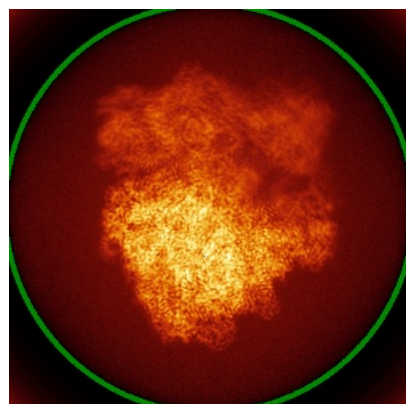


Y

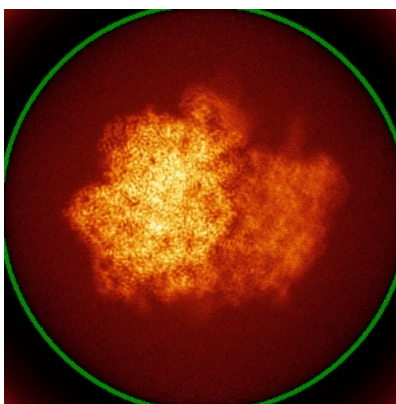


Z

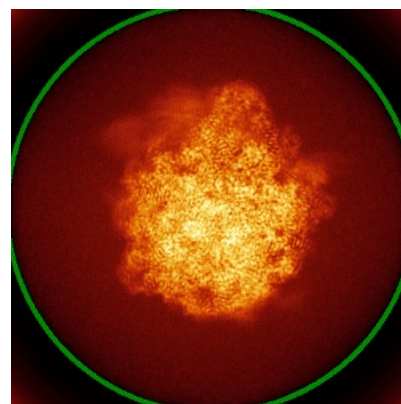
6.4.2 Raw map



X



Y

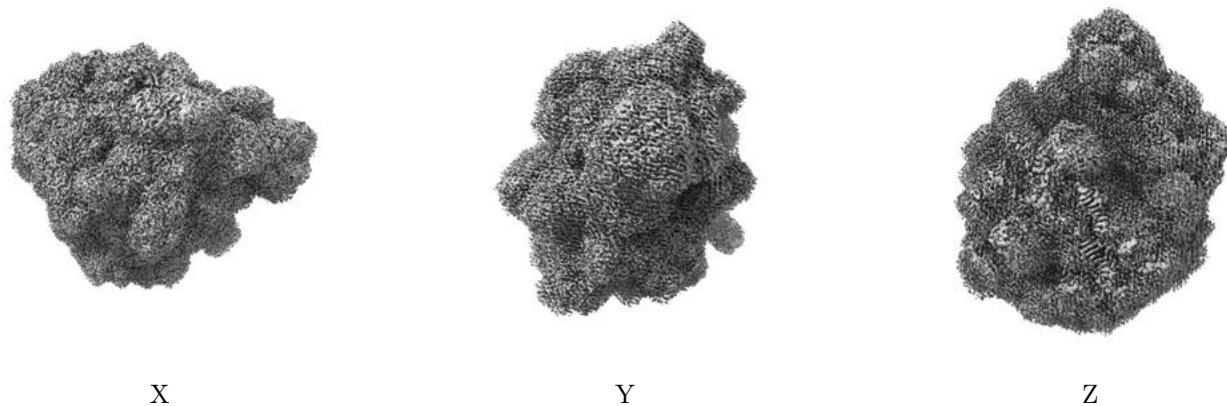


Z

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.

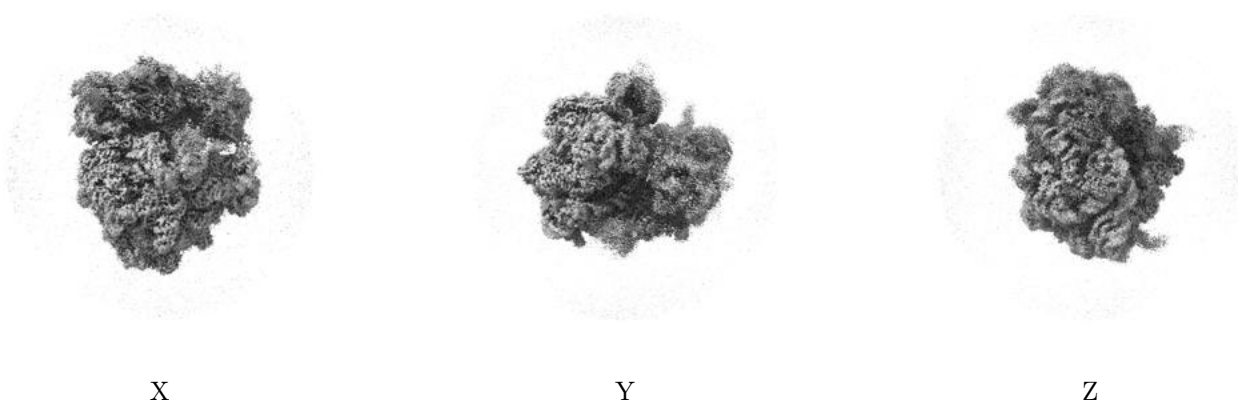
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

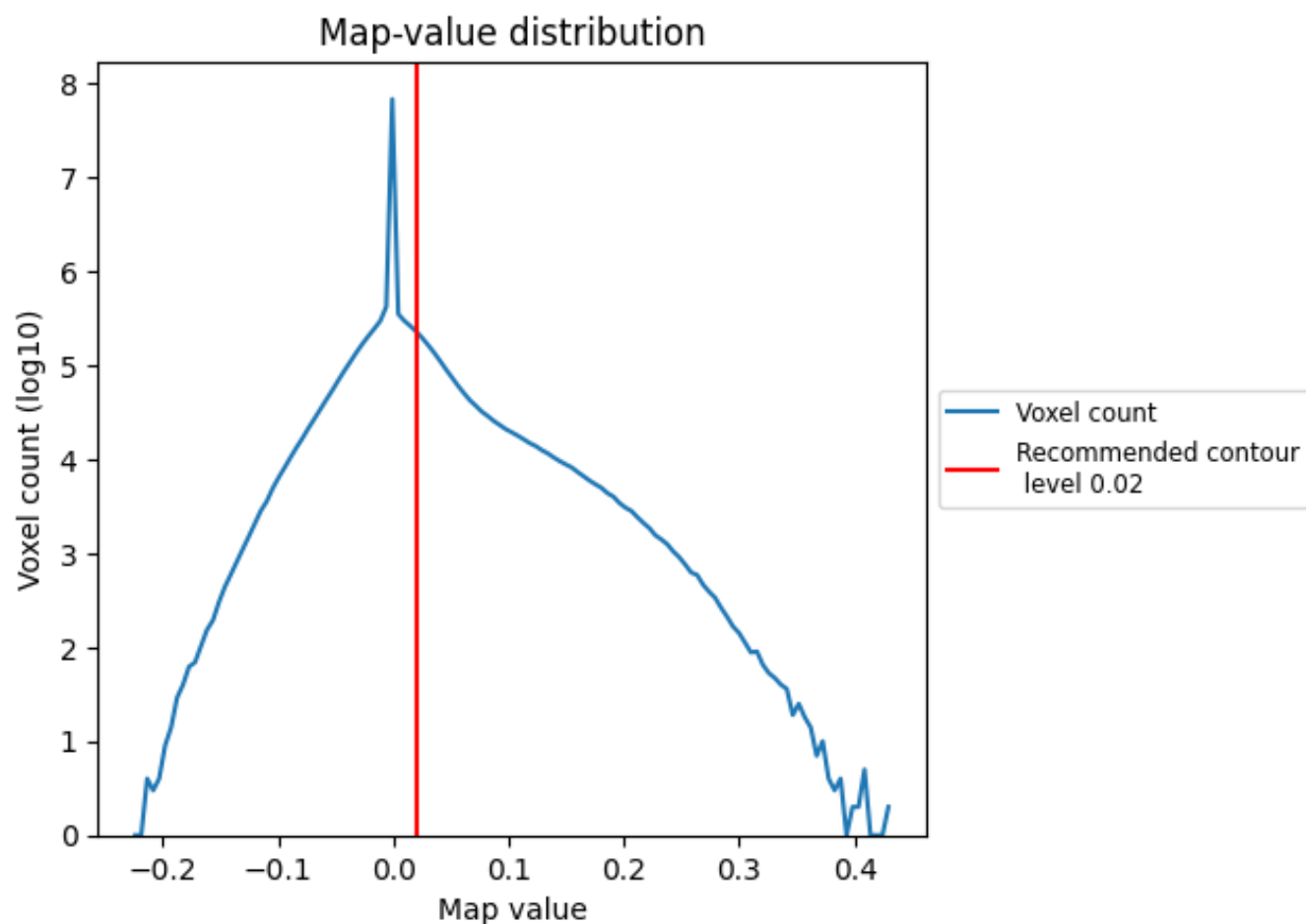
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

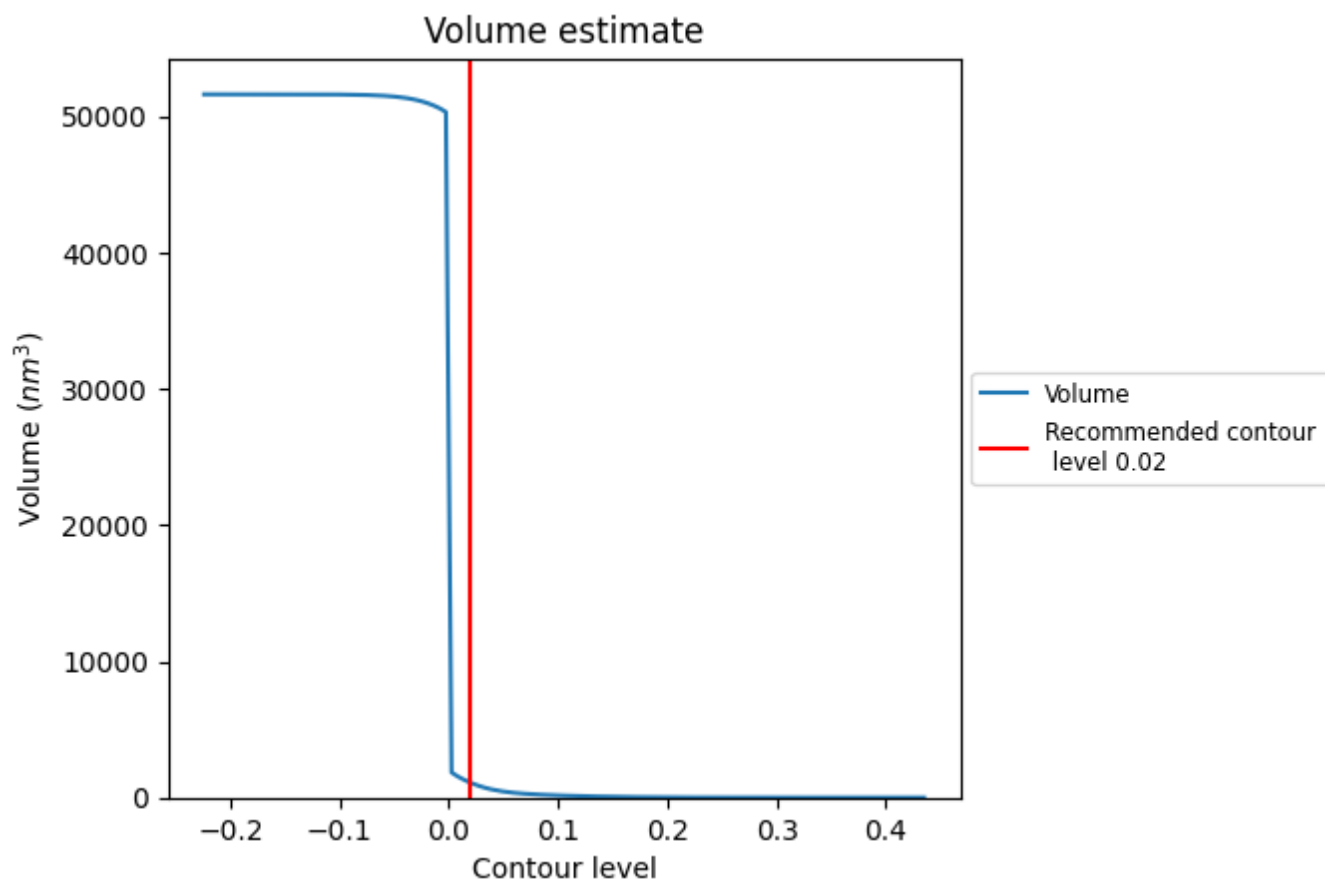
This section contains the results of statistical analysis of the map.

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.

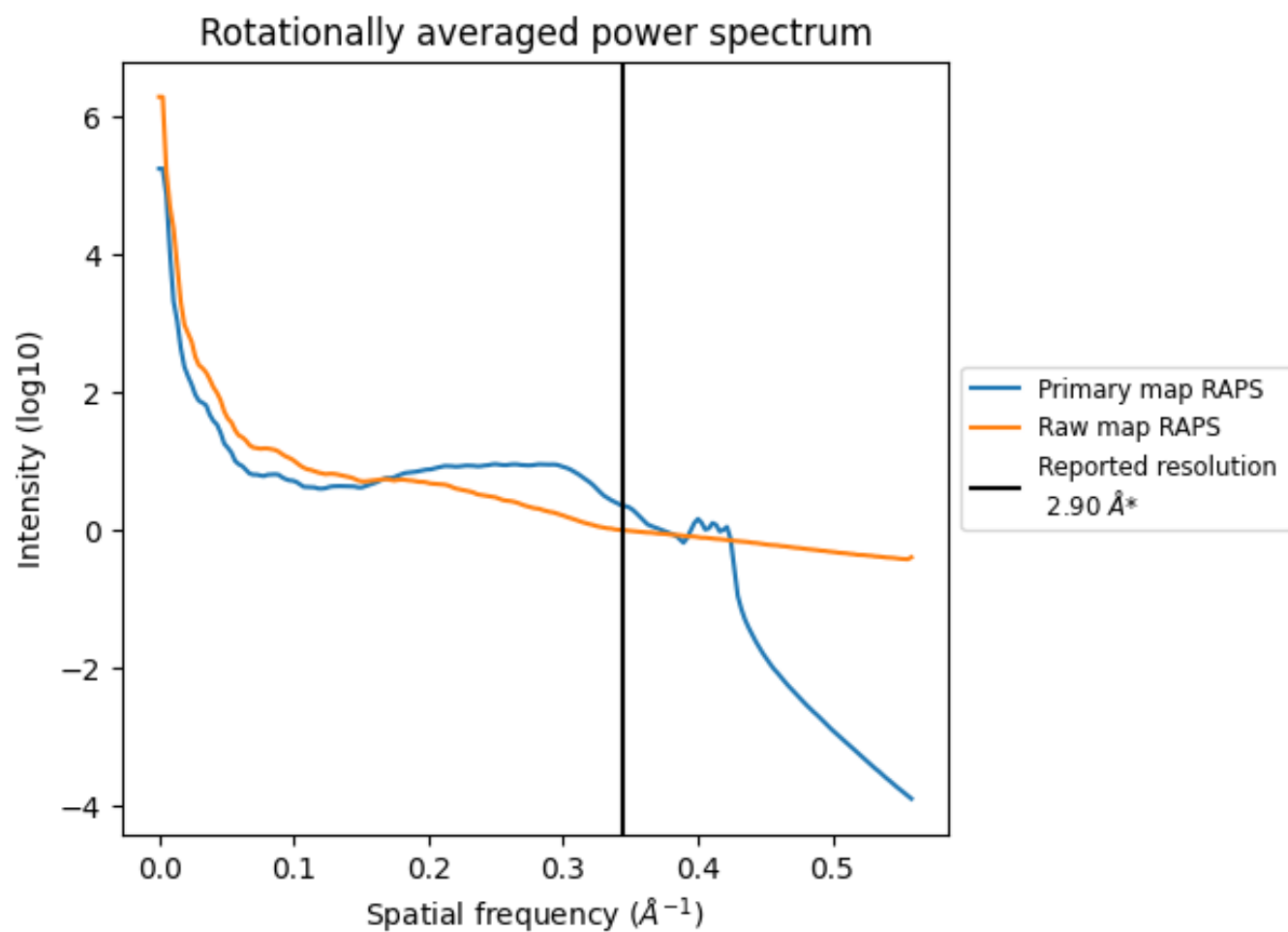
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1087 nm³; this corresponds to an approximate mass of 982 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 ⓘ

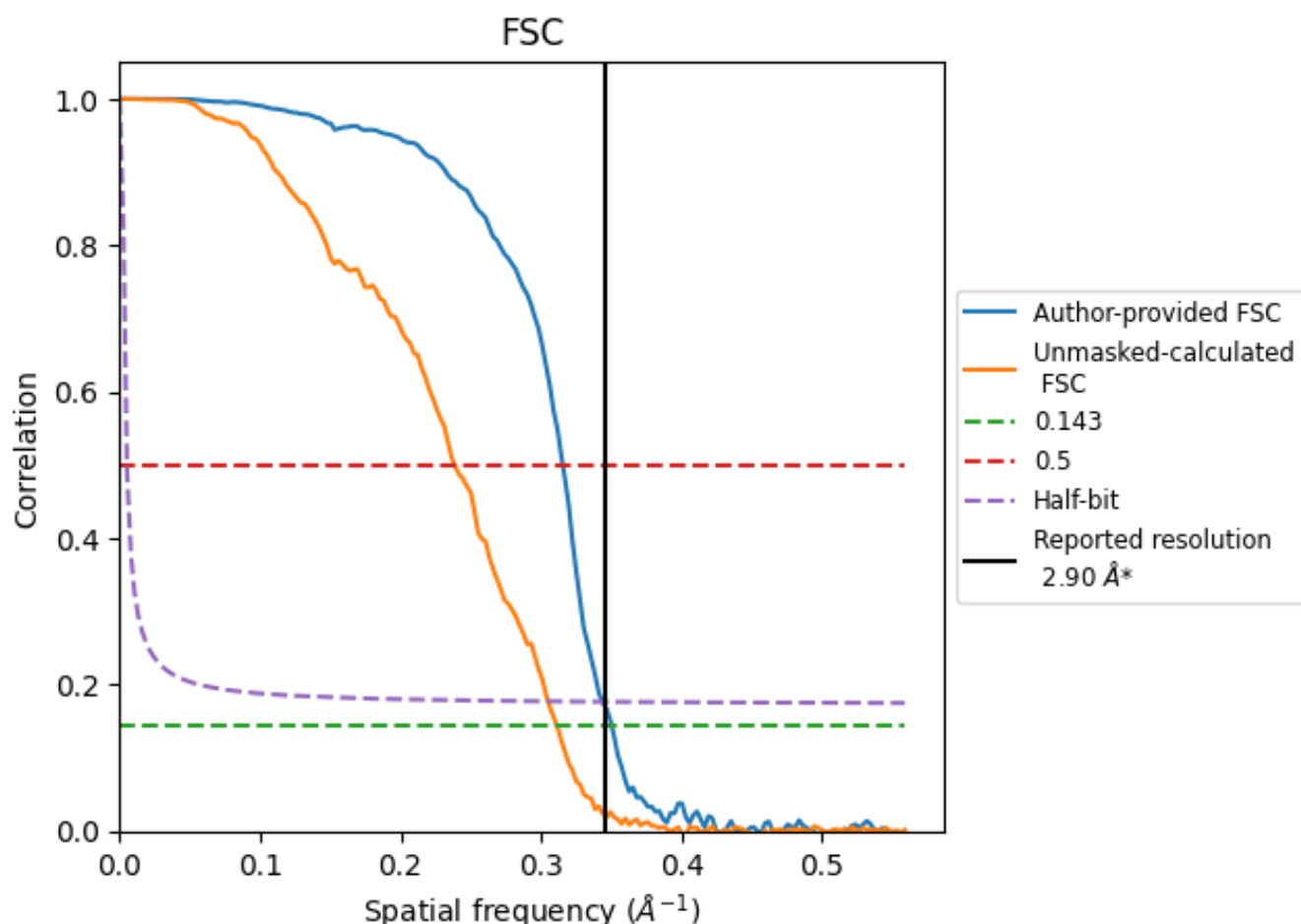


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

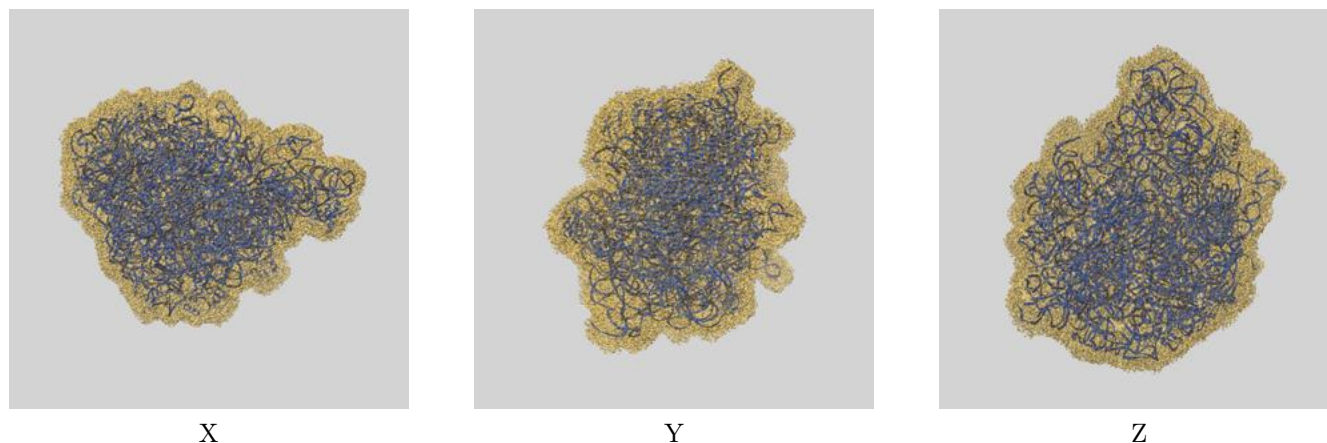
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.17	2.91
Unmasked-calculated*	3.21	4.19	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

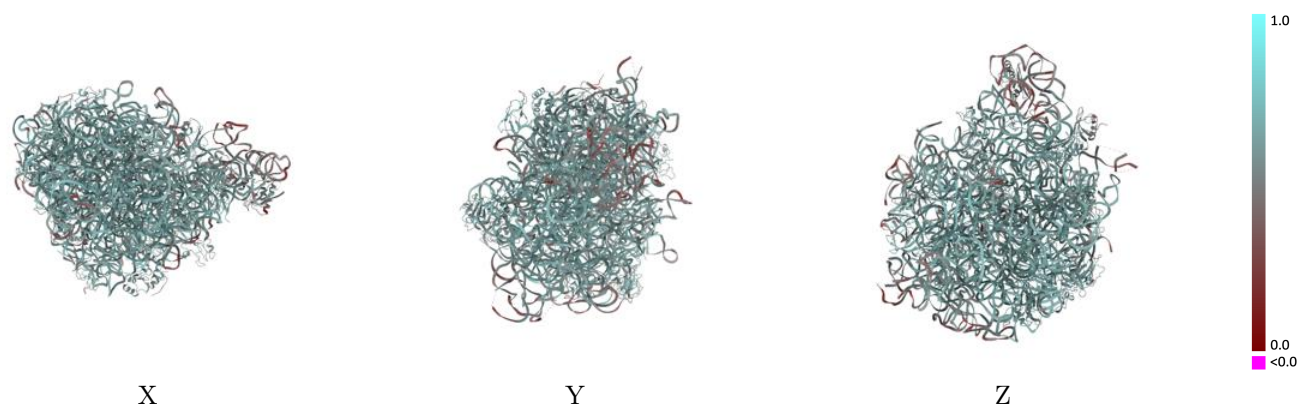
This section contains information regarding the fit between EMDB map EMD-21872 and PDB model 6WQN. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



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 [i](#)



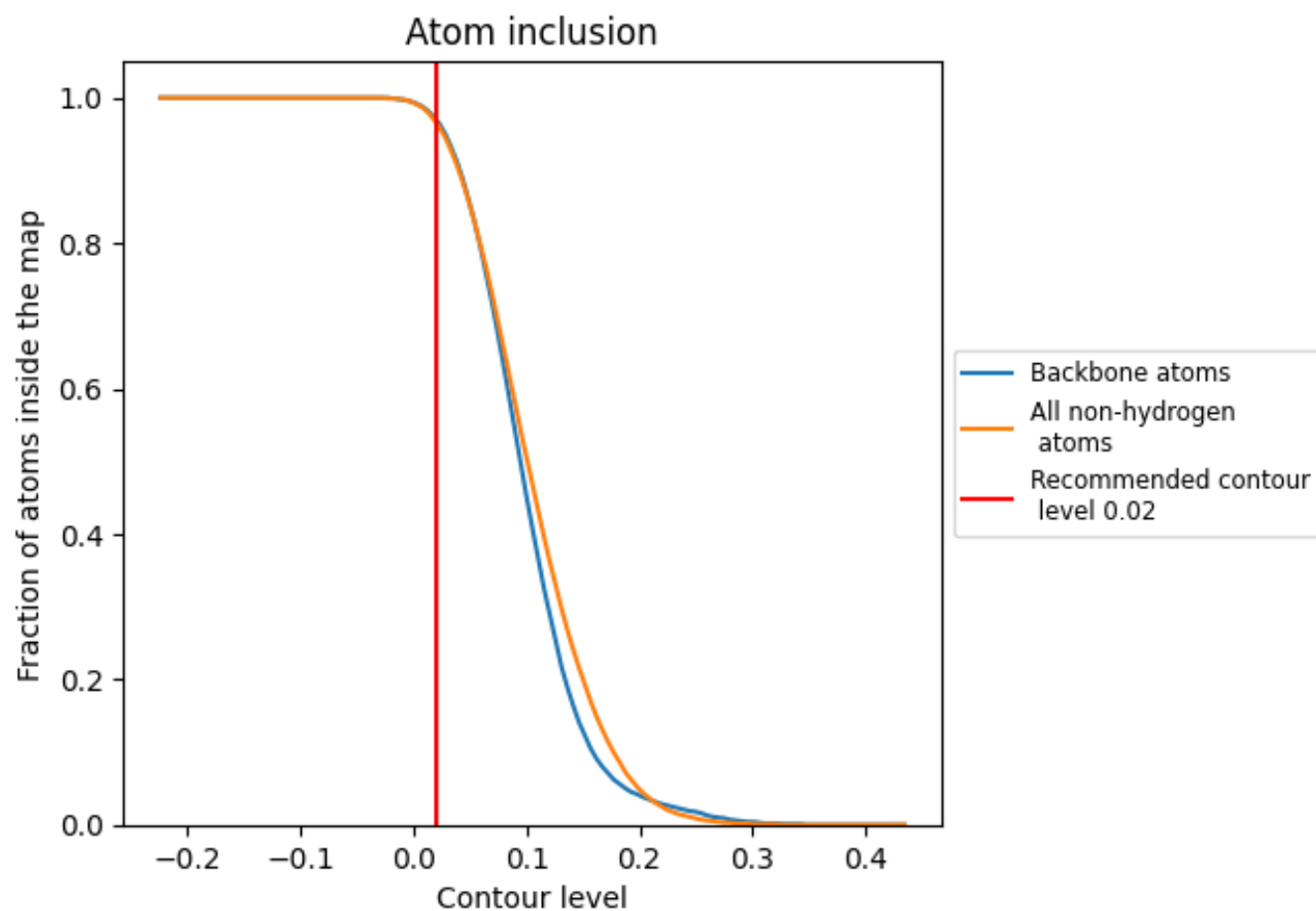
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.6010
1	 0.9680	 0.6040
2	 0.9400	 0.4950
A	 0.9660	 0.5960
B	 0.9690	 0.6230
C	 0.9920	 0.6480
D	 0.9530	 0.6090
E	 0.9830	 0.6390
F	 0.9560	 0.5870
G	 0.9290	 0.5440
H	 0.9030	 0.5040
I	 0.9900	 0.6410
J	 0.9460	 0.5890
K	 0.9340	 0.5600
L	 0.9750	 0.6200
M	 0.9650	 0.6180
N	 0.9690	 0.6140
O	 0.9440	 0.5800
P	 0.9890	 0.6630
Q	 0.9960	 0.6600
R	 0.9790	 0.6000
S	 0.9700	 0.6090
V	 0.9860	 0.6340
W	 0.9710	 0.6150
X	 0.9620	 0.6010
Y	 0.9740	 0.6160
Z	 0.9640	 0.6190
a	 0.9340	 0.5200

