



wwPDB EM Validation Summary Report ⓘ

Oct 30, 2025 – 06:38 PM EDT

PDB ID : 9NRI / pdb_00009nri
EMDB ID : EMD-49734
Title : Methanosarcina acetivorans 50S subunit obtained from acetate-grown cells
Authors : Ghosh, A.; Fordjour, G.N.R.; Armache, J.-P.; Ferry, J.G.; Murakami, K.S.; Bevilacqua, P.C.
Deposited on : 2025-03-14
Resolution : 2.85 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:

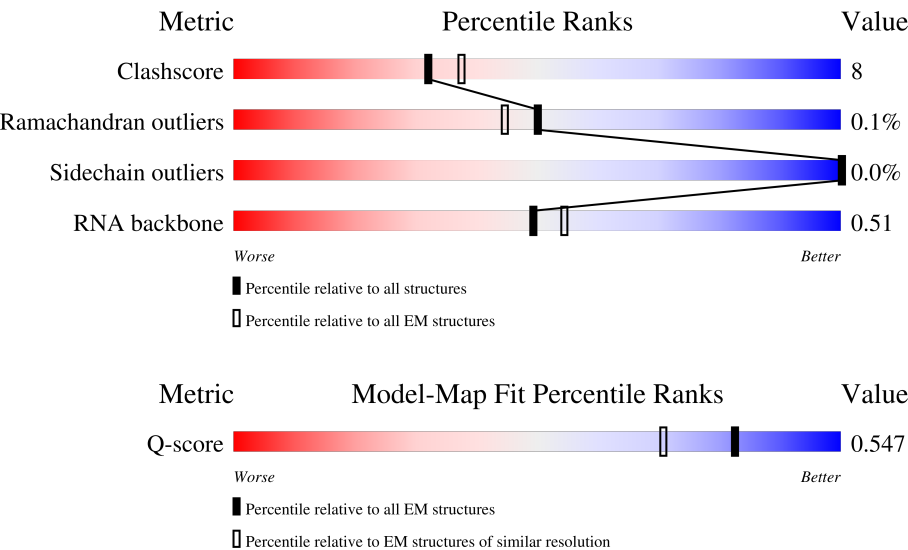
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

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 2.85 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	11965 (2.35 - 3.35)

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	BA	2899	
2	BB	129	
3	BC	238	





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Mol	Chain	Length	Quality of chain
4	BD	337	
5	BE	253	
6	BF	165	
7	BG	176	
8	BH	120	
9	BI	173	
10	BJ	143	
11	BK	132	
12	BL	140	
13	BM	196	
14	BN	174	
15	BO	126	
16	BP	151	
17	BQ	61	
18	BR	97	
19	BS	151	
20	BT	82	
21	BU	119	
22	BV	62	
23	BW	67	
24	BX	153	
25	BY	99	
26	BZ	89	
27	Ba	161	
28	Bb	94	

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Mol	Chain	Length	Quality of chain
29	Bc	56	 93% 7%
30	Bd	51	 75% 25%
31	Be	52	 10% 52% 33% 15%
32	Bf	92	 5% 70% 30%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 126100 atoms, of which 30897 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	BA	2884	Total	C	H	N	O	P	0	0
			92622	27552	30897	11225	20065	2883		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BB	128	Total	C	N	O	P	0	0
			2720	1214	481	897	128		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	BC	238	Total	C	N	O	S	0	0
			1808	1129	350	321	8		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	BD	337	Total	C	N	O	S	0	0
			2597	1639	474	476	8		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BE	252	Total	C	N	O	S	0	0
			1930	1208	368	353	1		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BF	165	Total	C	N	O	S	0	0
			1289	812	234	235	8		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BG	176	Total	C	N	O	S	0	0
			1371	876	235	254	6		

- Molecule 8 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BH	115	Total	C	N	O	S	0	0
			857	541	144	170	2		

- Molecule 9 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BI	159	Total	C	N	O	S	0	0
			1261	794	240	218	9		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	138	Total	C	N	O	S	0	0
			1086	683	200	199	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BK	132	Total	C	N	O	S	0	0
			999	623	185	182	9		

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BL	140	Total	C	N	O	S	0	0
			1058	643	204	205	6		

- Molecule 13 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BM	196	Total	C	N	O	S	0	0
			1593	986	329	273	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BN	174	Total	C	N	O	S	0	0
			1356	853	242	259	2		

- Molecule 15 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BO	126	Total	C	N	O	S	0	0
			962	608	173	178	3		

- Molecule 16 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BP	151	Total	C	N	O	S	0	0
			1195	739	242	210	4		

- Molecule 17 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	BQ	57	Total	C	N	O	0	0
			457	289	79	89		

- Molecule 18 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BR	96	Total	C	N	O	S	0	0
			766	475	146	141	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BS	151	Total	C	N	O	S	0	0
			1169	729	218	212	10		

- Molecule 20 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BT	82	Total	C	N	O	S	0	0
			656	418	108	122	8		

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BU	119	Total	C	N	O	S	0	0
			910	564	170	169	7		

- Molecule 22 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BV	62	Total	C	N	O	S	0	0
			499	316	88	87	8		

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BW	67	Total	C	N	O	S	0	0
			532	321	103	106	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BX	153	Total	C	N	O	S	0	0
			1237	779	230	222	6		

- Molecule 25 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BY	92	Total	C	N	O	S	0	0
			658	415	108	131	4		

- Molecule 26 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BZ	86	Total	C	N	O	S	0	0
			703	446	131	123	3		

- Molecule 27 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ba	132	Total	C	N	O	S	0	0
			1028	645	197	184	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ba	-2	MET	-	conflict	UNP A0A832W8Z7
Ba	-1	ILE	-	conflict	UNP A0A832W8Z7
Ba	0	MET	-	conflict	UNP A0A832W8Z7

- Molecule 28 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Bb	94	Total	C	N	O	S	0	0
			736	459	145	125	7		

- Molecule 29 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Bc	56	Total	C	N	O	S	0	0
			445	269	92	76	8		

- Molecule 30 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	51	Total	C	N	O	S	0	0
			439	272	101	64	2		

- Molecule 31 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Be	44	Total	C	N	O	S	0	0
			353	215	74	59	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	-2	MET	-	conflict	UNP Q8TJ19
Be	-1	THR	-	conflict	UNP Q8TJ19
Be	0	LYS	-	conflict	UNP Q8TJ19

- Molecule 32 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	92	Total	C	N	O	S	0	0
			760	480	151	122	7		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	BA	42	Total 42	Mg 42	0
33	Bc	1	Total 1	Mg 1	0

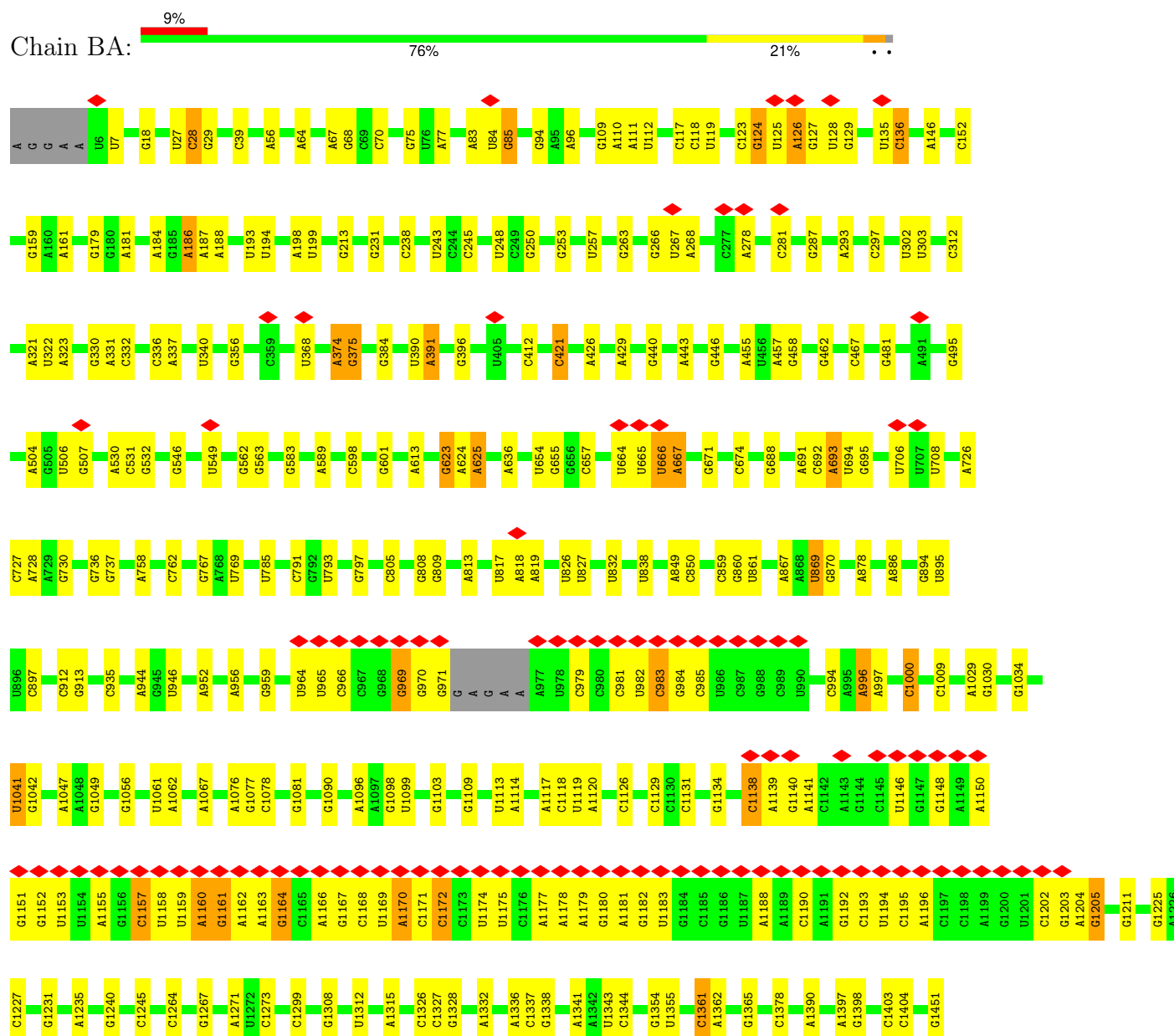
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	BV	1	Total 1	Zn 1	0
34	Bb	1	Total 1	Zn 1	0
34	Bc	1	Total 1	Zn 1	0
34	Be	1	Total 1	Zn 1	0
34	Bf	1	Total 1	Zn 1	0

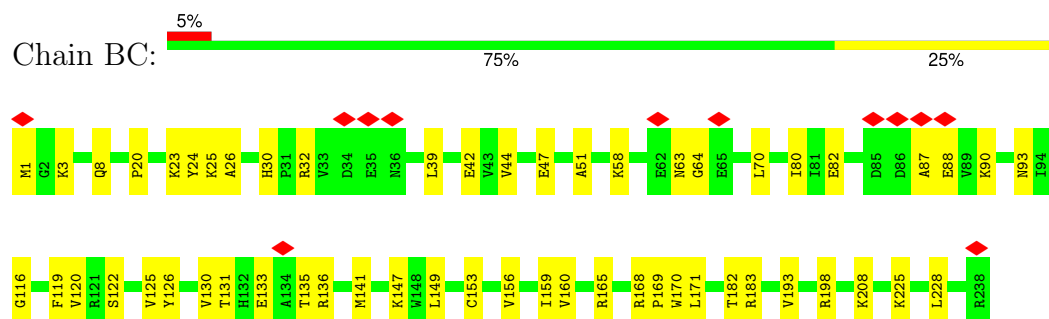
3 Residue-property plots

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.

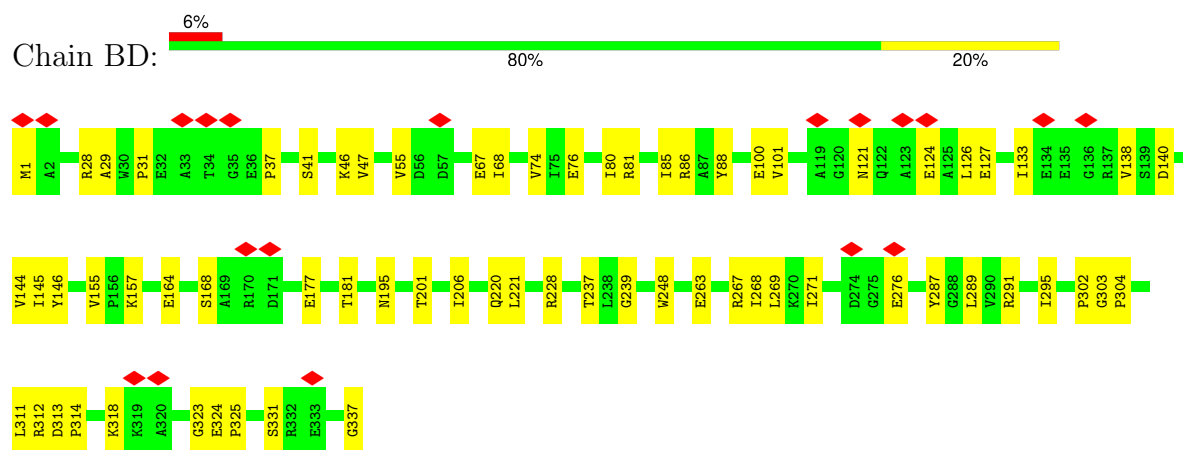
• Molecule 1: 23S rRNA



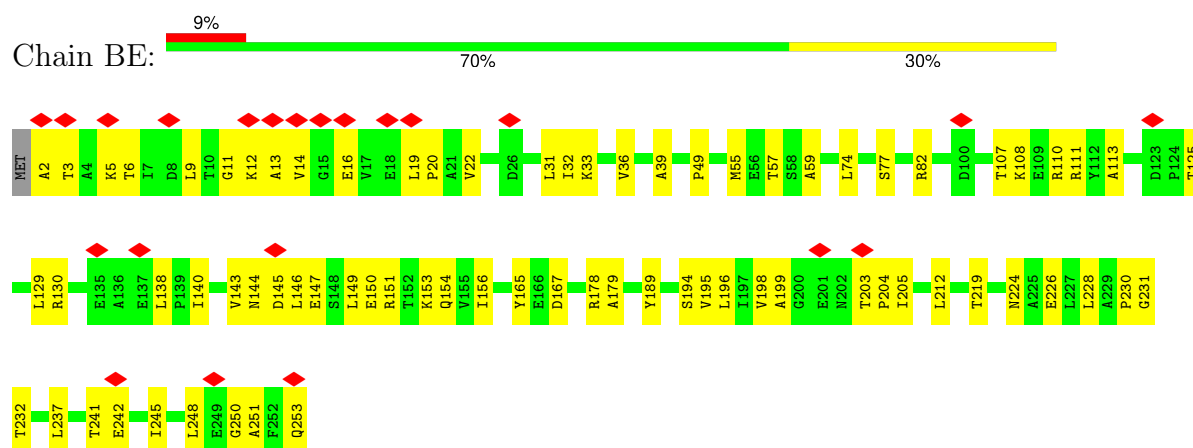
- Molecule 3: Large ribosomal subunit protein uL2



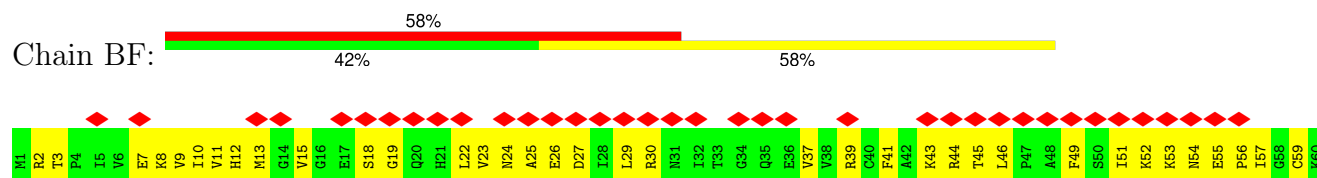
- Molecule 4: Large ribosomal subunit protein uL3

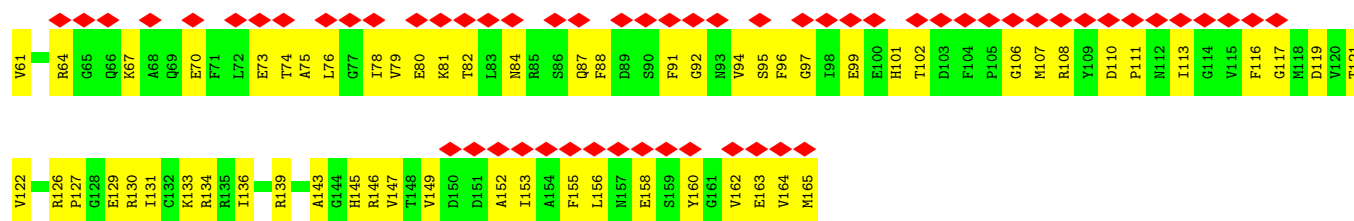


- Molecule 5: Large ribosomal subunit protein uL4

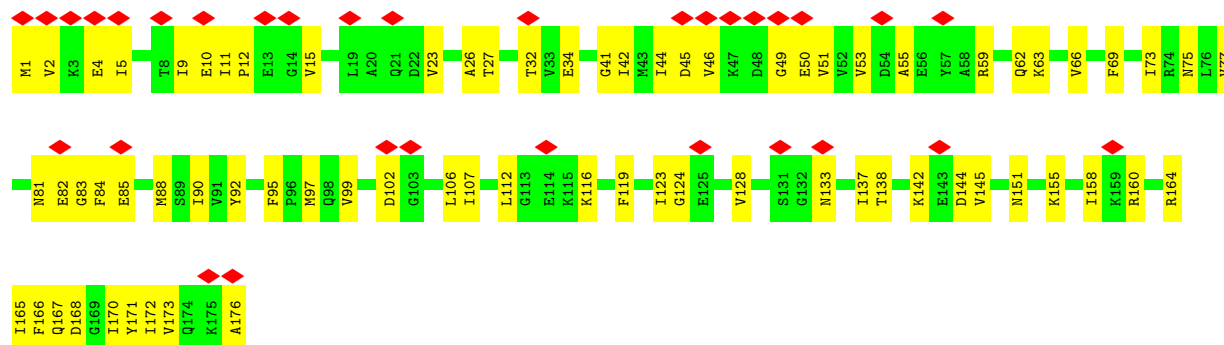


- Molecule 6: Large ribosomal subunit protein uL5

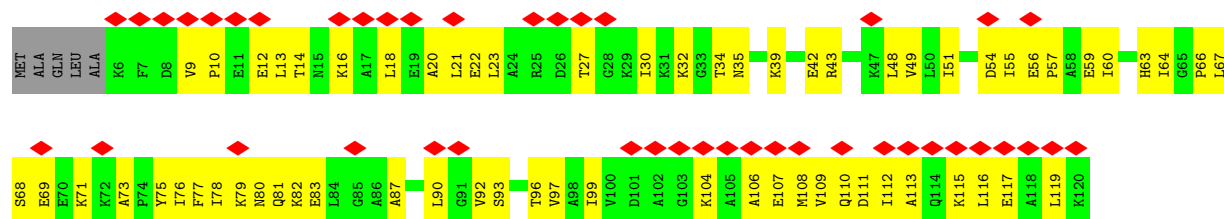




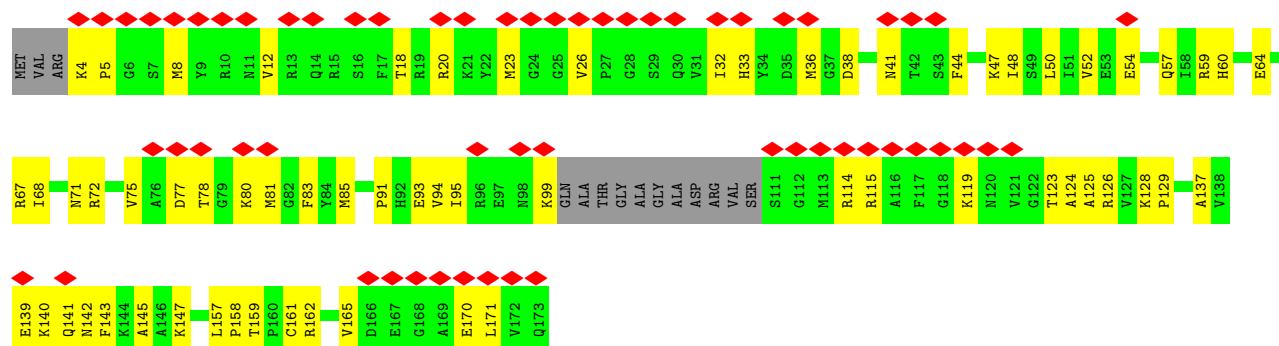
• Molecule 7: Large ribosomal subunit protein uL6



• Molecule 8: Large ribosomal subunit protein eL8

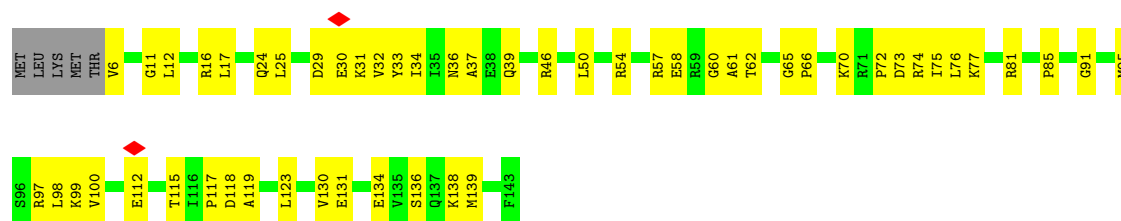


• Molecule 9: Large ribosomal subunit protein uL16




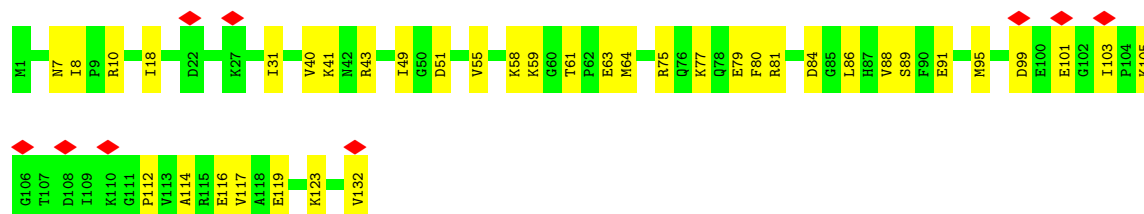
• Molecule 10: Large ribosomal subunit protein uL13

Chain BJ: 



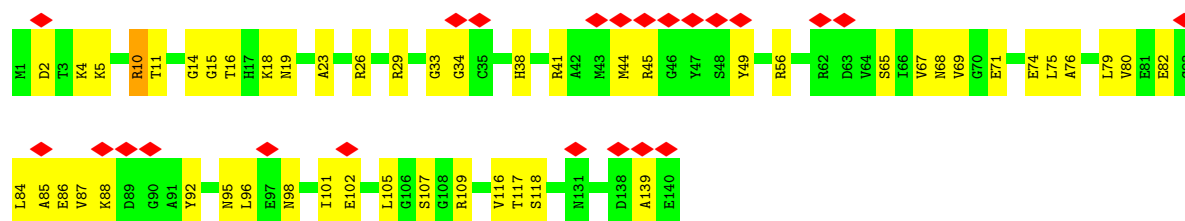
- Molecule 11: Large ribosomal subunit protein uL14

Chain BK: 




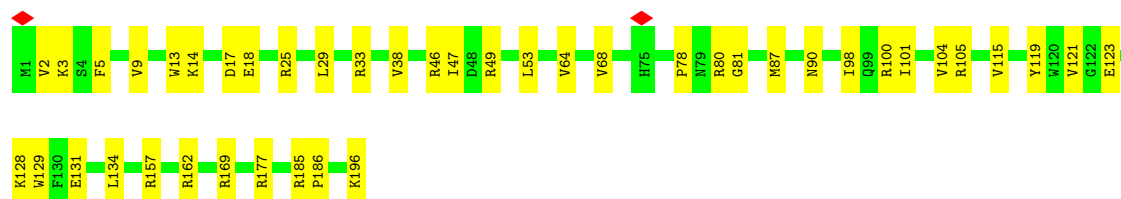
- Molecule 12: Large ribosomal subunit protein uL15

Chain BL: 



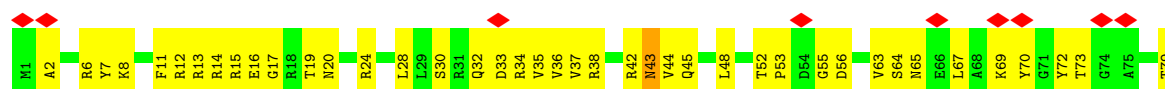
- Molecule 13: Large ribosomal subunit protein eL15

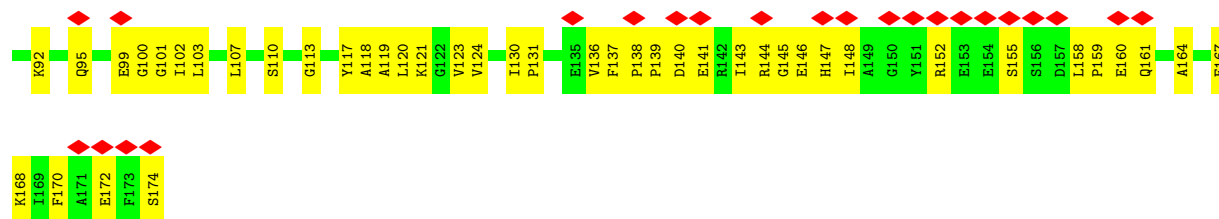
Chain BM: 



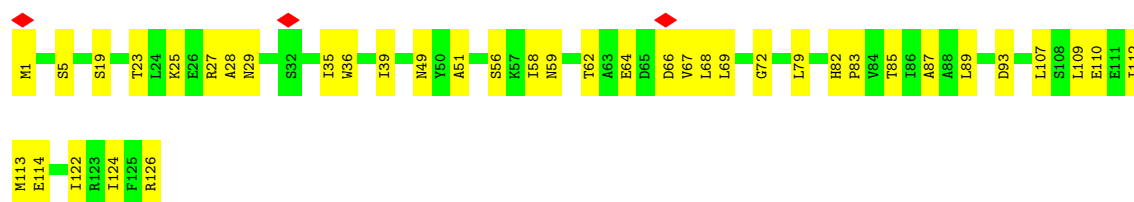
- Molecule 14: Large ribosomal subunit protein uL18

Chain BN: 

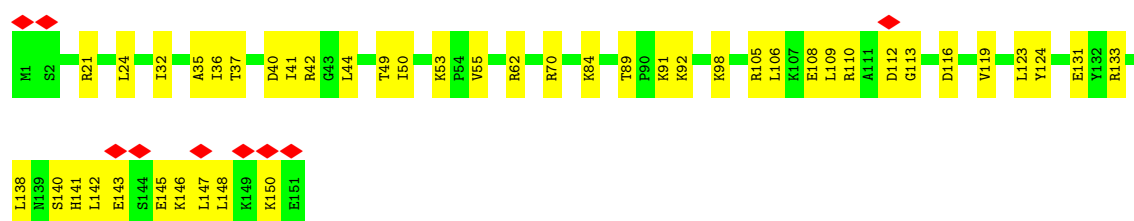
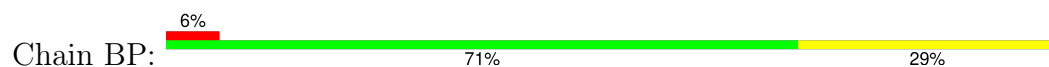




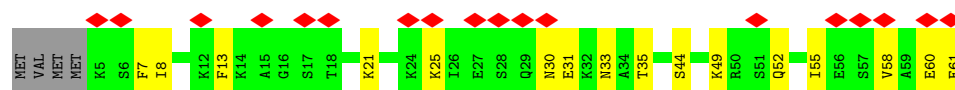
- Molecule 15: Large ribosomal subunit protein eL18



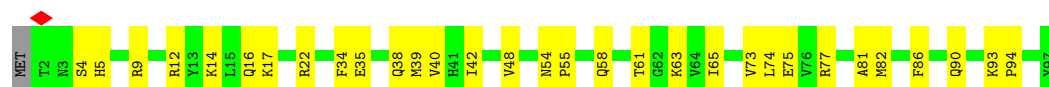
- Molecule 16: Large ribosomal subunit protein eL19



- Molecule 17: Large ribosomal subunit protein eL20

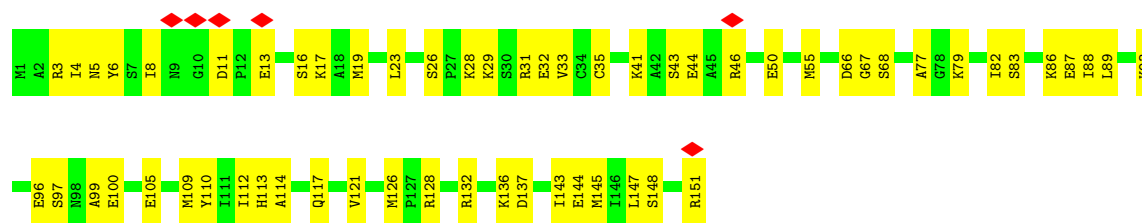


- Molecule 18: Large ribosomal subunit protein eL21



- Molecule 19: Large ribosomal subunit protein uL22

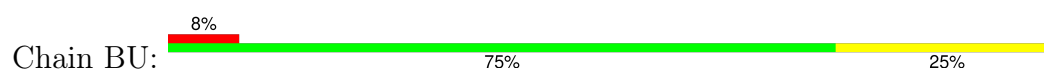




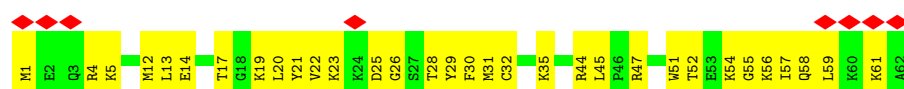
- Molecule 20: Large ribosomal subunit protein uL23



- Molecule 21: Large ribosomal subunit protein uL24



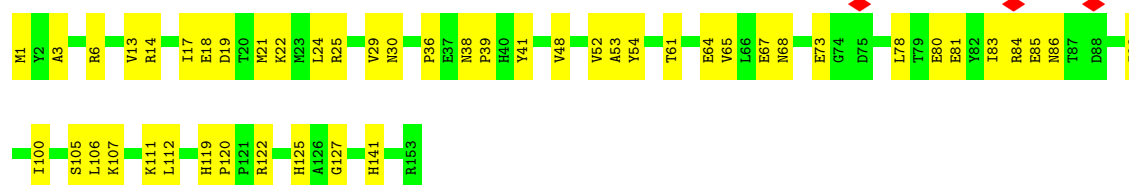
- Molecule 22: Large ribosomal subunit protein eL24



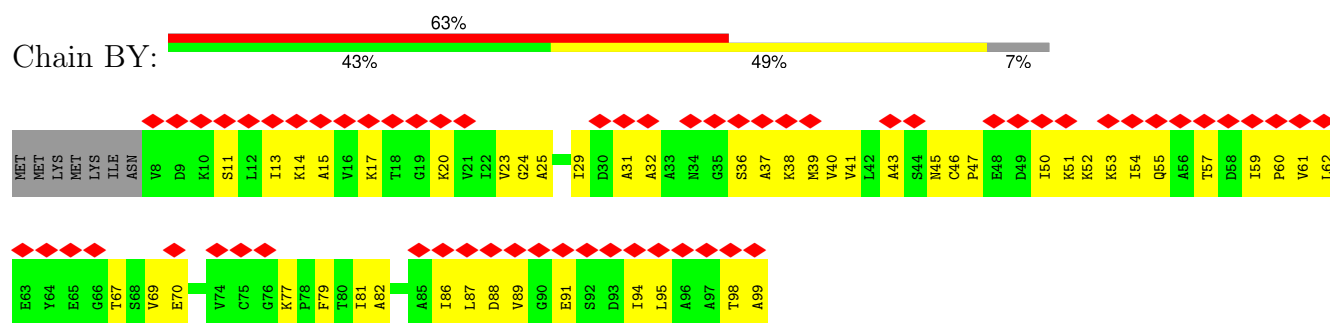
- Molecule 23: Large ribosomal subunit protein uL29



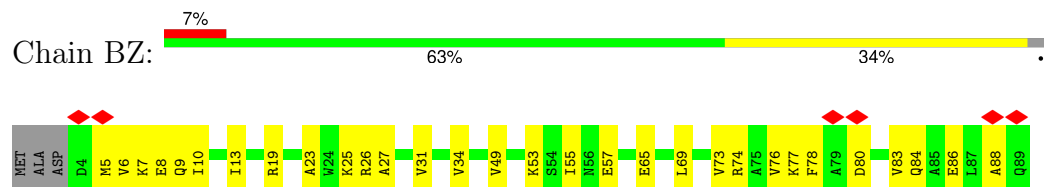
- Molecule 24: Large ribosomal subunit protein uL30



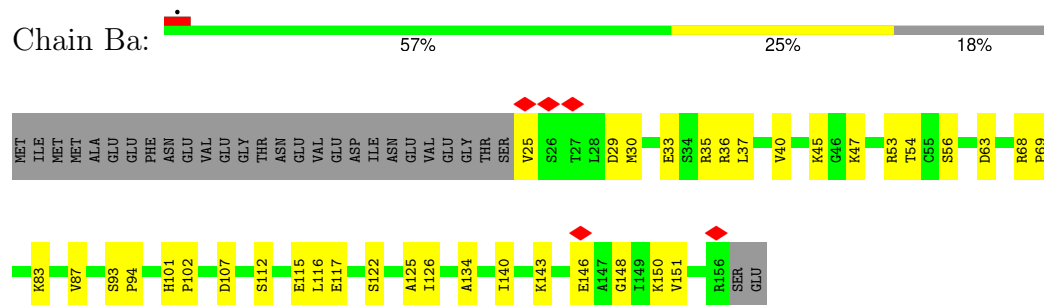
- Molecule 25: Large ribosomal subunit protein eL30



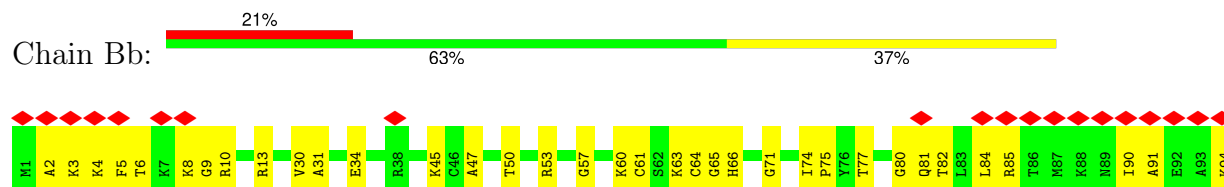
- Molecule 26: Large ribosomal subunit protein eL31



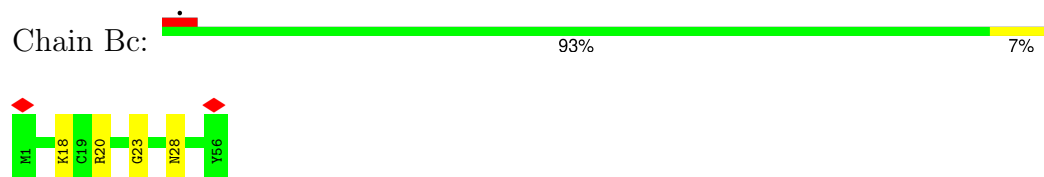
- Molecule 27: Large ribosomal subunit protein eL32



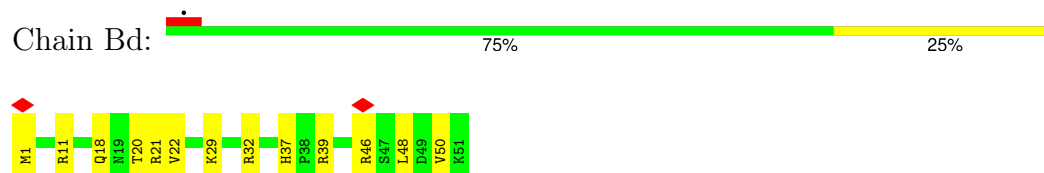
- Molecule 28: Large ribosomal subunit protein eL43



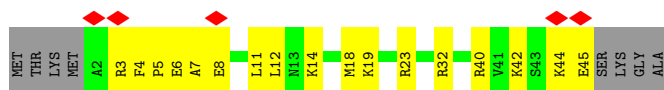
- Molecule 29: Large ribosomal subunit protein eL37



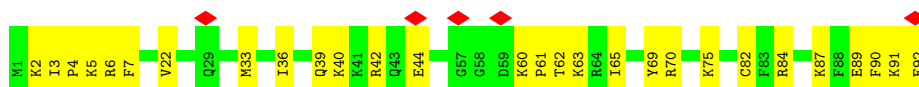
- Molecule 30: Large ribosomal subunit protein eL39



- Molecule 31: Large ribosomal subunit protein eL40



- Molecule 32: Large ribosomal subunit protein eL42



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.790	Depositor
Minimum map value	-0.426	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, ZN, MG, OMG, G7M

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	BA	0.30	0/69006	0.35	0/107607
2	BB	0.19	0/3037	0.26	0/4728
3	BC	0.26	0/1850	0.35	0/2497
4	BD	0.25	0/2646	0.30	0/3569
5	BE	0.25	0/1964	0.37	0/2654
6	BF	0.14	0/1310	0.36	0/1762
7	BG	0.17	0/1392	0.30	0/1870
8	BH	0.17	0/864	0.36	0/1161
9	BI	0.18	0/1284	0.33	0/1719
10	BJ	0.25	0/1101	0.38	0/1474
11	BK	0.23	0/1010	0.37	0/1355
12	BL	0.23	0/1071	0.39	0/1425
13	BM	0.28	0/1625	0.36	0/2176
14	BN	0.17	0/1382	0.33	0/1863
15	BO	0.25	0/975	0.37	0/1312
16	BP	0.24	0/1209	0.35	0/1602
17	BQ	0.18	0/464	0.33	0/614
18	BR	0.25	0/780	0.32	0/1042
19	BS	0.24	0/1189	0.36	0/1588
20	BT	0.21	0/664	0.35	0/884
21	BU	0.22	0/919	0.35	0/1227
22	BV	0.23	0/508	0.32	0/670
23	BW	0.19	0/534	0.35	0/716
24	BX	0.26	0/1259	0.34	0/1692
25	BY	0.13	0/663	0.28	0/897
26	BZ	0.22	0/715	0.34	0/960
27	Ba	0.29	0/1044	0.37	0/1397
28	Bb	0.22	0/749	0.36	0/997
29	Bc	0.36	0/452	0.36	0/593
30	Bd	0.30	0/448	0.42	0/595
31	Be	0.21	0/355	0.34	0/468
32	Bf	0.24	0/777	0.36	0/1029

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.28	0/103246	0.34	0/154143

There are no bond length outliers.

There are no bond angle outliers.

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	BA	61725	30897	31122	240	0
2	BB	2720	0	1382	68	0
3	BC	1808	0	1842	45	0
4	BD	2597	0	2692	44	0
5	BE	1930	0	1989	54	0
6	BF	1289	0	1317	108	0
7	BG	1371	0	1426	72	0
8	BH	857	0	898	69	0
9	BI	1261	0	1300	62	0
10	BJ	1086	0	1135	44	0
11	BK	999	0	1059	33	0
12	BL	1058	0	1044	42	0
13	BM	1593	0	1637	36	0
14	BN	1356	0	1358	79	0
15	BO	962	0	1021	32	0
16	BP	1195	0	1277	39	0
17	BQ	457	0	463	13	0
18	BR	766	0	777	29	0
19	BS	1169	0	1211	54	0
20	BT	656	0	688	25	0
21	BU	910	0	972	27	0
22	BV	499	0	515	29	0
23	BW	532	0	547	20	0
24	BX	1237	0	1269	38	0
25	BY	658	0	696	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	BZ	703	0	735	24	0
27	Ba	1028	0	1079	31	0
28	Bb	736	0	771	34	0
29	Bc	445	0	455	4	0
30	Bd	439	0	479	16	0
31	Be	353	0	374	18	0
32	Bf	760	0	797	29	0
33	BA	42	0	0	0	0
33	Bc	1	0	0	0	0
34	BV	1	0	0	0	0
34	Bb	1	0	0	0	0
34	Bc	1	0	0	0	0
34	Be	1	0	0	0	0
34	Bf	1	0	0	0	0
All	All	95203	30897	64327	1324	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 8.

The worst 5 of 1324 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BI:4:LYS:HD2	9:BI:8:MET:HE1	1.42	1.00
15:BO:35:ILE:HD11	15:BO:124:ILE:HD11	1.44	1.00
27:Ba:25:VAL:HG11	27:Ba:150:LYS:HB2	1.44	0.97
3:BC:42:GLU:HB3	3:BC:80:ILE:HG22	1.44	0.97
8:BH:23:LEU:HB3	8:BH:104:LYS:HE3	1.47	0.97

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	
3	BC	236/238 (99%)	223 (94%)	12 (5%)	1 (0%)	30	49
4	BD	335/337 (99%)	319 (95%)	16 (5%)	0	100	100
5	BE	250/253 (99%)	237 (95%)	13 (5%)	0	100	100
6	BF	163/165 (99%)	147 (90%)	16 (10%)	0	100	100
7	BG	174/176 (99%)	161 (92%)	13 (8%)	0	100	100
8	BH	113/120 (94%)	102 (90%)	11 (10%)	0	100	100
9	BI	155/173 (90%)	145 (94%)	10 (6%)	0	100	100
10	BJ	136/143 (95%)	128 (94%)	8 (6%)	0	100	100
11	BK	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
12	BL	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	19	36
13	BM	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	BN	172/174 (99%)	161 (94%)	11 (6%)	0	100	100
15	BO	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
16	BP	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
17	BQ	55/61 (90%)	49 (89%)	6 (11%)	0	100	100
18	BR	94/97 (97%)	88 (94%)	6 (6%)	0	100	100
19	BS	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
20	BT	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
21	BU	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
22	BV	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
23	BW	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
24	BX	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
25	BY	90/99 (91%)	87 (97%)	3 (3%)	0	100	100
26	BZ	84/89 (94%)	77 (92%)	7 (8%)	0	100	100
27	Ba	130/161 (81%)	120 (92%)	10 (8%)	0	100	100
28	Bb	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
29	Bc	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
30	Bd	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
31	Be	42/52 (81%)	39 (93%)	3 (7%)	0	100	100
32	Bf	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3871/4010 (96%)	3624 (94%)	245 (6%)	2 (0%)	50	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	BL	10	ARG
3	BC	120	VAL

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	
3	BC	188/188 (100%)	188 (100%)	0	100	100
4	BD	277/277 (100%)	277 (100%)	0	100	100
5	BE	197/198 (100%)	197 (100%)	0	100	100
6	BF	140/140 (100%)	140 (100%)	0	100	100
7	BG	148/148 (100%)	148 (100%)	0	100	100
8	BH	88/91 (97%)	88 (100%)	0	100	100
9	BI	132/141 (94%)	132 (100%)	0	100	100
10	BJ	114/119 (96%)	114 (100%)	0	100	100
11	BK	109/109 (100%)	109 (100%)	0	100	100
12	BL	108/108 (100%)	108 (100%)	0	100	100
13	BM	166/166 (100%)	166 (100%)	0	100	100
14	BN	143/143 (100%)	142 (99%)	1 (1%)	81	91
15	BO	104/104 (100%)	104 (100%)	0	100	100
16	BP	123/123 (100%)	123 (100%)	0	100	100
17	BQ	50/54 (93%)	50 (100%)	0	100	100
18	BR	85/86 (99%)	85 (100%)	0	100	100
19	BS	124/124 (100%)	124 (100%)	0	100	100
20	BT	73/73 (100%)	73 (100%)	0	100	100
21	BU	100/100 (100%)	100 (100%)	0	100	100
22	BV	54/54 (100%)	54 (100%)	0	100	100
23	BW	57/57 (100%)	57 (100%)	0	100	100
24	BX	134/134 (100%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BY	71/78 (91%)	71 (100%)	0	100	100
26	BZ	76/78 (97%)	76 (100%)	0	100	100
27	Ba	109/135 (81%)	109 (100%)	0	100	100
28	Bb	76/76 (100%)	76 (100%)	0	100	100
29	Bc	49/49 (100%)	49 (100%)	0	100	100
30	Bd	48/48 (100%)	48 (100%)	0	100	100
31	Be	37/43 (86%)	37 (100%)	0	100	100
32	Bf	82/82 (100%)	82 (100%)	0	100	100
All	All	3262/3326 (98%)	3261 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	BN	43	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
10	BJ	39	GLN
27	Ba	57	HIS
14	BN	43	ASN
24	BX	46	GLN
14	BN	20	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	BA	2881/2899 (99%)	480 (16%)	11 (0%)
2	BB	127/129 (98%)	20 (15%)	1 (0%)
All	All	3008/3028 (99%)	500 (16%)	12 (0%)

5 of 500 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	BA	7	U
1	BA	28	C
1	BA	29	G

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Mol	Chain	Res	Type
1	BA	39	C
1	BA	56	A

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	2168	A
1	BA	2374	G
2	BB	25	G
1	BA	2463	U
1	BA	1712	U

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

3 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	G7M	BA	2251	1	20,26,27	2.38	4 (20%)	16,39,42	0.87	1 (6%)
1	OMU	BA	2563	1	19,22,23	0.54	0	25,31,34	1.26	4 (16%)
1	OMG	BA	2564	1	19,26,27	1.20	3 (15%)	21,38,41	1.42	3 (14%)

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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	BA	2251	1	-	0/3/25/26	0/3/3/3
1	OMU	BA	2563	1	-	1/9/27/28	0/2/2/2
1	OMG	BA	2564	1	-	2/5/27/28	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	2251	G7M	O6-C6	8.15	1.42	1.23
1	BA	2251	G7M	C2-N2	4.79	1.45	1.34
1	BA	2251	G7M	C6-N1	-3.45	1.32	1.37
1	BA	2564	OMG	C5-C6	-3.20	1.41	1.47
1	BA	2564	OMG	C2-N2	3.00	1.41	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	2564	OMG	O6-C6-C5	3.76	131.77	124.32
1	BA	2564	OMG	O6-C6-N1	-3.21	116.81	120.62
1	BA	2563	OMU	C4-N3-C2	-2.68	123.28	126.61
1	BA	2564	OMG	N1-C2-N3	2.56	128.00	123.32
1	BA	2251	G7M	C2-N1-C6	-2.49	120.56	125.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	BA	2563	OMU	C3'-C2'-O2'-CM2
1	BA	2564	OMG	C3'-C4'-C5'-O5'
1	BA	2564	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BA	2251	G7M	1	0
1	BA	2563	OMU	1	0
1	BA	2564	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

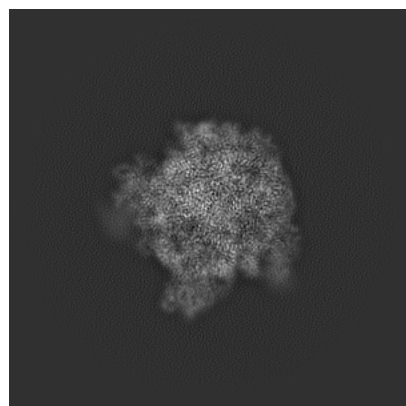
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49734. These allow visual inspection of the internal detail of the map and identification of artifacts.

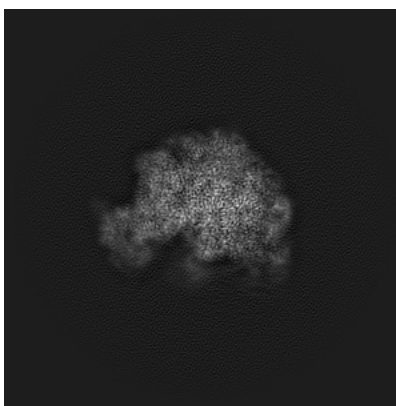
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

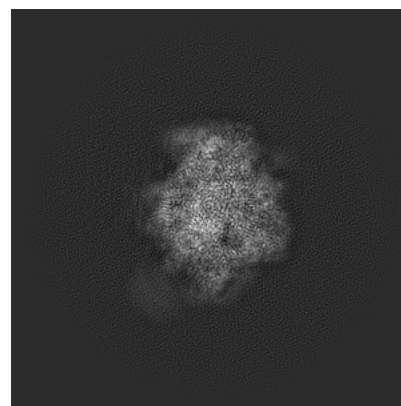
6.1.1 Primary map



X

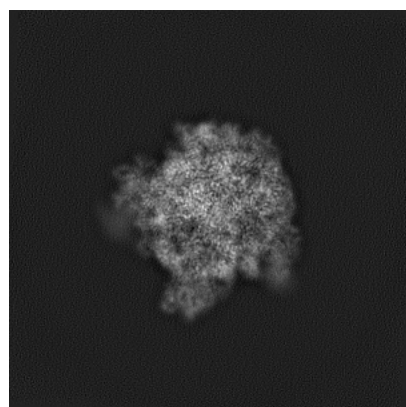


Y

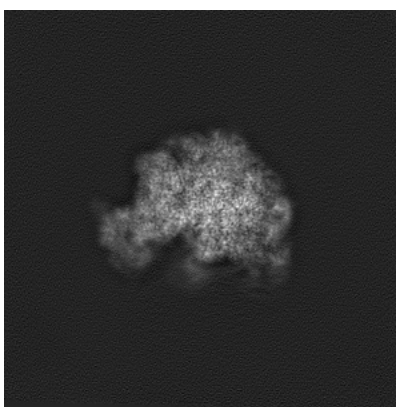


Z

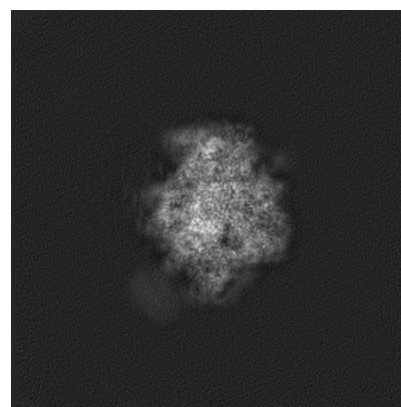
6.1.2 Raw map



X



Y

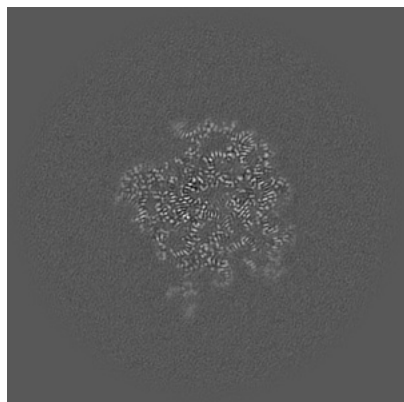


Z

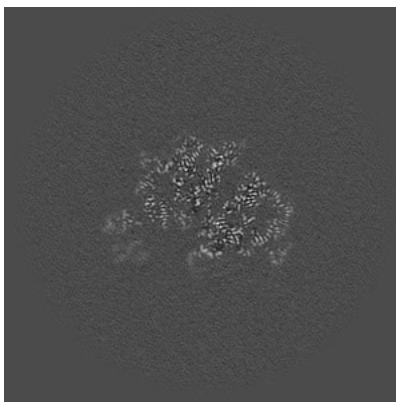
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

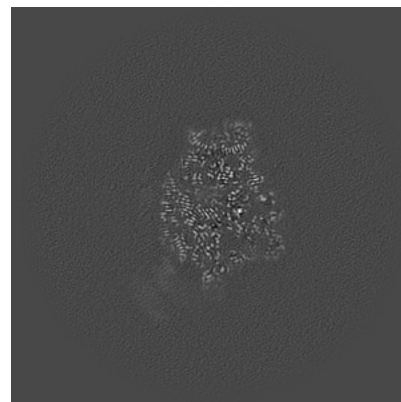
6.2.1 Primary map



X Index: 200

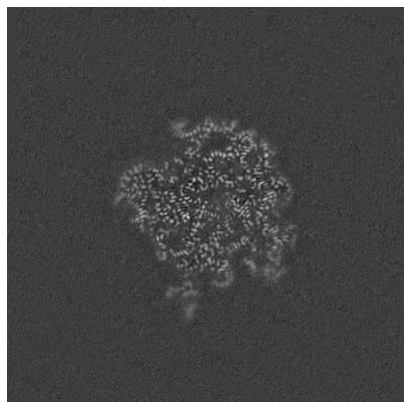


Y Index: 200

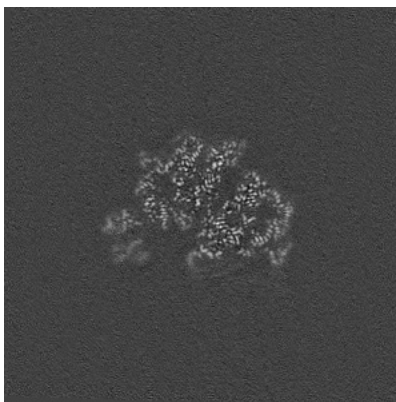


Z Index: 200

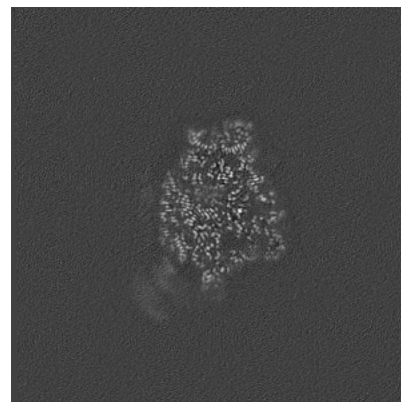
6.2.2 Raw map



X Index: 200



Y Index: 200

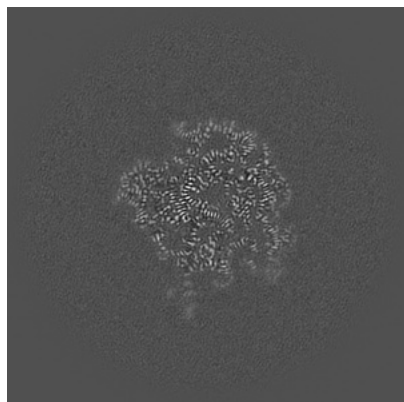


Z Index: 200

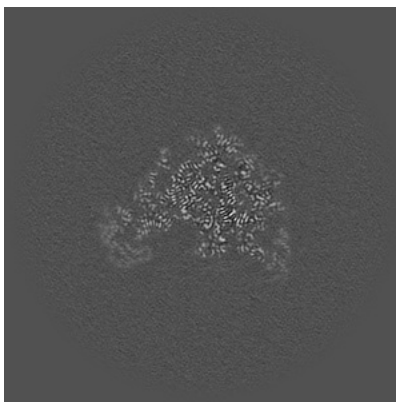
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

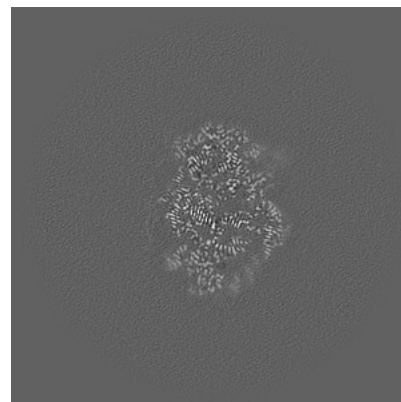
6.3.1 Primary map



X Index: 201

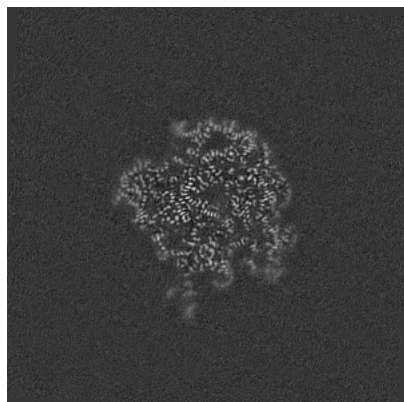


Y Index: 189

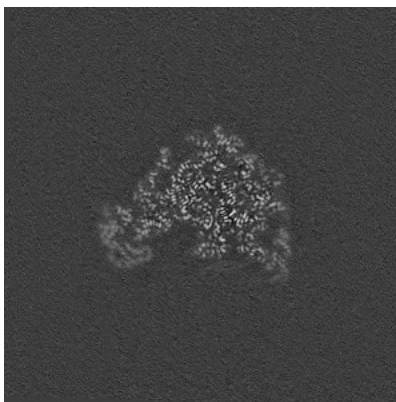


Z Index: 220

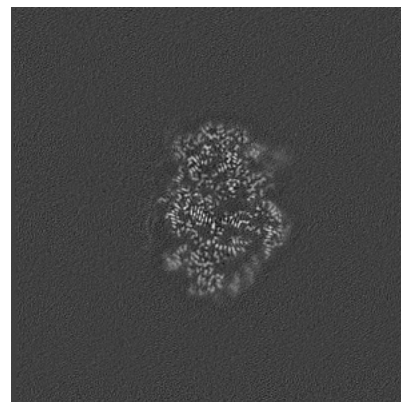
6.3.2 Raw map



X Index: 201



Y Index: 189

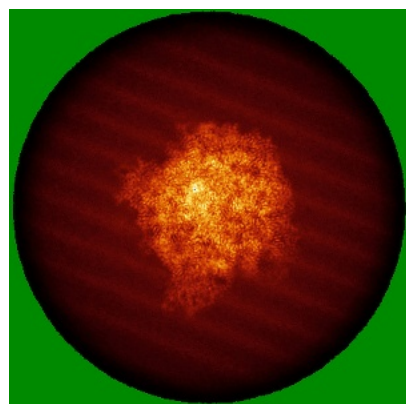


Z Index: 220

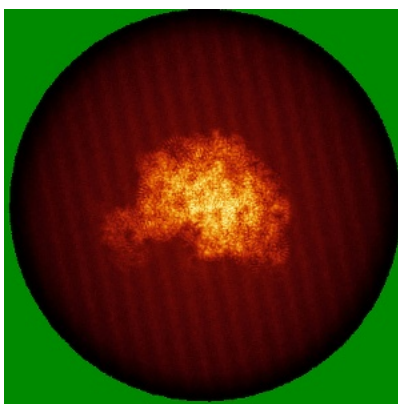
The images above show the largest variance slices of the map in three orthogonal directions.

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

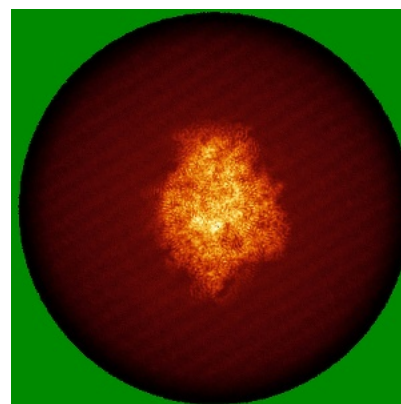
6.4.1 Primary map



X

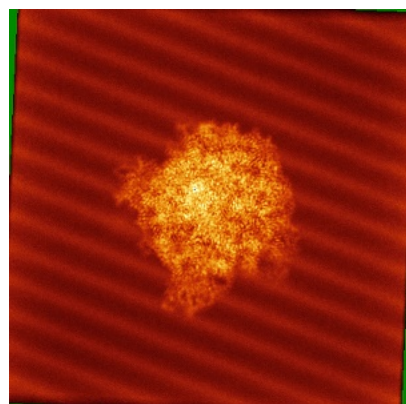


Y

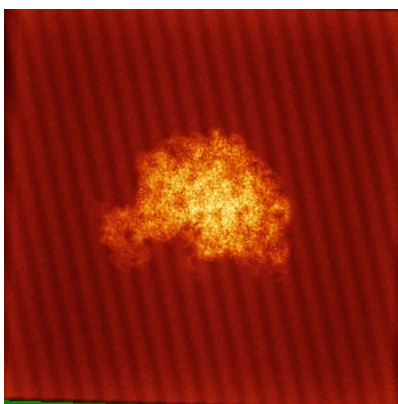


Z

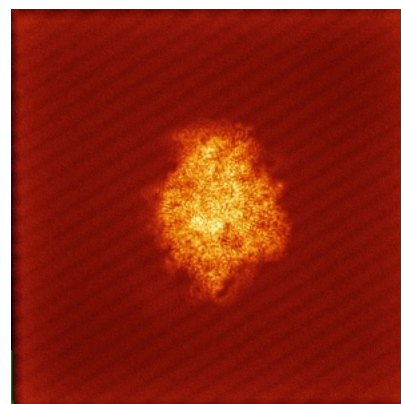
6.4.2 Raw map



X



Y

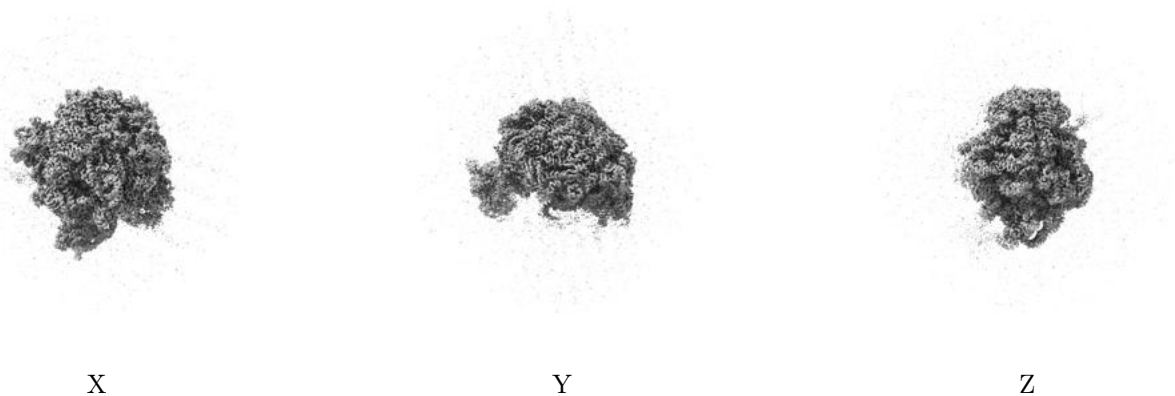


Z

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.

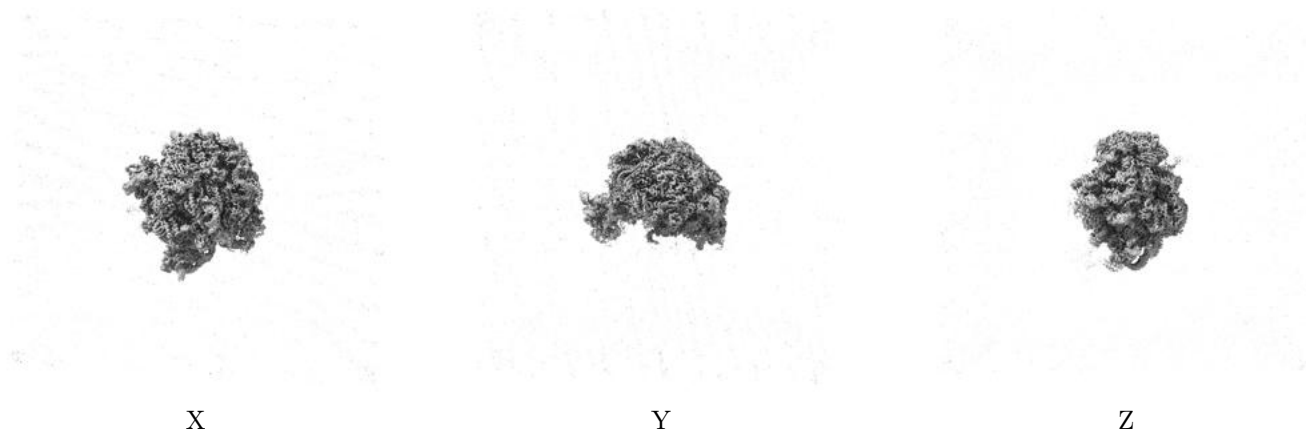
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

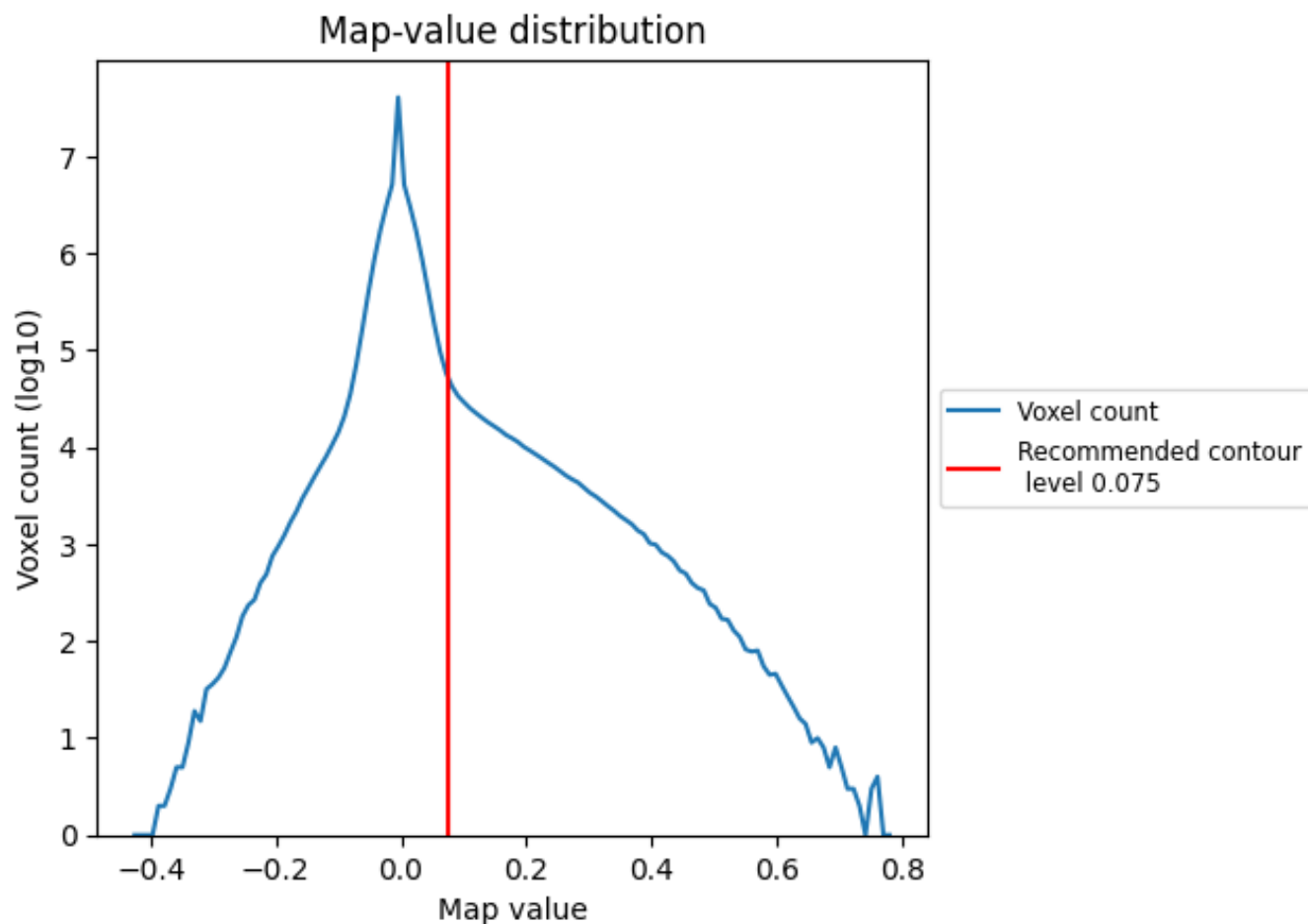
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

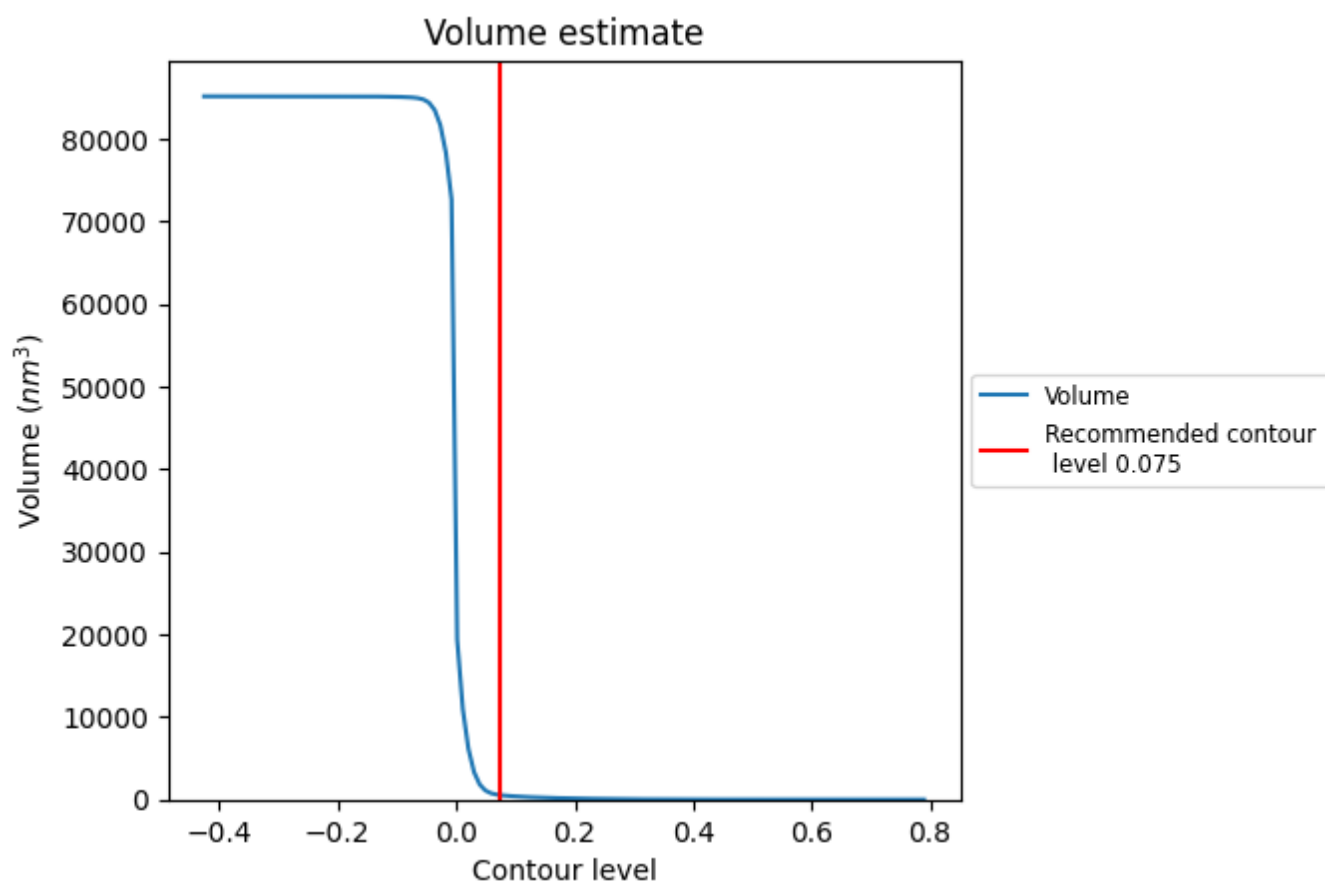
This section contains the results of statistical analysis of the map.

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.

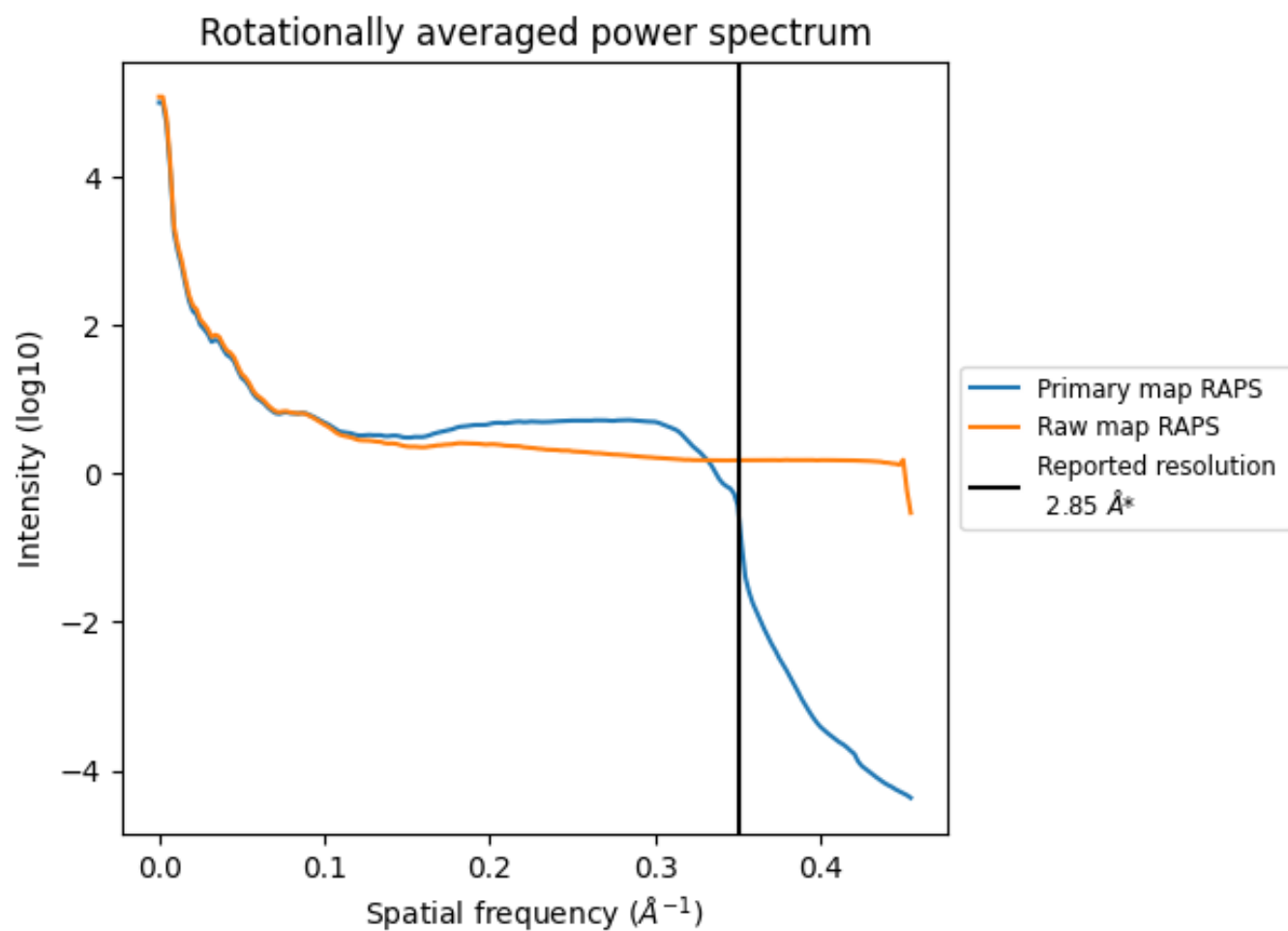
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm^3 ; this corresponds to an approximate mass of 483 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 ⓘ

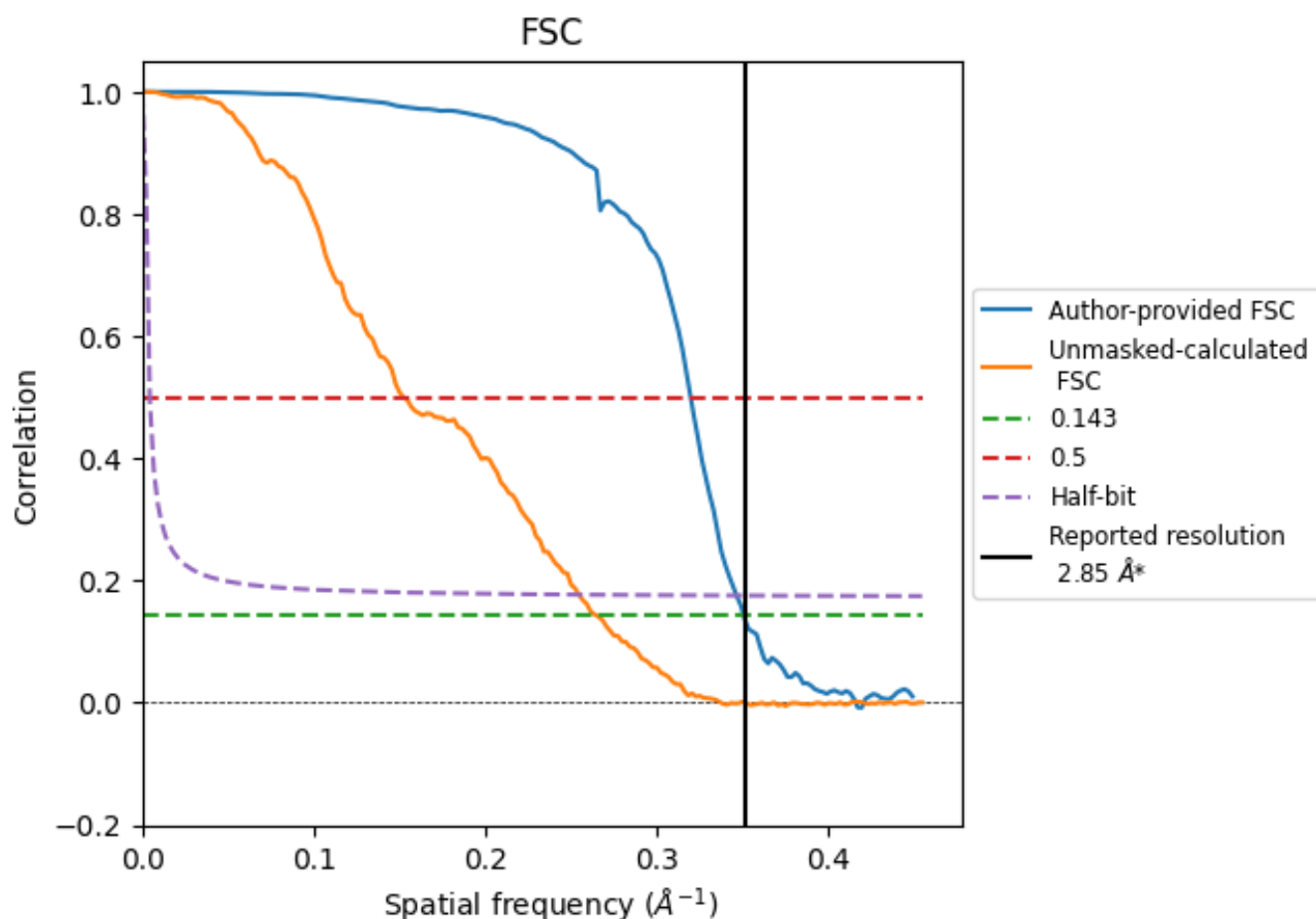


*Reported resolution corresponds to spatial frequency of 0.351 \AA^{-1}

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 0.351 Å⁻¹

8.2 Resolution estimates

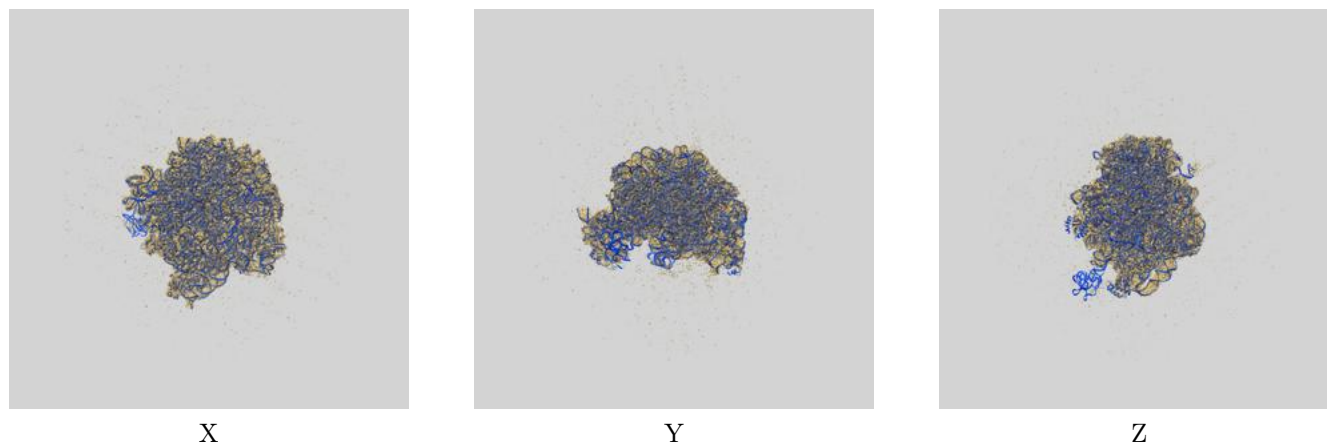
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.85	3.13	2.89
Unmasked-calculated*	3.78	6.57	3.93

*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 3.78 differs from the reported value 2.85 by more than 10 %

9 Map-model fit [i](#)

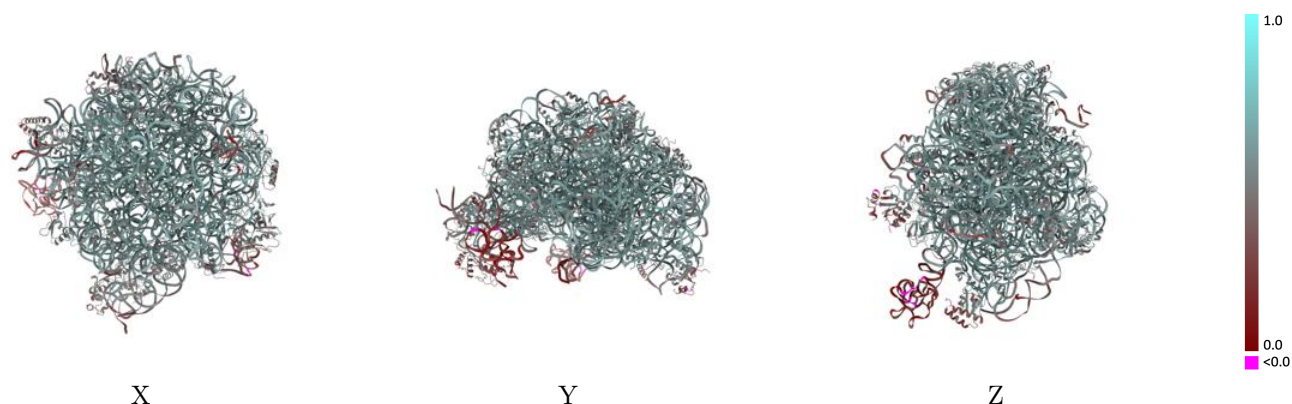
This section contains information regarding the fit between EMDB map EMD-49734 and PDB model 9NRI. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



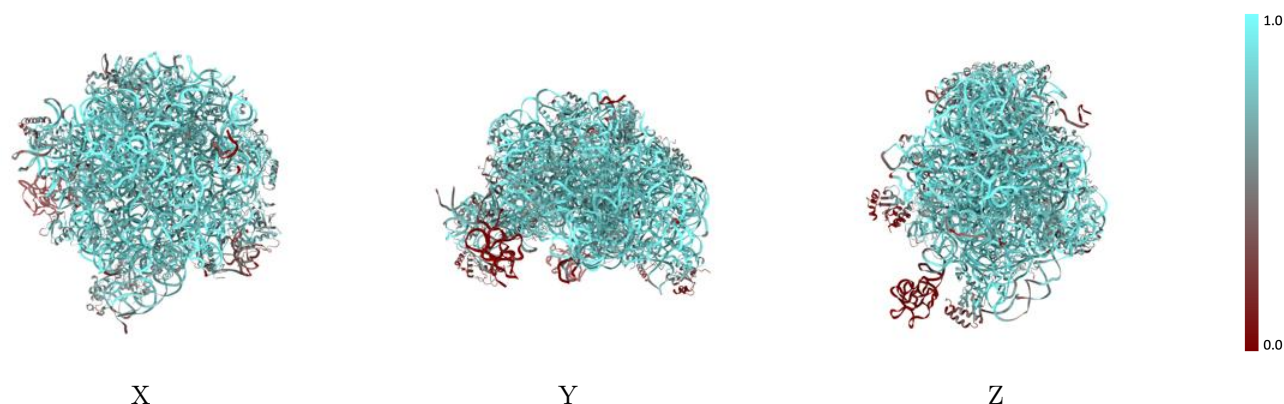
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



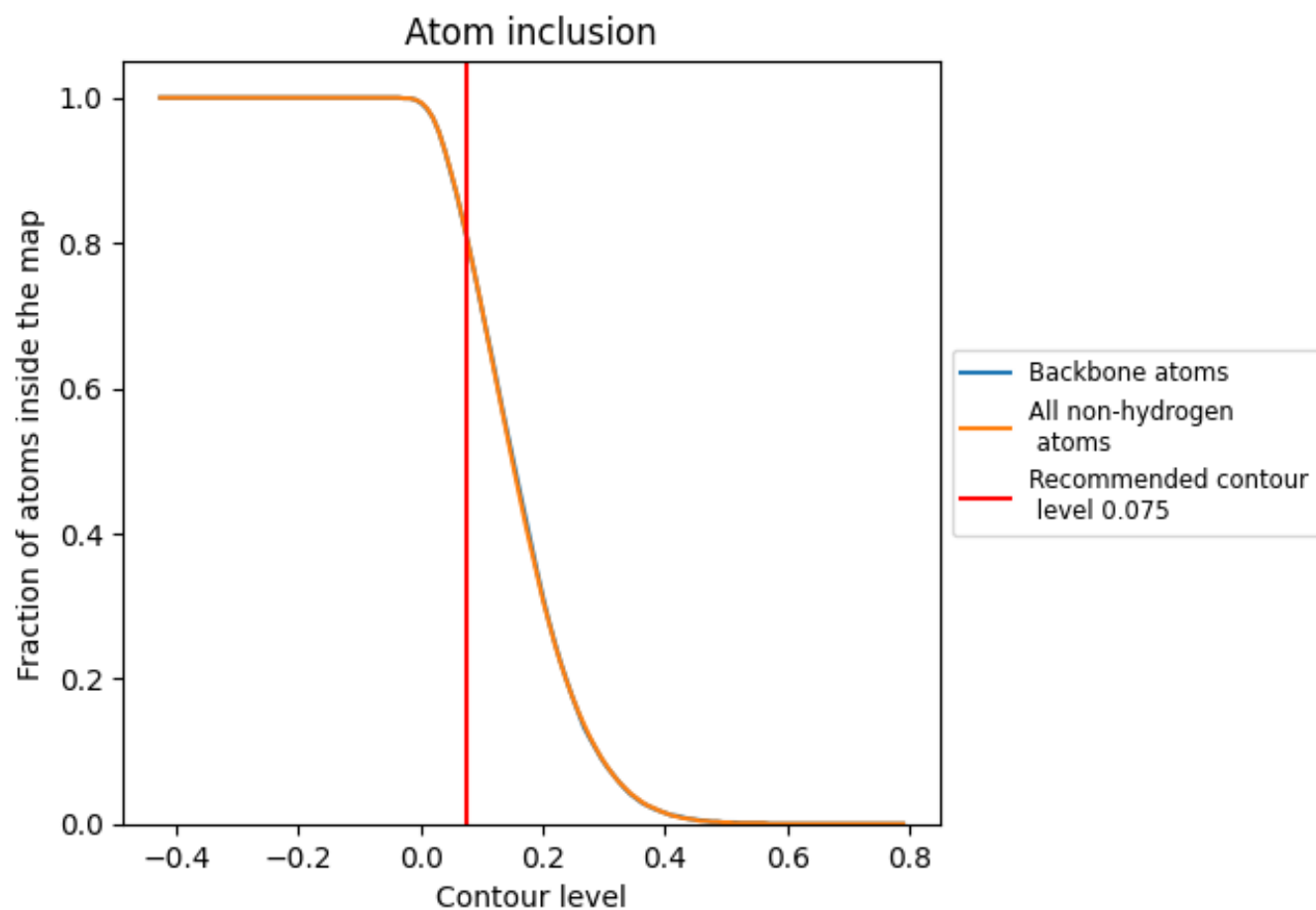
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8110	 0.5470
BA	 0.8640	 0.5590
BB	 0.8040	 0.4940
BC	 0.8050	 0.5720
BD	 0.8090	 0.5670
BE	 0.7760	 0.5600
BF	 0.3540	 0.3600
BG	 0.5820	 0.4710
BH	 0.4870	 0.4280
BI	 0.5200	 0.5020
BJ	 0.7890	 0.5510
BK	 0.7210	 0.5590
BL	 0.6710	 0.5300
BM	 0.8520	 0.5810
BN	 0.6230	 0.4520
BO	 0.7750	 0.5460
BP	 0.7810	 0.5390
BQ	 0.5190	 0.4940
BR	 0.8030	 0.5660
BS	 0.7640	 0.5530
BT	 0.7050	 0.5230
BU	 0.7500	 0.5330
BV	 0.7030	 0.5390
BW	 0.6540	 0.4700
BX	 0.8060	 0.5510
BY	 0.2840	 0.3730
BZ	 0.7540	 0.5440
Ba	 0.7910	 0.5590
Bb	 0.6610	 0.5050
Bc	 0.9070	 0.6070
Bd	 0.8380	 0.5800
Be	 0.7110	 0.5180
Bf	 0.7890	 0.5580

