



## wwPDB EM Validation Summary Report ⓘ

Mar 24, 2025 – 03:14 pm GMT

PDB ID : 9HC4  
EMDB ID : EMD-52036  
Title : Cryo-EM structure of *P. urativorans* 70S ribosome with 2 copies of bS20.  
Authors : Helena-Bueno, K.; Hill, C.H.; Melnikov, S.V.  
Deposited on : 2024-11-08  
Resolution : 3.20 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
MolProbity : 4.02b-467  
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) : 2.41.5

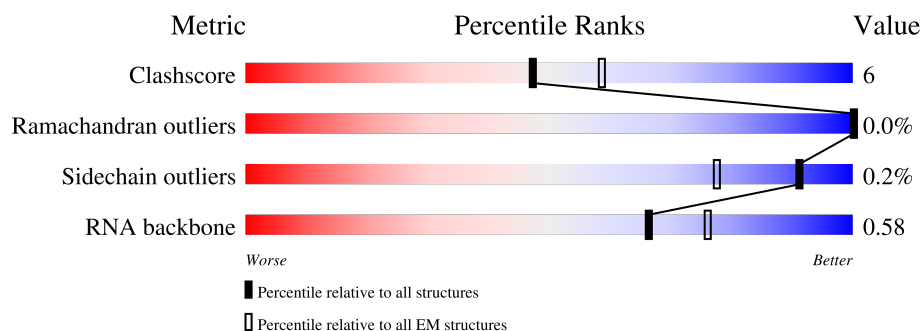
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	128	
2	C1	166	
3	R3	76	
4	A4	269	
5	E5	171	
6	L6	124	
7	F7	178	


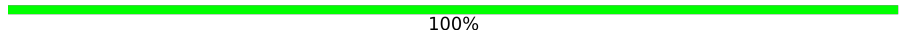
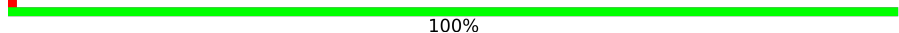
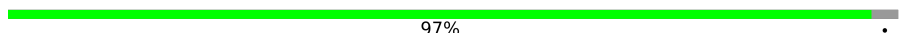
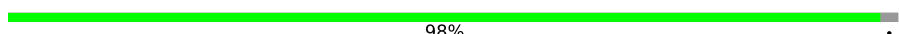
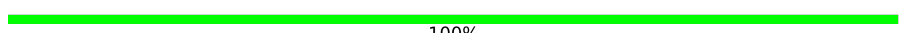
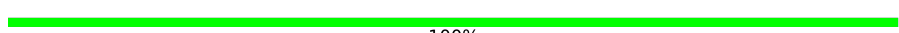







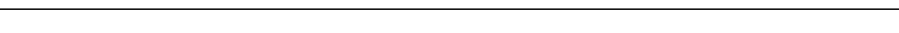
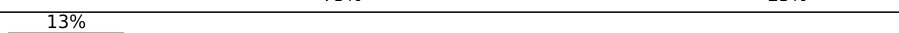
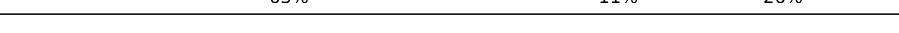
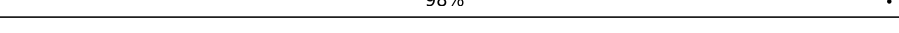
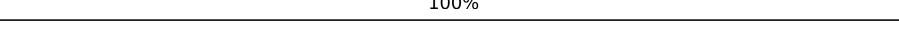


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Mol	Chain	Length	Quality of chain
8	E9	200	
9	aA	60	
10	MB	119	
11	UC	219	
12	WD	78	
13	XE	65	
14	RF	109	
15	FG	134	
16	VH	85	
17	TI	105	
18	fJ	93	
19	HK	101	
20	OL	88	
21	MM	118	
22	PO	118	
23	SP	91	
24	BQ	132	
25	GR	177	
26	GS	157	
27	CT	241	
28	KU	129	
29	NV	71	
30	YW	59	
31	IX	142	
32	JY	103	

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Mol	Chain	Length	Quality of chain
33	QZ	91	
34	Ba	44	
35	Qb	103	
36	Nc	116	
37	Kd	146	
38	Je	122	
39	Af	212	
40	Lg	137	
41	dh	65	
42	Oi	130	
43	Pj	89	
44	bk	51	
45	Cl	274	
46	Dm	213	
47	Sn	116	
48	A	88	
48	To	88	
49	ep	38	
50	D8	115	
51	iN	1589	
52	Z2	2882	

## 2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 136434 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 Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	125	Total	C	N	O	S	0	0
			948	592	179	176	1		

- Molecule 2 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	49	Total	C	N	O	S	0	0
			374	244	64	65	1		

- Molecule 3 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	R3	56	Total	C	N	O	0	0
			457	290	80	87		

- Molecule 4 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A4	233	Total	C	N	O	S	0	0
			1807	1138	327	335	7		

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E5	156	Total	C	N	O	S	0	0
			1151	716	218	211	6		

- Molecule 6 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L6	122	Total	C	N	O	S	0	0
			946	583	193	165	5		

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F7	177	Total	C	N	O	S	0	0
			1356	870	234	246	6		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E9	199	Total	C	N	O	S	0	0
			1537	966	282	284	5		

- Molecule 9 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aA	53	Total	C	N	O	S	0	0
			446	267	101	75	3		

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	MB	119	Total	C	N	O	S	0	0
			947	587	188	164	8		

- Molecule 11 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UC	96	Total	C	N	O	S	0	0
			750	479	135	135	1		

- Molecule 12 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	WD	76	Total	C	N	O	S	0	0
			618	383	131	101	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	XE	62	Total	C	N	O	S	0	0
			502	307	99	95	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	RF	109	Total	C	N	O	S	0	0
			834	521	159	151	3		

- Molecule 15 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	FG	102	Total	C	N	O	S	0	0
			849	535	154	158	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	VH	78	Total	C	N	O	S	0	0
			587	365	115	104	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	TI	102	Total	C	N	O	S	0	0
			784	487	149	148			

- Molecule 18 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	fJ	55	Total	C	N	O	S	0	0
			443	282	74	86	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	HK	100	Total	C	N	O	S	0	0
			811	498	162	144	7		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	OL	86	Total	C	N	O	S	0	0
			694	427	137	128	2		

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	MM	110	Total	C	N	O	S	0	0
			858	528	172	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	PO	116	Total	C	N	O	S	0	0
			935	586	199	148	2		

- Molecule 23 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SP	80	Total	C	N	O	S	0	0
			637	405	121	108	3		

- Molecule 24 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BQ	131	Total	C	N	O	S	0	0
			974	602	179	187	6		

- Molecule 25 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	GR	173	Total	C	N	O	S	0	0
			1339	836	244	257	2		

- Molecule 26 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	GS	152	Total	C	N	O	S	0	0
			1190	738	230	215	7		

- Molecule 27 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CT	204	Total	C	N	O	S	0	0
			1606	1009	301	290	6		

- Molecule 28 is a protein called Small ribosomal subunit protein uS11.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	KU	114	Total	C	N	O	S	0	0
			836	518	162	155	1		

- Molecule 29 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	NV	57	Total	C	N	O	S	0	0
			472	299	95	77	1		

- Molecule 30 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	YW	56	Total	C	N	O	S	0	0
			438	272	88	76	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	IX	142	Total	C	N	O	S	0	0
			1108	710	198	197	3		

- Molecule 32 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	JY	95	Total	C	N	O	S	0	0
			760	472	145	141	2		

- Molecule 33 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	QZ	79	Total	C	N	O	S	0	0
			632	395	119	116	2		

- Molecule 34 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ba	44	Total	C	N	O	S	0	0
			369	227	89	51	2		

- Molecule 35 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Qb	103	Total	C	N	O	S	0	0
			827	524	153	148	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Nc	113	Total	C	N	O	S	0	0
			852	530	170	152			

- Molecule 37 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Kd	143	Total	C	N	O	S	1	0
			1053	651	205	194	3		

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Je	122	Total	C	N	O	S	0	0
			937	585	181	166	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Af	211	Total	C	N	O	S	0	0
			1548	954	292	296	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lg	137	Total	C	N	O	S	0	0
			1093	697	210	179	7		

- Molecule 41 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	dh	64	Total	C	N	O	S	0	0
			519	326	107	82	4		

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Oi	115	Total	C	N	O		
			917	572	184	161	0	0

- Molecule 43 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Pj	81	Total	C	N	O	S	
			648	409	126	111	2	0

- Molecule 44 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	bk	49	Total	C	N	O	S	
			394	254	68	69	3	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Cl	272	Total	C	N	O	S	
			2103	1302	431	364	6	0

- Molecule 46 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Dm	212	Total	C	N	O	S	
			1688	1058	318	309	3	0

- Molecule 47 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Sn	87	Total	C	N	O	S	
			690	442	124	122	2	0

- Molecule 48 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	To	86	Total	C	N	O	S	
			675	410	144	119	2	0
48	A	65	Total	C	N	O	S	
			462	285	93	82	2	0

- Molecule 49 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	ep	38	Total	C	N	O	S	0	0
			298	182	66	46	4		

- Molecule 50 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	D8	115	Total	C	N	O	P	0	0
			2446	1093	436	802	115		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D8	85	U	-	insertion	GB 930356181
D8	88	A	C	variant	GB 930356181

- Molecule 51 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	iN	1503	Total	C	N	O	P	0	0
			32246	14388	5917	10438	1503		

- Molecule 52 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Z2	2705	Total	C	N	O	P	0	0
			58043	25910	10660	18768	2705		


There is a discrepancy between the modelled and reference sequences:

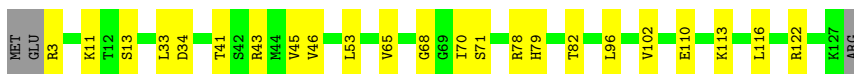
Chain	Residue	Modelled	Actual	Comment	Reference
Z2	1717	U	G	conflict	GB 930356181

### 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.

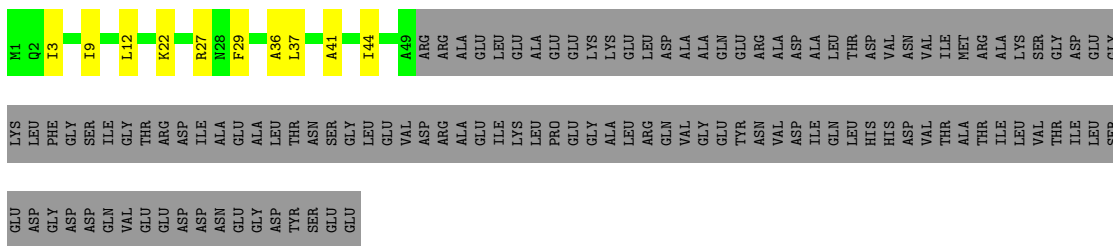
- Molecule 1: Small ribosomal subunit protein uS9

Chain F: 



- Molecule 2: Large ribosomal subunit protein bL9

Chain C1: 



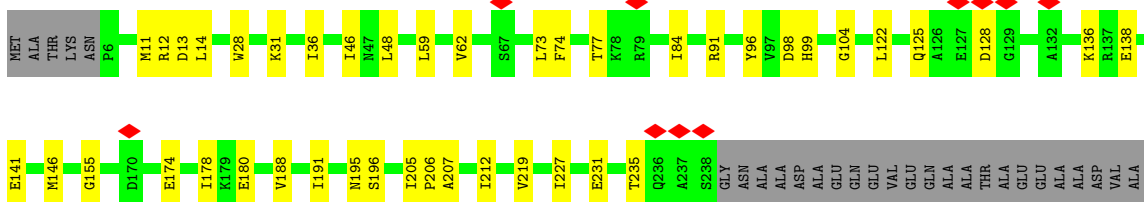
- Molecule 3: Small ribosomal subunit protein bS18

Chain R3: 




- Molecule 4: Small ribosomal subunit protein uS2

Chain A4: 




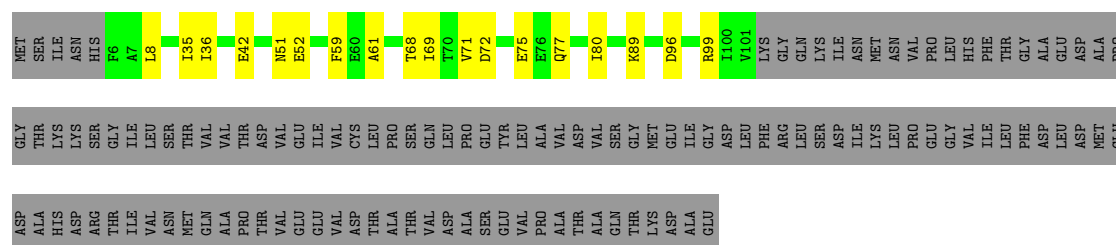


Chain MB:  85% 15%




- Molecule 11: Large ribosomal subunit protein bL25

Chain UC:  36% 8% 56%



- Molecule 12: Large ribosomal subunit protein bL28

Chain WD:  82% 15% 3%




- Molecule 13: Large ribosomal subunit protein uL29

Chain XE:  66% 29% 5%



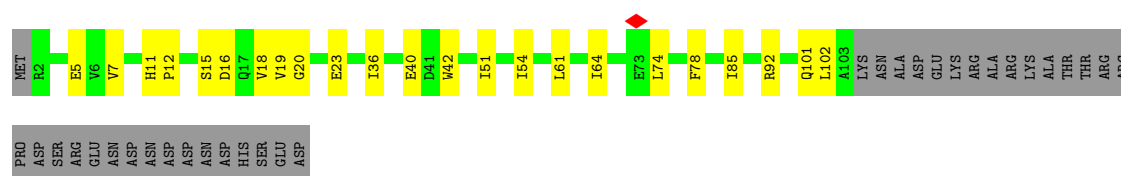
- Molecule 14: Large ribosomal subunit protein uL22

Chain RF:  83% 17% 0%



- Molecule 15: Small ribosomal subunit protein bS6

Chain FG:  59% 17% 24%



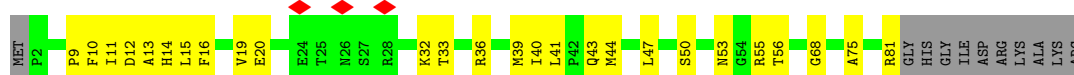
- Molecule 16: Large ribosomal subunit protein bL27







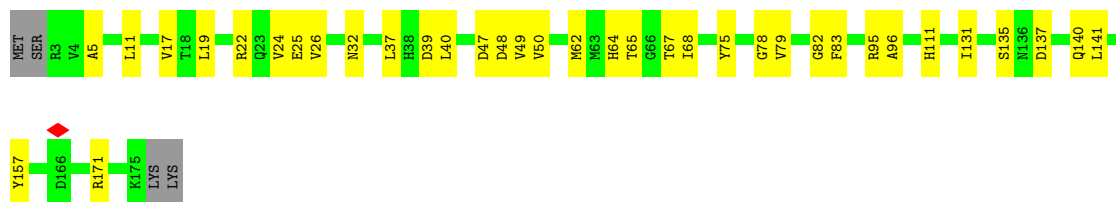
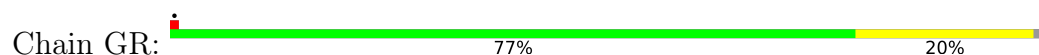
- Molecule 23: Small ribosomal subunit protein uS19



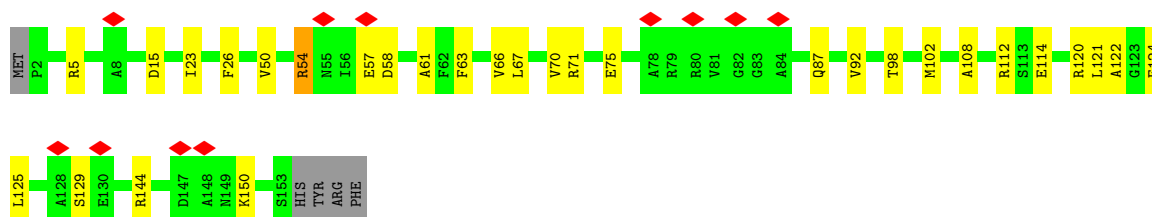
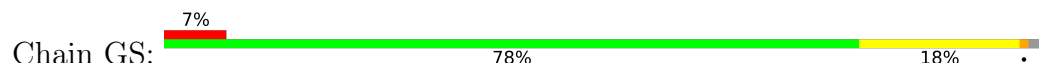
- Molecule 24: Small ribosomal subunit protein uS8



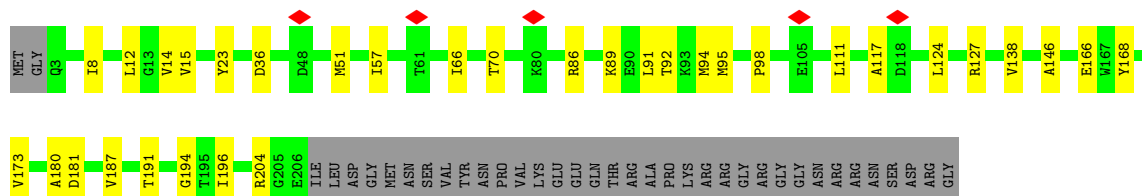
- Molecule 25: Large ribosomal subunit protein uL6



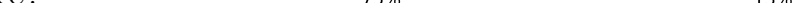
- Molecule 26: Small ribosomal subunit protein uS7



- Molecule 27: Small ribosomal subunit protein uS3



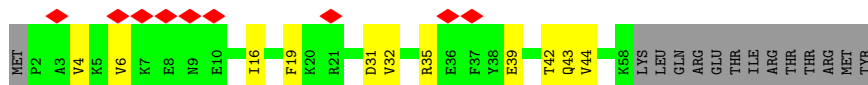
- Molecule 28: Small ribosomal subunit protein uS11

Chain KU:  75% 13% 12%




- Molecule 29: Small ribosomal subunit protein bS21

Chain NV: 

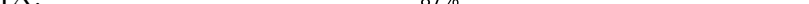


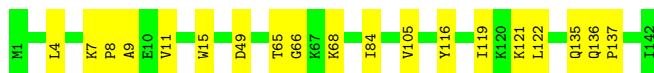
- Molecule 30: Large ribosomal subunit protein uL30

Chain YW:  76% 19% 5%



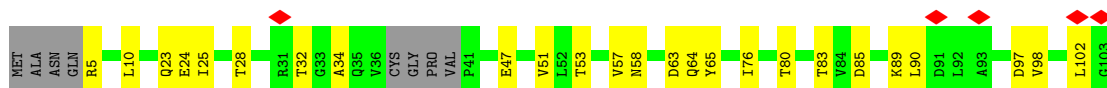
- Molecule 31: Large ribosomal subunit protein uL13

Chain IX:  87% 13%



- Molecule 32: Small ribosomal subunit protein uS10

Chain JY: 



- Molecule 33: Small ribosomal subunit protein uS17

Chain QZ:  69% 18% 13%



- Molecule 34: Large ribosomal subunit protein bL34

Chain Ba: 

There are no outlier residues recorded for this chain.

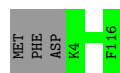
- Molecule 35: Large ribosomal subunit protein bL21

Chain Qb:  100%



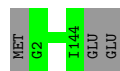
- Molecule 36: Large ribosomal subunit protein uL18

Chain Nc:  97%



- Molecule 37: Large ribosomal subunit protein uL15

Chain Kd:  98%



- Molecule 38: Large ribosomal subunit protein uL14

Chain Je:  100%

There are no outlier residues recorded for this chain.

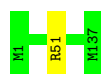
- Molecule 39: Large ribosomal subunit protein uL3

Chain Af:  100%



- Molecule 40: Large ribosomal subunit protein uL16

Chain Lg:  99%




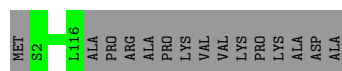
- Molecule 41: Large ribosomal subunit protein bL35

Chain dh:  94% 5%



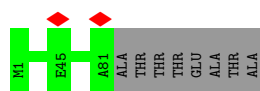
- Molecule 42: Large ribosomal subunit protein bL19

Chain Oi:  88% 12%



- Molecule 43: Small ribosomal subunit protein bS16

Chain Pj:  91% 9%



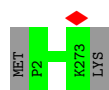
- Molecule 44: Large ribosomal subunit protein bL33

Chain bk:  96%



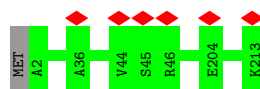
- Molecule 45: Large ribosomal subunit protein uL2

Chain Cl:  99%




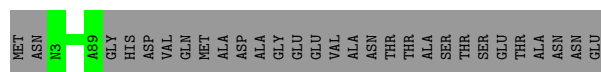
- Molecule 46: Small ribosomal subunit protein uS4

Chain Dm:  100%



- Molecule 47: Large ribosomal subunit protein uL23

Chain Sn:  75% 25%



- Molecule 48: Small ribosomal subunit protein bS20

Chain To:  98%



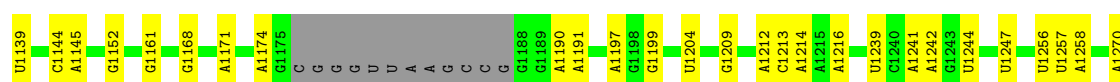
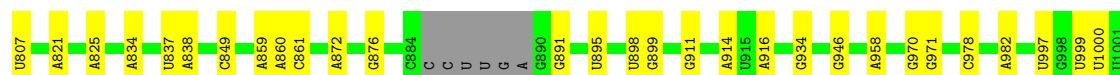
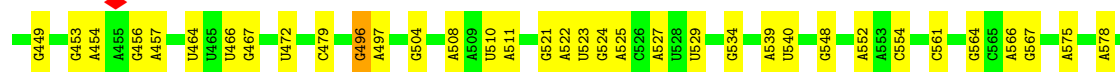
- Molecule 48: Small ribosomal subunit protein bS20

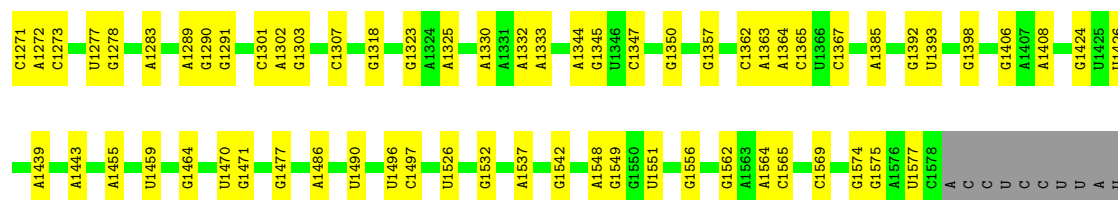


- Molecule 50: 5S rRNA



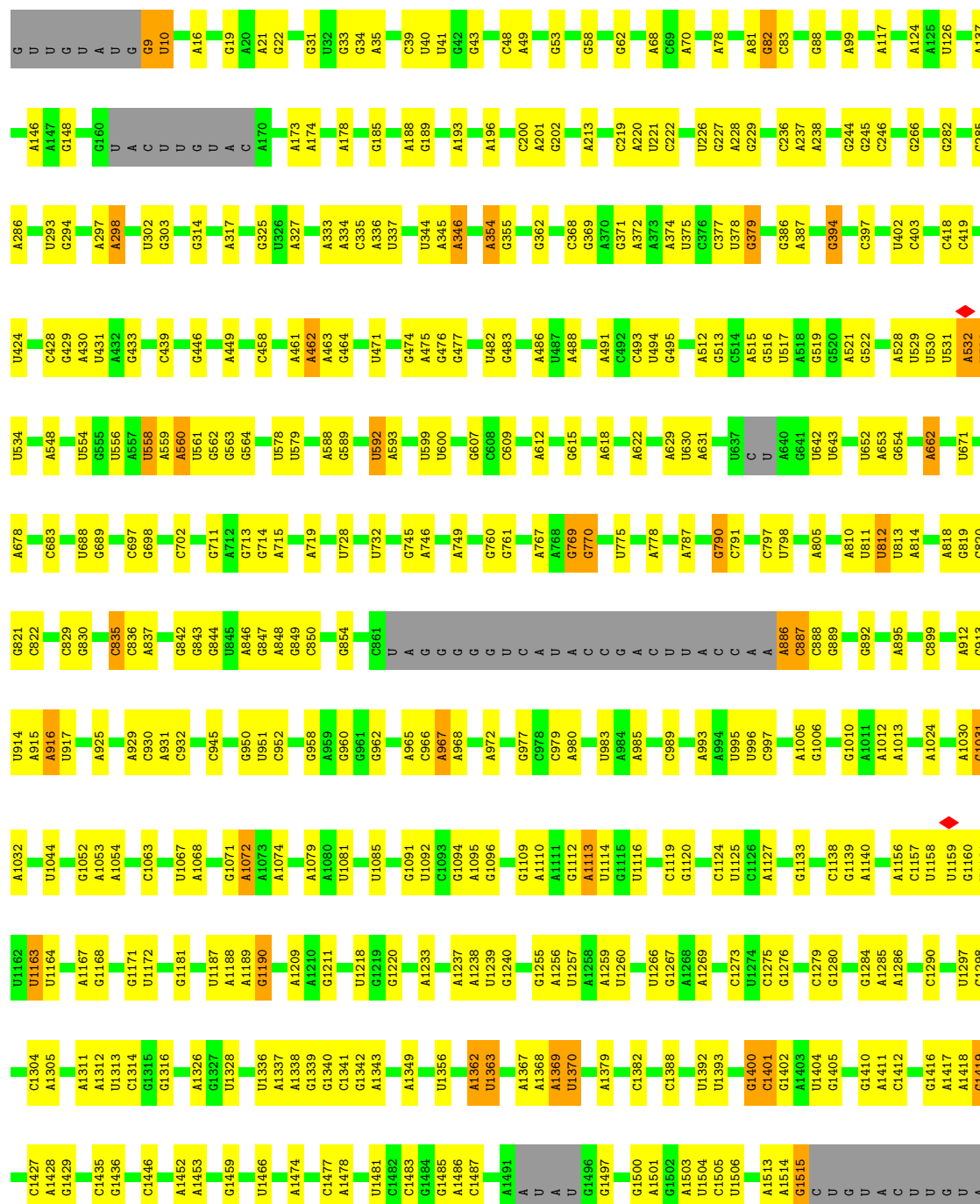
- [illegible]





## • Molecule 52: 23S rRNA

Chain Z2: 68% 24% 6%



G2814	U2870	G2515	U2363	G2221	G	U	A1956	A1769	C
G2818	G2671	G2527	A2364	G2222	C	G	U1957	A	A
G2823	U2872	G2530	G2365	G2233	C	A	G1958	G	G
A2826	C2673	A2536	G2366	C2241	A	C	U1968	A1531	C
U2831	G2674	G2537	U2367	A2249	U	U	C1976	A1532	A1532
G2832	G2675	U2538	C2368	A2250	C	G	U1977	G1536	G1536
U2836	G2685	U2545	U2385	A2261	U	A	U1978	G1548	G1548
U2837	A2688	U2546	U2389	U2266	A	U	U1979	U1551	U1551
A2838	G2692	A2547	C2400	U2277	A	G	C1983	C1552	C1552
A2839	G2697	A2548	A2401	A2270	U	U	G1998	A1554	A1554
C2840	C2706	A2549	C2407	A2271	A	C	A1999	U1681	U1681
C2841	U2707	A2551	A2408	A2276	C	A	A2000	G1685	G1685
A2849	A2708	C2556	A2409	U2274	C	G	A2001	A1686	A1686
U2850	C2709	G2561	C2410	G2275	C	A	A2005	G1688	G1688
U2858	G2710	G2564	G2411	G2276	C	U	A2007	G1690	G1690
G2865	U2711	G2565	G2412	G2286	U	G	C2008	G1691	G1691
A2866	G2714	G2566	A2422	G2287	G	G	U2009	G1695	G1695
C2867	G2715	G2567	C2423	U2288	U	U	G2017	U1706	U1706
C2868	A2716	G2578	G2425	C2289	C	G	G2018	G1707	G1707
U	A2724	A2581	U2426	G2290	A	G	A2019	A1708	A1708
A	C2725	A2585	A2431	G2291	U	A	A2017	U1709	U1709
C	G2726	G2586	A2433	U2302	U	G	G2018	A1710	A1710
C	G2727	U2587	A2452	G2303	C	C	U2024	G1711	G1711
A	A2731	U2592	G2453	G2304	G	U	G2025	G1712	G1712
A	U2739	U2596	A2459	A2305	G	U	C2029	A	A
C	A2740	A2597	C2469	G2306	U	U	C2030	C	C
C	G2760	U2598	U2472	U2307	U	G	U2037	U	U
A	A2761	G2610	U2473	U2309	A	A	A2038	U	U
A	U2762	U2611	U2474	A2310	G	G	G2041	G1718	G1718
A	U2763	G2612	U2479	A2311	C	C	G2042	C1721	C1721
G	A2764	G2613	C2479	A2312	C	C	A2046	U1722	U1722
C2771	C2771	A2615	G2485	A2328	G	G	G2047	G1723	G1723
C2772	U2772	U2619	U2486	A2329	A	A	U2048	G1724	G1724
A2774	A2774	G2621	U2487	C2330	G	C	C2049	A1725	A1725
A2775	U2775	U2620	U2488	C2333	C	C	G2053	G1732	G1732
A2776	G2776	G2621	U2489	G2334	G	G	U2054	G1739	G1739
U2784	U2784	C2629	C2498	A2337	U	U	G2055	G1742	G1742
G2785	G2785	U2630	U2499	C2338	C	C	A2057	G1750	G1750
A2786	A2786	G2631	U2501	C2339	G	G	C2058	U1759	U1759
A2787	C2804	A2640	U2502	C2340	C	C	U2073	C1633	C1633
G2805	C2805	G2644	C2503	C2347	U	U	A2074	C1634	C1634
C2806	A2907	U2645	G2512	A2348	G	G	U2078	U1635	U1635
U2813	U2813	G2646	A2360	A2349	U	U	G2079	U1636	U1636
				C2357	G	G	A2080	G1762	G1762
				G2206	U	U	U2084	U1765	U1765
				G2207	C	C		U1768	U1768
				A2208	C	C			
				C2209	U	U			
				A2210	U	U			
				U2211	G	G			
				U2212	C	C			
				G2213	U	U			
				U2219	G	G			
				G2220	A	A			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19576	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1250	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	420.30002, 420.30002, 420.30002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.934, 0.934, 0.934	Depositor



## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	F	0.27	0/961	0.52	0/1293
2	C1	0.28	0/379	0.50	0/511
3	R3	0.24	0/465	0.42	0/629
4	A4	0.27	0/1838	0.46	0/2481
5	E5	0.27	0/1163	0.50	0/1564
6	L6	0.26	0/959	0.50	0/1282
7	F7	0.28	0/1377	0.49	0/1851
8	E9	0.27	0/1559	0.47	0/2103
9	aA	0.25	0/454	0.52	0/600
10	MB	0.26	0/961	0.48	0/1282
11	UC	0.27	0/763	0.46	0/1028
12	WD	0.25	0/628	0.48	0/841
13	XE	0.27	0/503	0.47	0/670
14	RF	0.26	0/840	0.51	0/1125
15	FG	0.25	0/864	0.47	0/1169
16	VH	0.27	0/595	0.48	0/793
17	TI	0.25	0/790	0.47	0/1057
18	fJ	0.28	0/458	0.59	0/626
19	HK	0.27	0/821	0.50	0/1091
20	OL	0.25	0/702	0.42	0/941
21	MM	0.32	0/866	0.57	0/1166
22	PO	0.26	0/947	0.51	0/1261
23	SP	0.27	0/652	0.51	0/879
24	BQ	0.25	0/982	0.46	0/1318
25	GR	0.26	0/1359	0.49	0/1839
26	GS	0.27	0/1208	0.50	1/1619 (0.1%)
27	CT	0.27	0/1630	0.51	0/2192
28	KU	0.27	0/851	0.48	0/1150
29	NV	0.26	0/478	0.41	0/632
30	YW	0.28	0/442	0.51	0/590
31	IX	0.26	0/1134	0.46	0/1529
32	JY	0.28	0/768	0.54	0/1033
33	QZ	0.24	0/638	0.46	0/858
34	Ba	0.29	0/373	0.54	0/489

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	Qb	0.26	0/839	0.50	0/1127
36	Nc	0.26	0/863	0.50	0/1158
37	Kd	0.25	0/1064	0.49	0/1417
38	Je	0.26	0/946	0.48	0/1271
39	Af	0.26	0/1566	0.49	0/2103
40	Lg	0.26	0/1112	0.50	1/1483 (0.1%)
41	dh	0.26	0/524	0.57	0/686
42	Oi	0.26	0/927	0.49	0/1239
43	Pj	0.27	0/660	0.48	0/887
44	bk	0.26	0/401	0.43	0/534
45	Cl	0.26	0/2143	0.49	0/2879
46	Dm	0.27	0/1712	0.50	0/2296
47	Sn	0.27	0/697	0.47	0/928
48	A	0.25	0/465	0.39	0/626
48	To	0.27	0/679	0.45	0/904
49	ep	0.27	0/300	0.47	0/395
50	D8	0.18	0/2733	0.72	0/4256
51	iN	0.20	0/36108	0.76	5/56315 (0.0%)
52	Z2	0.22	0/65009	0.75	3/101385 (0.0%)
All	All	0.23	0/148156	0.69	10/221381 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
5	E5	0	1
41	dh	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	iN	997	U	C5-C6-N1	6.03	125.71	122.70
52	Z2	1297	U	C2-N1-C1'	5.83	124.70	117.70
51	iN	496	G	O4'-C1'-N9	5.67	112.74	108.20
40	Lg	51	ARG	NE-CZ-NH1	5.39	123.00	120.30
26	GS	54	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E5	82	ASN	Peptide
1	F	11	LYS	Peptide
41	dh	31	HIS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	948	0	967	15	0
2	C1	374	0	406	9	0
3	R3	457	0	466	6	0
4	A4	1807	0	1827	25	0
5	E5	1151	0	1205	21	0
6	L6	946	0	1008	8	0
7	F7	1356	0	1391	23	0
8	E9	1537	0	1590	21	0
9	aA	446	0	443	0	0
10	MB	947	0	988	13	0
11	UC	750	0	767	12	0
12	WD	618	0	637	8	0
13	XE	502	0	527	13	0
14	RF	834	0	898	12	0
15	FG	849	0	838	18	0
16	VH	587	0	592	3	0
17	TI	784	0	820	10	0
18	fJ	443	0	391	0	0
19	HK	811	0	845	11	0
20	OL	694	0	710	9	0
21	MM	858	0	897	21	0
22	PO	935	0	999	15	0
23	SP	637	0	665	20	0
24	BQ	974	0	1009	10	0
25	GR	1339	0	1371	23	0
26	GS	1190	0	1224	23	0
27	CT	1606	0	1667	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	KU	836	0	845	19	0
29	NV	472	0	520	13	0
30	YW	438	0	476	10	0
31	IX	1108	0	1145	14	0
32	JY	760	0	789	25	0
33	QZ	632	0	676	13	0
34	Ba	369	0	418	0	0
35	Qb	827	0	862	0	0
36	Nc	852	0	880	0	0
37	Kd	1053	0	1117	0	0
38	Je	937	0	1003	0	0
39	Af	1548	0	1574	0	0
40	Lg	1093	0	1188	0	0
41	dh	519	0	581	0	0
42	Oi	917	0	969	0	0
43	Pj	648	0	661	0	0
44	bk	394	0	412	0	0
45	Cl	2103	0	2184	0	0
46	Dm	1688	0	1745	0	0
47	Sn	690	0	744	0	0
48	A	462	0	453	8	0
48	To	675	0	716	0	0
49	ep	298	0	334	0	0
50	D8	2446	0	1241	14	0
51	iN	32246	0	16224	0	0
52	Z2	58043	0	29179	308	0
All	All	136434	0	92084	735	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 6.

The worst 5 of 735 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:LEU:HD11	1:F:46:VAL:HG11	1.47	0.93
52:Z2:2786:A:O2'	52:Z2:2787:A:OP1	1.89	0.89
22:PO:49:ASP:OD2	52:Z2:517:U:O2'	1.92	0.88
52:Z2:1109:G:OP2	52:Z2:1110:A:O2'	1.92	0.87
4:A4:77:THR:OG1	4:A4:174:GLU:OE2	1.94	0.85

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	123/128 (96%)	118 (96%)	5 (4%)	0	100	100
2	C1	47/166 (28%)	47 (100%)	0	0	100	100
3	R3	54/76 (71%)	54 (100%)	0	0	100	100
4	A4	231/269 (86%)	228 (99%)	3 (1%)	0	100	100
5	E5	154/171 (90%)	152 (99%)	2 (1%)	0	100	100
6	L6	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
7	F7	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
8	E9	197/200 (98%)	193 (98%)	4 (2%)	0	100	100
9	aA	51/60 (85%)	51 (100%)	0	0	100	100
10	MB	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
11	UC	94/219 (43%)	88 (94%)	6 (6%)	0	100	100
12	WD	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
13	XE	60/65 (92%)	60 (100%)	0	0	100	100
14	RF	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
15	FG	100/134 (75%)	97 (97%)	3 (3%)	0	100	100
16	VH	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
17	TI	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
18	fJ	53/93 (57%)	52 (98%)	1 (2%)	0	100	100
19	HK	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
20	OL	84/88 (96%)	79 (94%)	5 (6%)	0	100	100
21	MM	108/118 (92%)	104 (96%)	4 (4%)	0	100	100
22	PO	114/118 (97%)	114 (100%)	0	0	100	100
23	SP	78/91 (86%)	74 (95%)	4 (5%)	0	100	100
24	BQ	129/132 (98%)	128 (99%)	1 (1%)	0	100	100
25	GR	171/177 (97%)	170 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	GS	150/157 (96%)	149 (99%)	1 (1%)	0	100	100
27	CT	202/241 (84%)	199 (98%)	3 (2%)	0	100	100
28	KU	112/129 (87%)	110 (98%)	2 (2%)	0	100	100
29	NV	55/71 (78%)	55 (100%)	0	0	100	100
30	YW	54/59 (92%)	53 (98%)	1 (2%)	0	100	100
31	IX	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
32	JY	91/103 (88%)	86 (94%)	5 (6%)	0	100	100
33	QZ	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
34	Ba	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
35	Qb	101/103 (98%)	101 (100%)	0	0	100	100
36	Nc	111/116 (96%)	109 (98%)	2 (2%)	0	100	100
37	Kd	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
38	Je	120/122 (98%)	120 (100%)	0	0	100	100
39	Af	209/212 (99%)	202 (97%)	7 (3%)	0	100	100
40	Lg	135/137 (98%)	134 (99%)	1 (1%)	0	100	100
41	dh	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	3	22
42	Oi	113/130 (87%)	112 (99%)	1 (1%)	0	100	100
43	Pj	79/89 (89%)	79 (100%)	0	0	100	100
44	bk	47/51 (92%)	47 (100%)	0	0	100	100
45	Cl	270/274 (98%)	265 (98%)	5 (2%)	0	100	100
46	Dm	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
47	Sn	85/116 (73%)	85 (100%)	0	0	100	100
48	A	63/88 (72%)	61 (97%)	2 (3%)	0	100	100
48	To	84/88 (96%)	83 (99%)	1 (1%)	0	100	100
49	ep	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	5505/6229 (88%)	5391 (98%)	112 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	dh	32	ILE
41	dh	33	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	97/105 (92%)	96 (99%)	1 (1%)	73	87
2	C1	39/135 (29%)	39 (100%)	0	100	100
3	R3	51/67 (76%)	51 (100%)	0	100	100
4	A4	186/211 (88%)	185 (100%)	1 (0%)	86	93
5	E5	118/131 (90%)	118 (100%)	0	100	100
6	L6	102/103 (99%)	102 (100%)	0	100	100
7	F7	138/146 (94%)	138 (100%)	0	100	100
8	E9	159/159 (100%)	159 (100%)	0	100	100
9	aA	47/53 (89%)	47 (100%)	0	100	100
10	MB	101/102 (99%)	101 (100%)	0	100	100
11	UC	78/184 (42%)	78 (100%)	0	100	100
12	WD	67/71 (94%)	66 (98%)	1 (2%)	60	81
13	XE	54/57 (95%)	54 (100%)	0	100	100
14	RF	88/88 (100%)	88 (100%)	0	100	100
15	FG	92/121 (76%)	91 (99%)	1 (1%)	70	86
16	VH	58/62 (94%)	58 (100%)	0	100	100
17	TI	83/85 (98%)	83 (100%)	0	100	100
18	fJ	47/81 (58%)	47 (100%)	0	100	100
19	HK	87/88 (99%)	87 (100%)	0	100	100
20	OL	75/77 (97%)	75 (100%)	0	100	100
21	MM	91/99 (92%)	88 (97%)	3 (3%)	33	64
22	PO	88/90 (98%)	88 (100%)	0	100	100
23	SP	71/79 (90%)	71 (100%)	0	100	100
24	BQ	103/104 (99%)	103 (100%)	0	100	100
25	GR	147/151 (97%)	147 (100%)	0	100	100
26	GS	123/128 (96%)	123 (100%)	0	100	100

*Continued on next page...*

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	CT	167/198 (84%)	166 (99%)	1 (1%)	84	92
28	KU	84/98 (86%)	84 (100%)	0	100	100
29	NV	49/63 (78%)	49 (100%)	0	100	100
30	YW	50/52 (96%)	50 (100%)	0	100	100
31	IX	116/117 (99%)	116 (100%)	0	100	100
32	JY	84/90 (93%)	84 (100%)	0	100	100
33	QZ	73/84 (87%)	73 (100%)	0	100	100
34	Ba	37/37 (100%)	37 (100%)	0	100	100
35	Qb	89/89 (100%)	89 (100%)	0	100	100
36	Nc	81/85 (95%)	81 (100%)	0	100	100
37	Kd	107/110 (97%)	107 (100%)	0	100	100
38	Je	102/102 (100%)	102 (100%)	0	100	100
39	Af	161/162 (99%)	161 (100%)	0	100	100
40	Lg	114/114 (100%)	114 (100%)	0	100	100
41	dh	55/56 (98%)	55 (100%)	0	100	100
42	Oi	97/108 (90%)	97 (100%)	0	100	100
43	Pj	63/68 (93%)	63 (100%)	0	100	100
44	bk	42/46 (91%)	42 (100%)	0	100	100
45	Cl	218/221 (99%)	218 (100%)	0	100	100
46	Dm	177/181 (98%)	177 (100%)	0	100	100
47	Sn	75/97 (77%)	75 (100%)	0	100	100
48	A	39/69 (56%)	39 (100%)	0	100	100
48	To	66/69 (96%)	66 (100%)	0	100	100
49	ep	33/33 (100%)	33 (100%)	0	100	100
All	All	4569/5126 (89%)	4561 (100%)	8 (0%)	91	97

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	CT	127	ARG
21	MM	110	LYS
21	MM	59	GLN
15	FG	92	ARG
21	MM	92	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
9	aA	4	GLN
28	KU	118	HIS
39	Af	47	GLN
47	Sn	73	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	D8	114/115 (99%)	9 (7%)	0
51	iN	1498/1589 (94%)	291 (19%)	0
52	Z2	2698/2882 (93%)	344 (12%)	8 (0%)
All	All	4310/4586 (93%)	644 (14%)	8 (0%)

5 of 644 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	D8	13	A
50	D8	28	C
50	D8	33	U
50	D8	39	C
50	D8	50	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	Z2	2195	A
52	Z2	1856	U
52	Z2	1053	A
52	Z2	886	A
52	Z2	1580	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

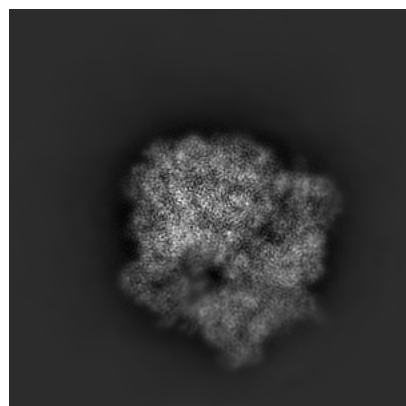
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52036. These allow visual inspection of the internal detail of the map and identification of artifacts.

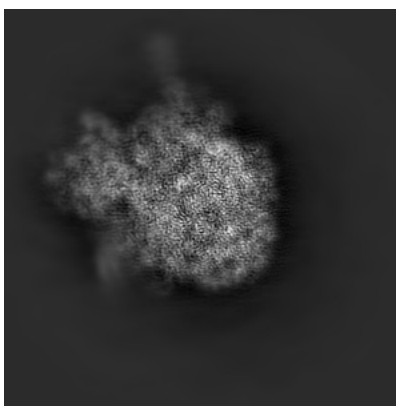
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

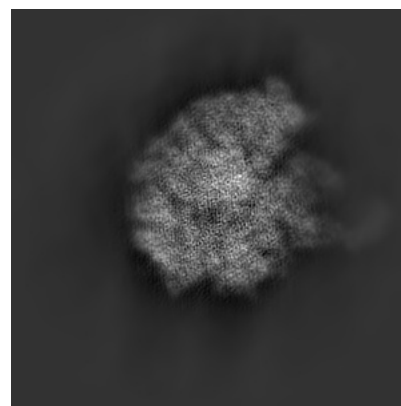
#### 6.1.1 Primary map



X

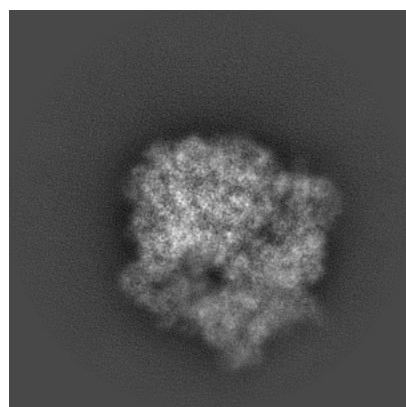


Y

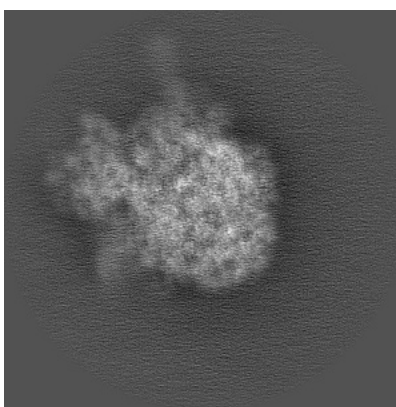


Z

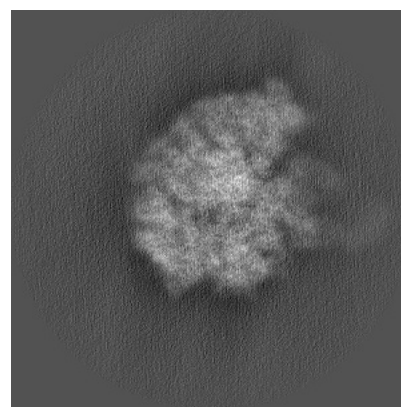
#### 6.1.2 Raw map



X



Y

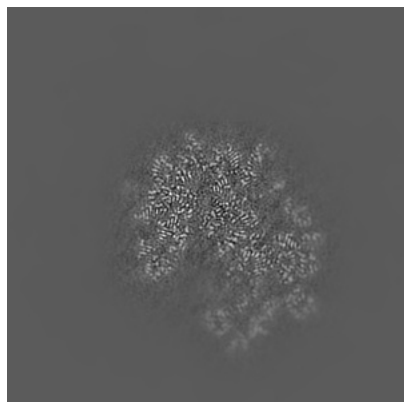


Z

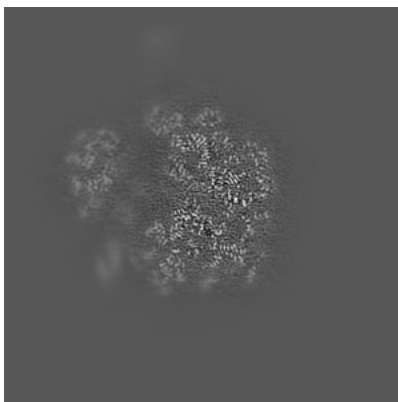
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

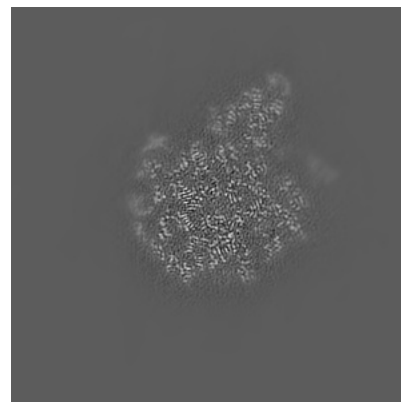
### 6.2.1 Primary map



X Index: 225

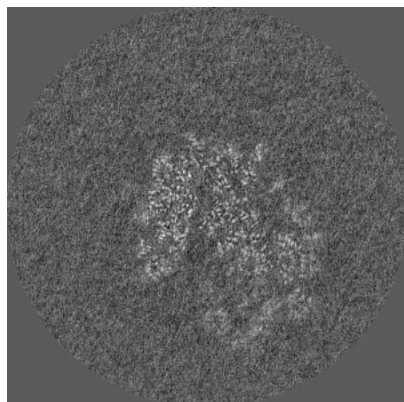


Y Index: 225

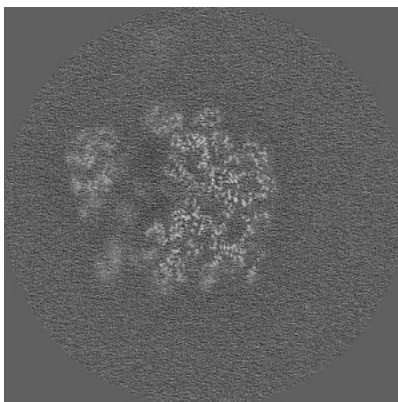


Z Index: 225

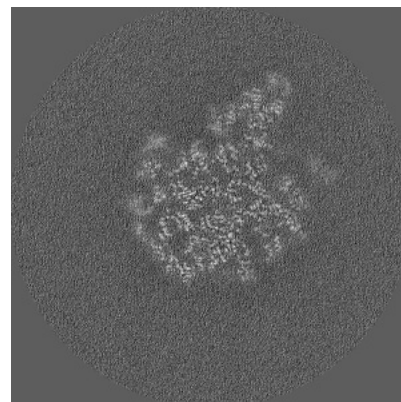
### 6.2.2 Raw map



X Index: 225



Y Index: 225

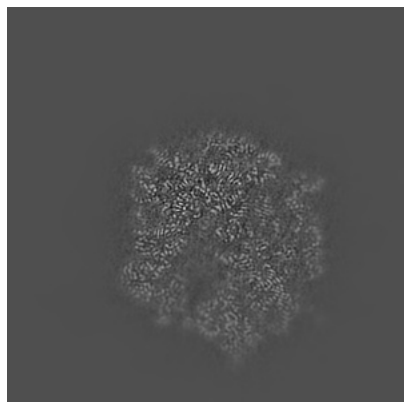


Z Index: 225

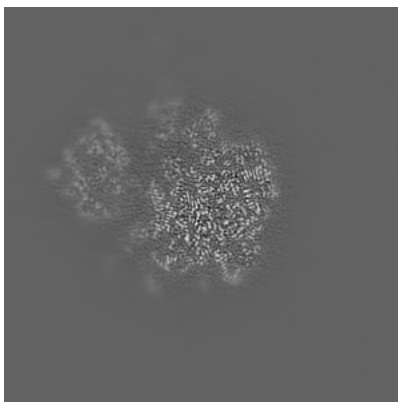
The images above show central slices of the map in three orthogonal directions.

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

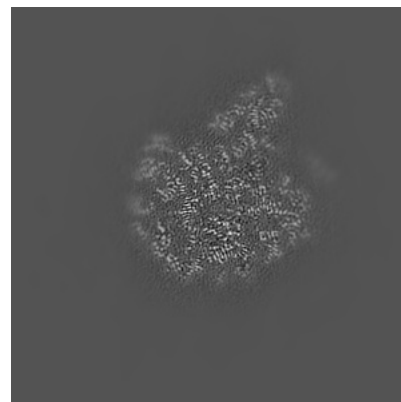
### 6.3.1 Primary map



X Index: 246

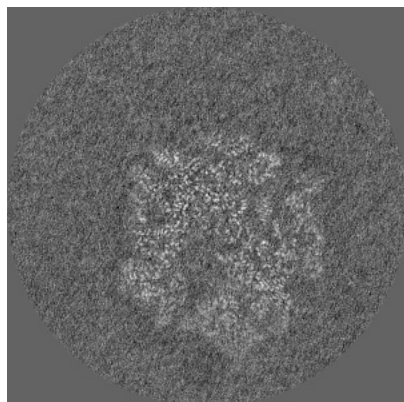


Y Index: 238

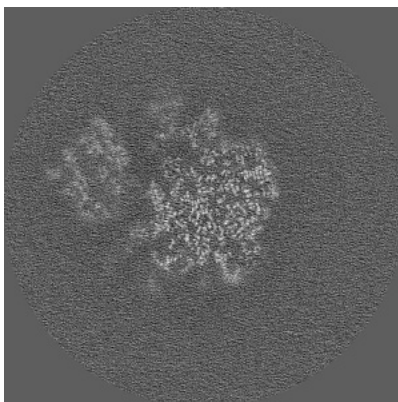


Z Index: 228

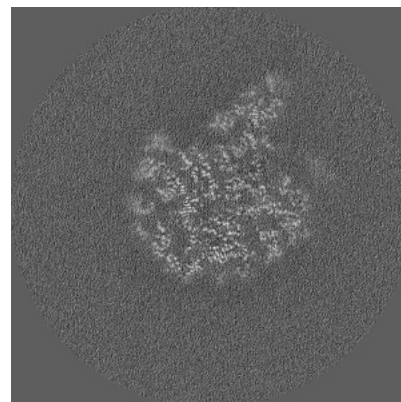
### 6.3.2 Raw map



X Index: 247



Y Index: 238



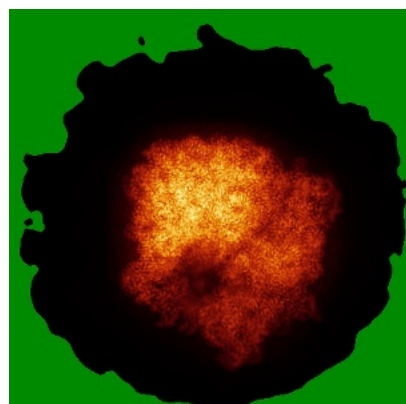
Z Index: 228

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

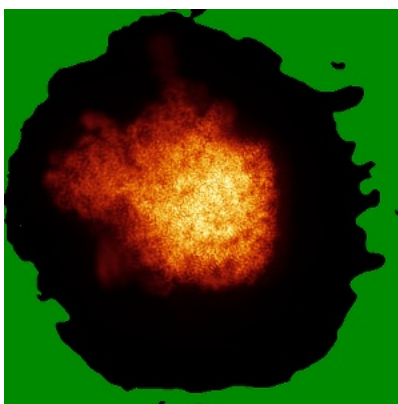


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

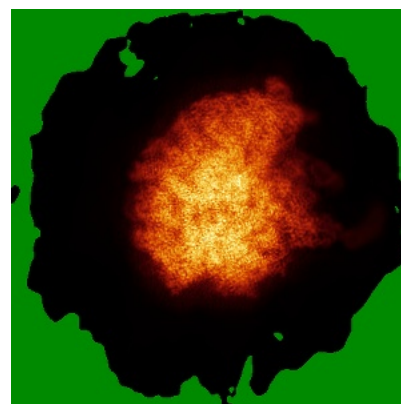
### 6.4.1 Primary map



X

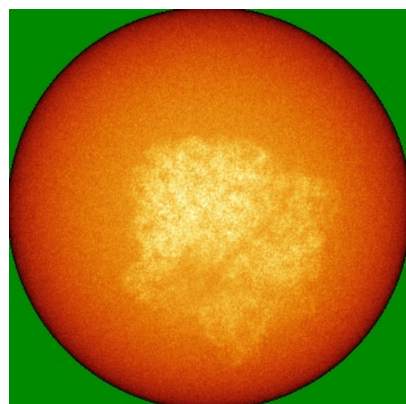


Y

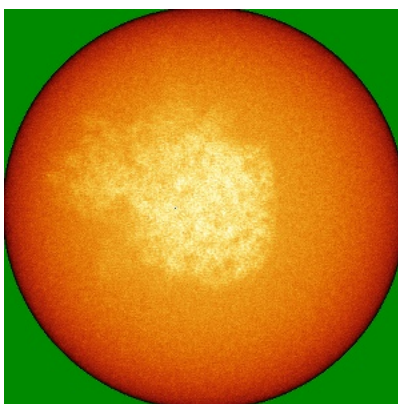


Z

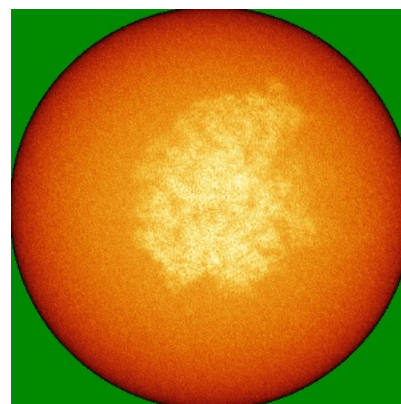
### 6.4.2 Raw map



X



Y



Z

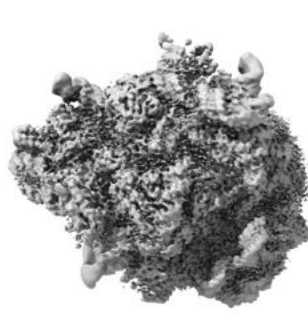
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

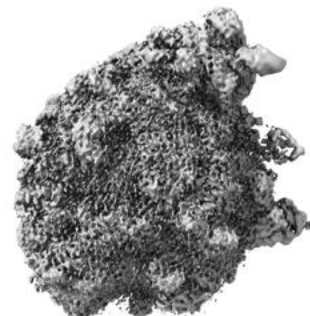
### 6.5.1 Primary map



X



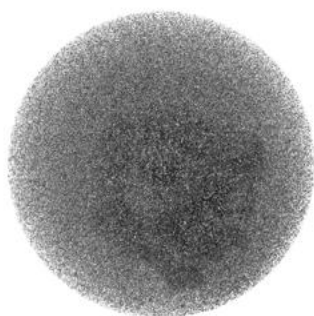
Y



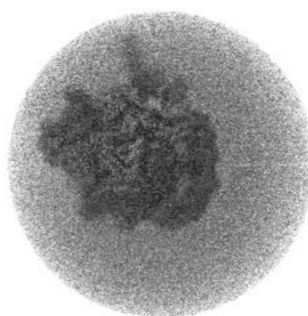
Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

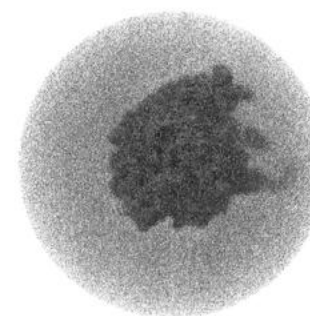
### 6.5.2 Raw map



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.

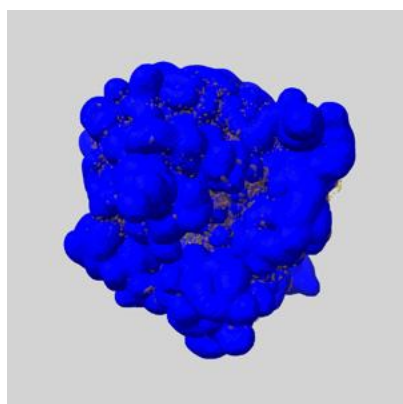
## 6.6 Mask visualisation [i](#)

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

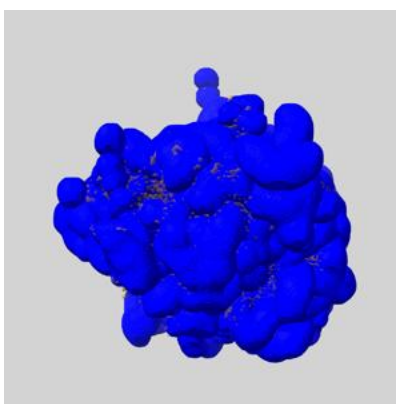
A mask typically either:

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

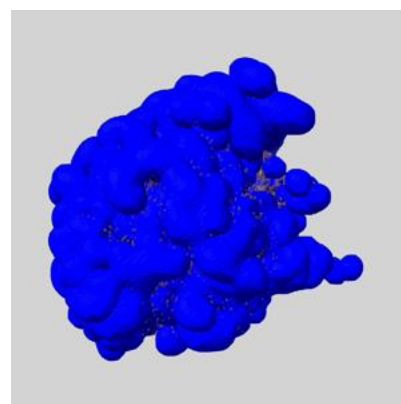
### 6.6.1 emd\_52036\_msk\_1.map [i](#)



X



Y



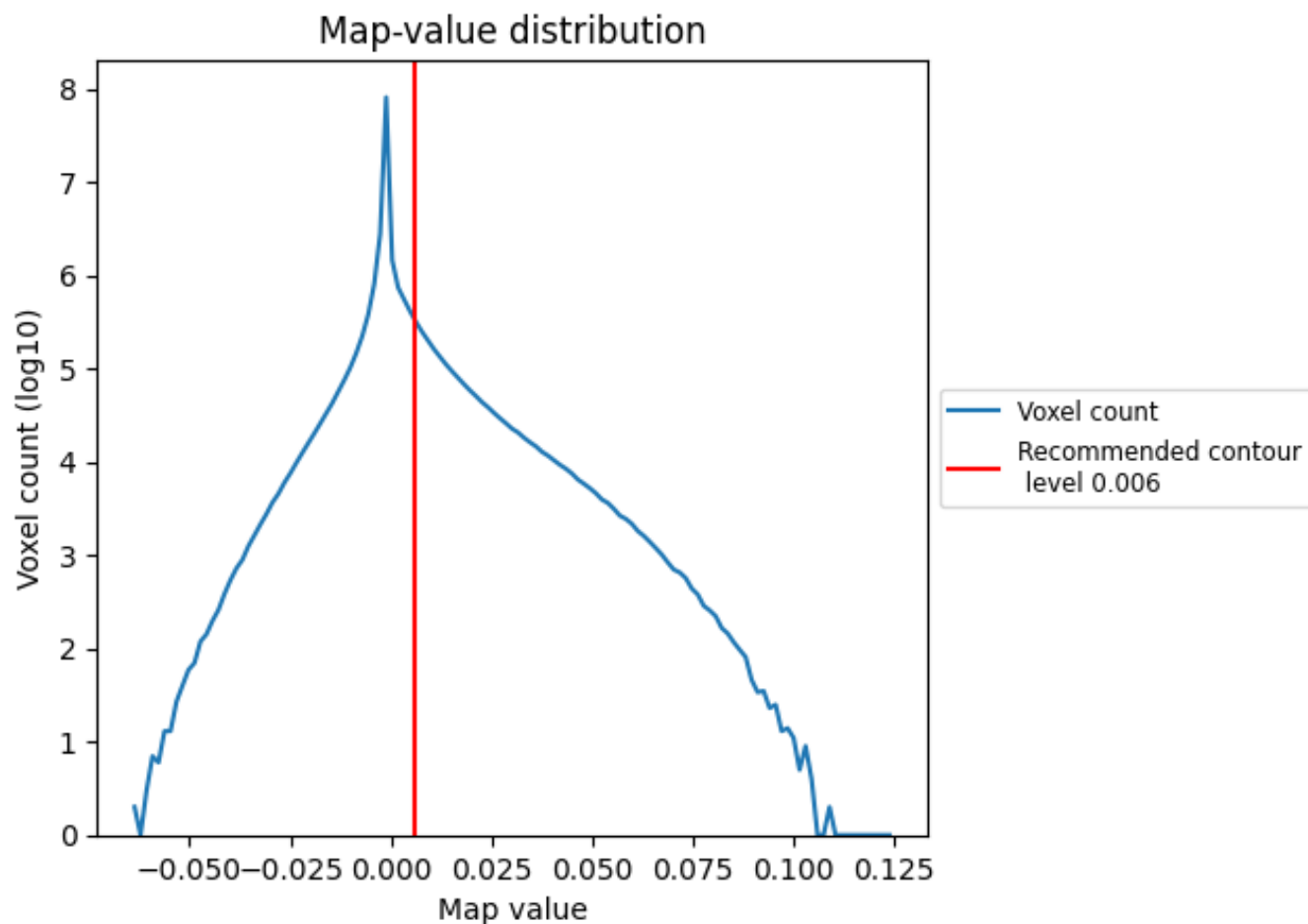
Z



## 7 Map analysis [i](#)

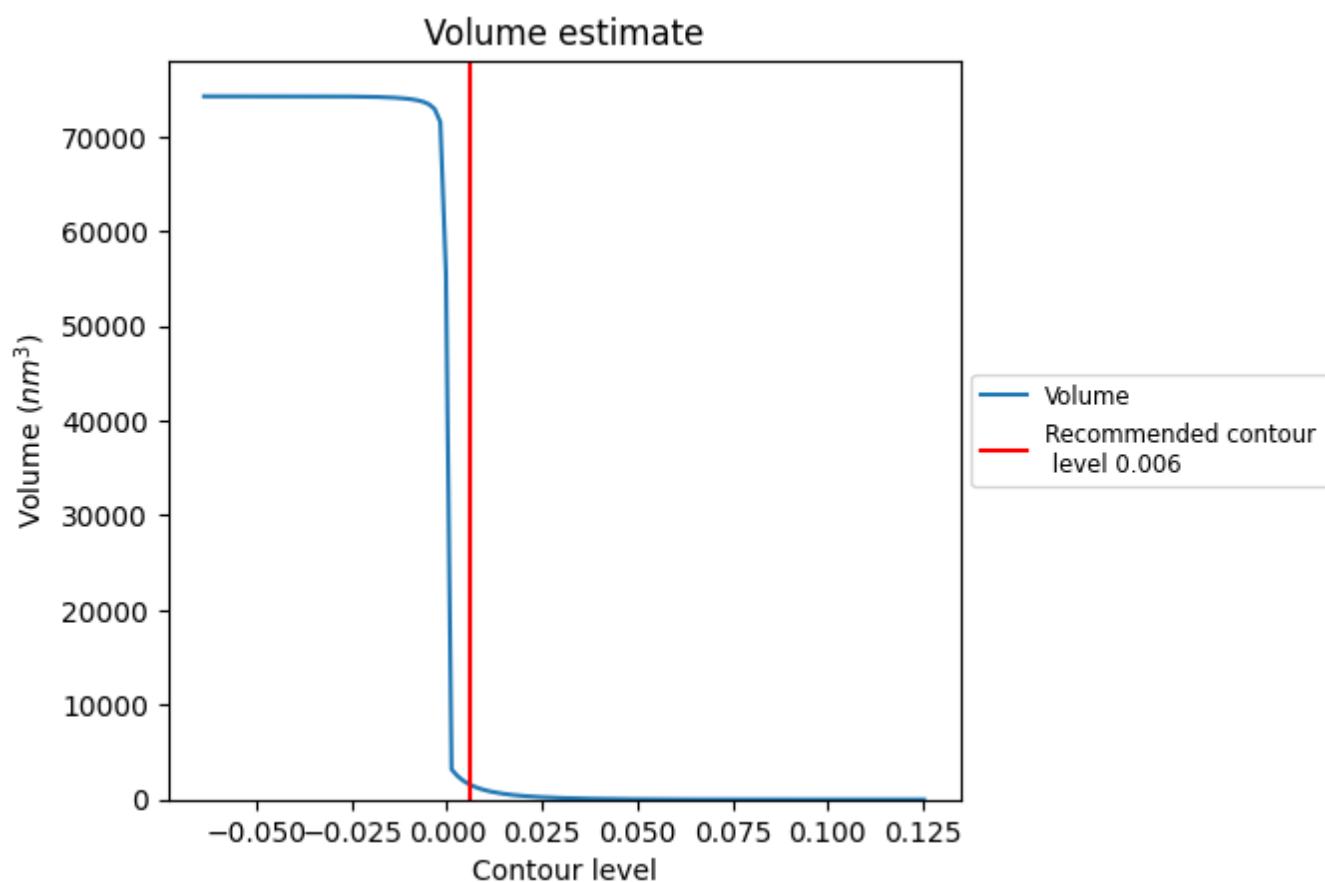
This section contains the results of statistical analysis of the map.

### 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.

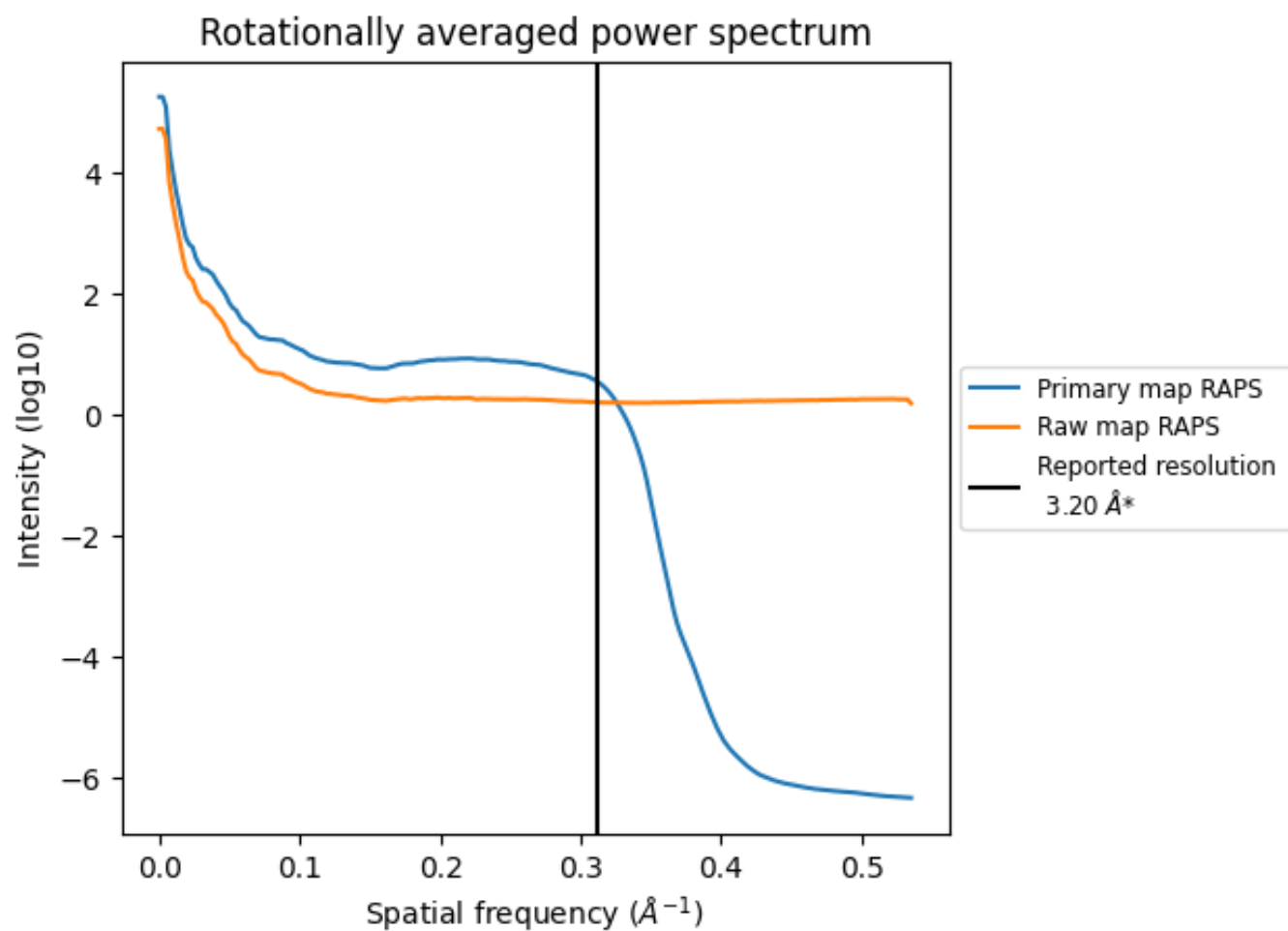
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1603  $\text{nm}^3$ ; this corresponds to an approximate mass of 1448 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 ⓘ

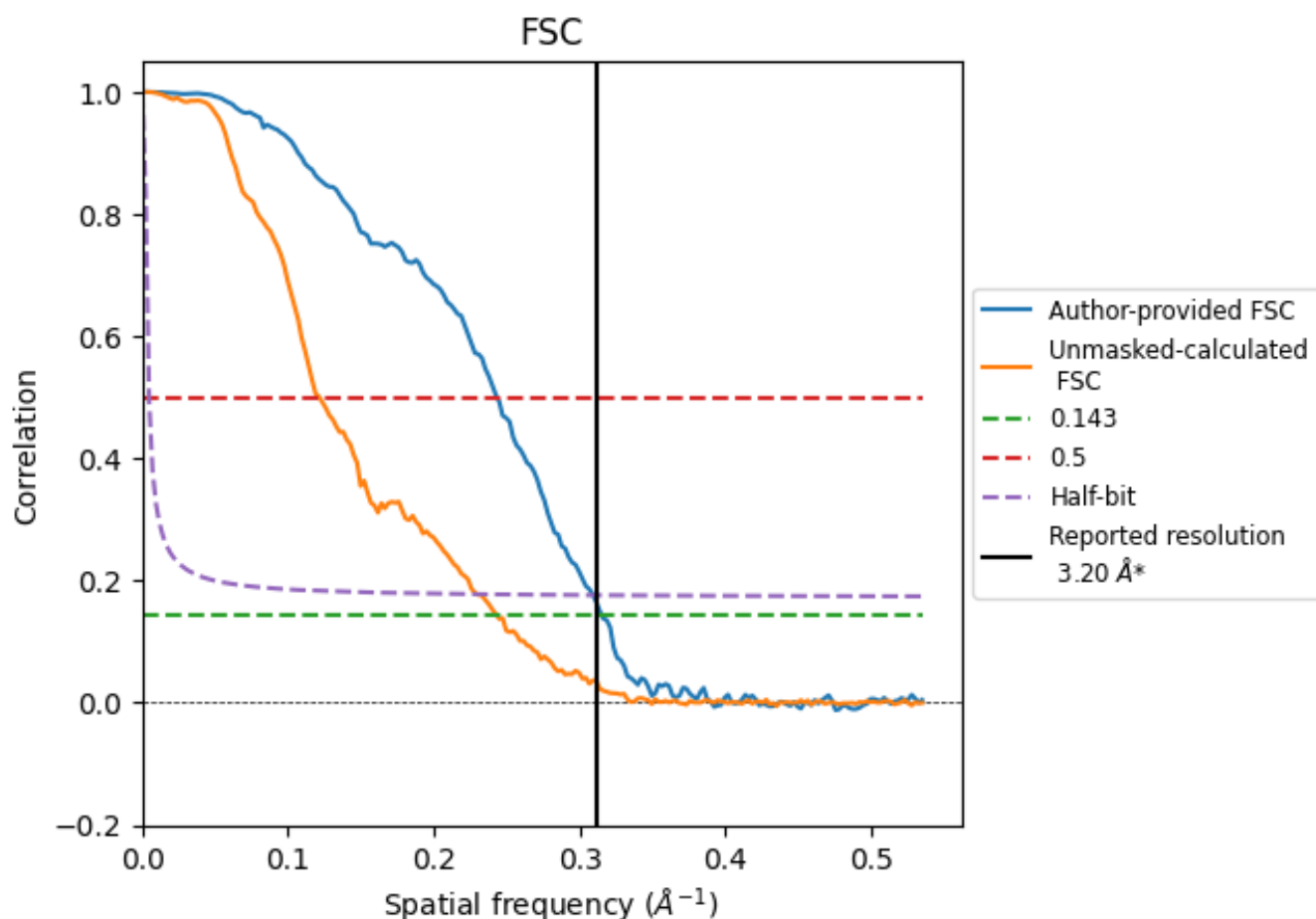


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 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 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

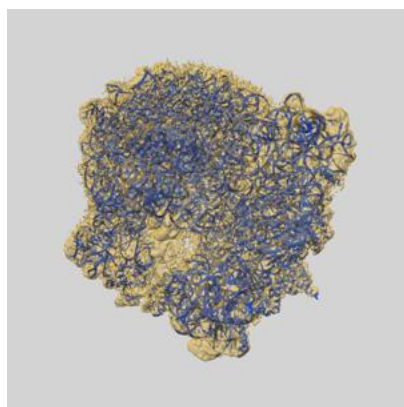
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	4.11	3.23
Unmasked-calculated*	4.11	8.22	4.35

\*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 4.11 differs from the reported value 3.2 by more than 10 %

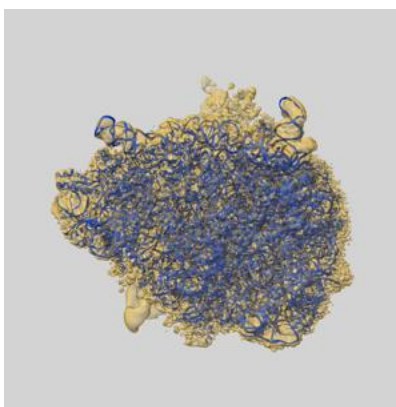
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52036 and PDB model 9HC4. Per-residue inclusion information can be found in section [3](#) on page [13](#).

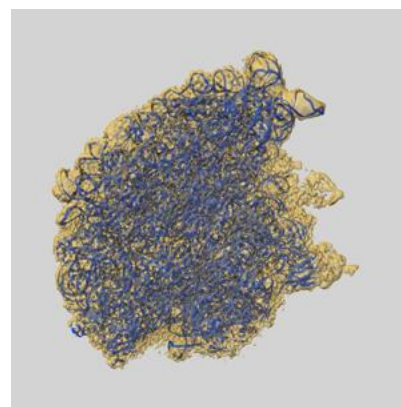
### 9.1 Map-model overlay [i](#)



X



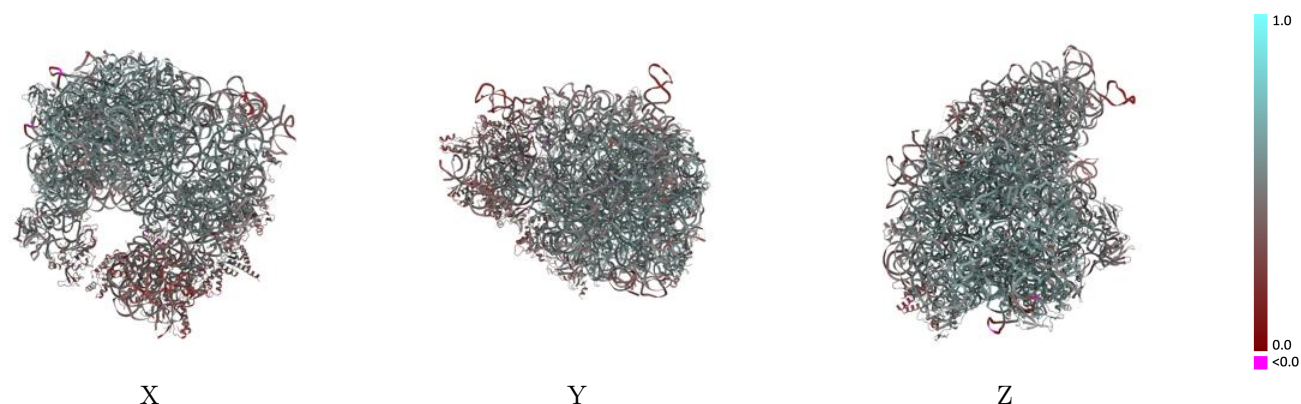
Y



Z

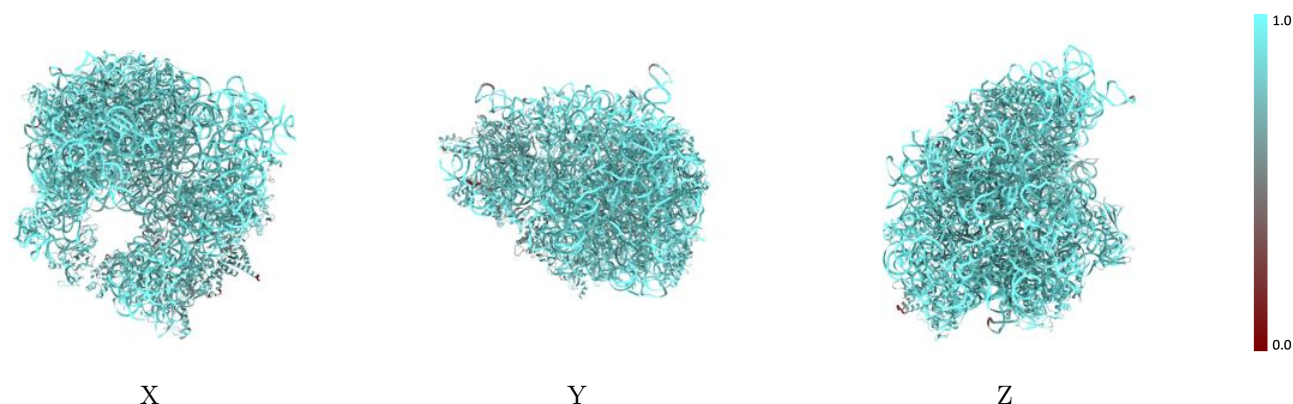
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



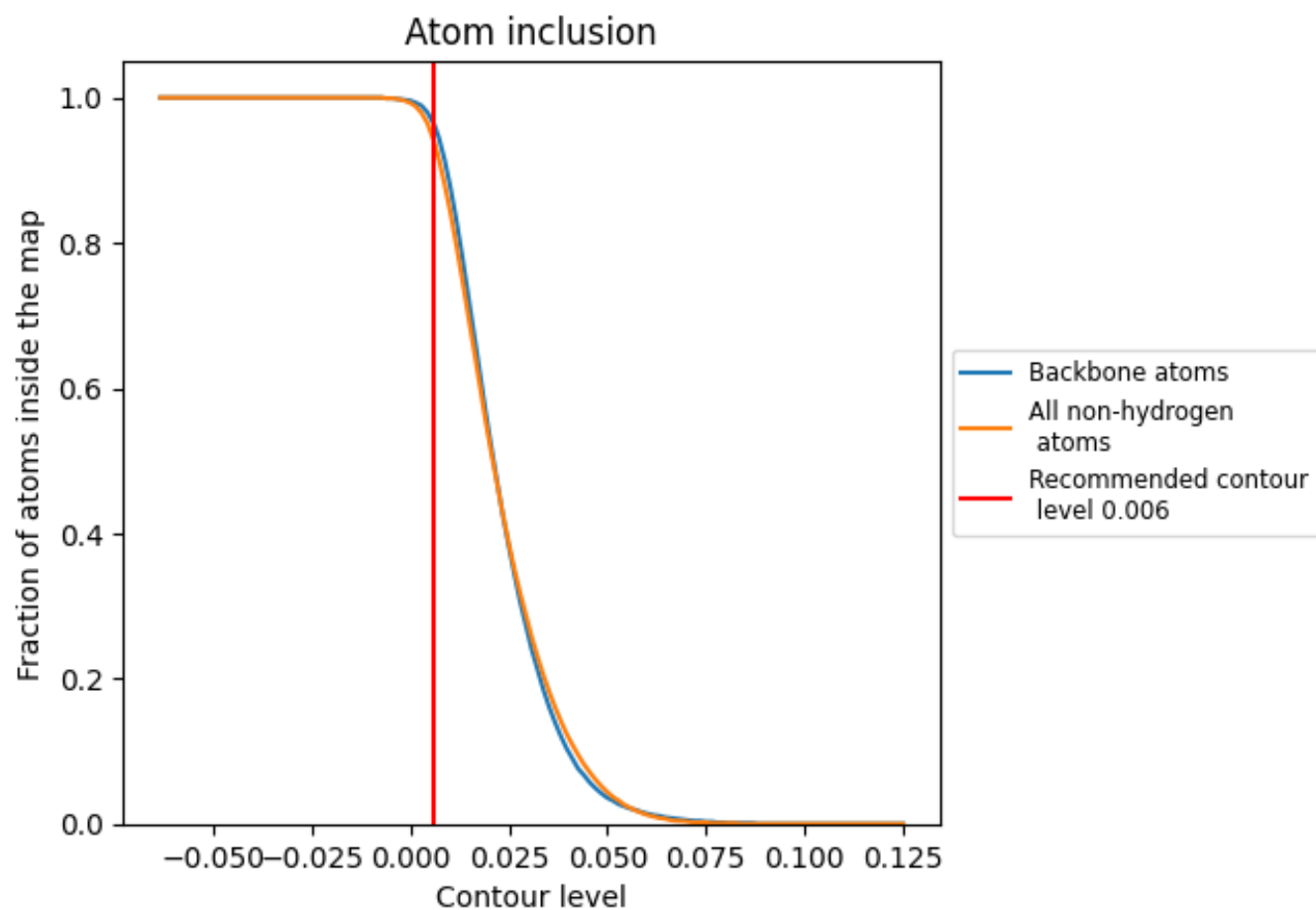
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.5020
A	 0.6920	 0.3280
A4	 0.7700	 0.3910
Af	 0.9350	 0.5330
BQ	 0.9070	 0.5050
Ba	 0.9370	 0.5390
C1	 0.8730	 0.4280
CT	 0.7810	 0.4000
Cl	 0.9240	 0.5250
D8	 0.9760	 0.4910
Dm	 0.8230	 0.4180
E5	 0.8620	 0.4570
E9	 0.9070	 0.5060
F	 0.8440	 0.3900
F7	 0.8270	 0.4080
FG	 0.8150	 0.4120
GR	 0.8750	 0.4530
GS	 0.7680	 0.3670
HK	 0.8270	 0.3970
IX	 0.9430	 0.5400
JY	 0.7660	 0.3800
Je	 0.8980	 0.5370
KU	 0.7800	 0.3960
Kd	 0.9260	 0.5280
L6	 0.8610	 0.5080
Lg	 0.8880	 0.5060
MB	 0.9610	 0.5480
MM	 0.7420	 0.3400
NV	 0.6300	 0.3370
Nc	 0.9240	 0.4890
OL	 0.8720	 0.4710
Oi	 0.8880	 0.4970
PO	 0.9600	 0.5520
Pj	 0.8840	 0.4650
QZ	 0.8700	 0.4660



*Continued on next page...*

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Chain	Atom inclusion	Q-score
Qb	 0.9140	 0.5170
R3	 0.8050	 0.4390
RF	 0.9410	 0.5400
SP	 0.7810	 0.3500
Sn	 0.9130	 0.5090
TI	 0.8810	 0.4480
To	 0.9040	 0.4700
UC	 0.9120	 0.5040
VH	 0.9350	 0.5520
WD	 0.9230	 0.5240
XE	 0.9180	 0.4640
YW	 0.9090	 0.5250
Z2	 0.9760	 0.5430
aA	 0.9220	 0.5040
bk	 0.9430	 0.5080
dh	 0.9260	 0.5120
ep	 0.9240	 0.5040
fJ	 0.8450	 0.3650
iN	 0.9640	 0.4800