



Full wwPDB EM Validation Report ⓘ

Feb 19, 2024 – 01:44 PM JST

PDB ID : 8WI9
EMDB ID : EMD-37561
Title : Cryo- EM structure of Mycobacterium smegmatis 30S ribosomal subunit (body 2) of 70S ribosome, bS1 and RafH.
Authors : Kumar, N.; Sharma, S.; Kaushal, P.S.
Deposited on : 2023-09-24
Resolution : 3.50 Å (reported)
Based on initial model : 8WHX

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

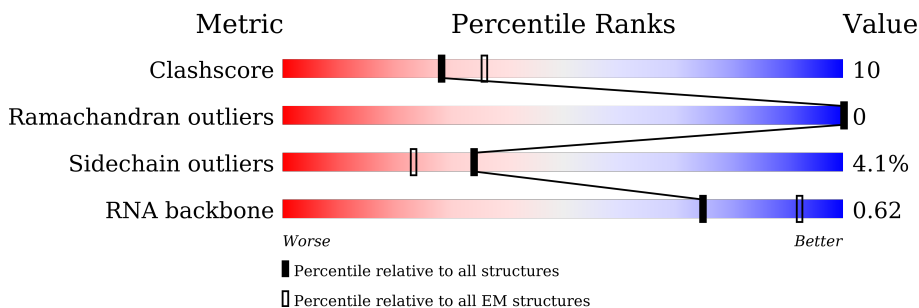
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



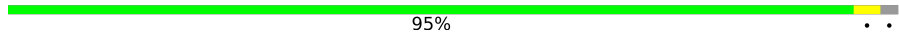
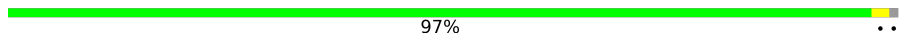



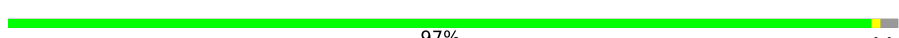




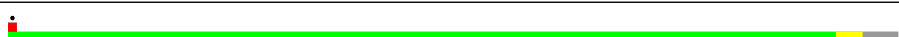


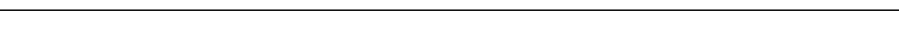
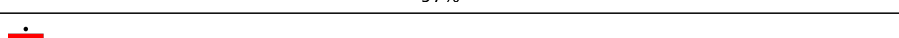
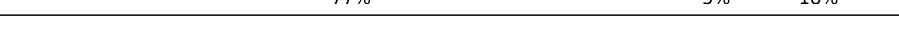
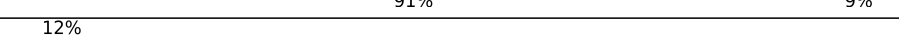
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	1528	
2	b	479	
3	v	33	
4	d	275	
5	e	201	
6	f	214	
7	g	96	

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Mol	Chain	Length	Quality of chain
8	h	156	 95%
9	i	132	 97%
10	j	150	 79% 5% 16%
11	k	101	 19% 78% 21%
12	l	138	 82% 17%
13	m	124	 97%
14	n	124	 88% 6% 6%
15	o	61	 89% 10%
16	p	89	 98%
17	q	156	 71% 28%
18	r	98	 93%
19	s	84	 77% 23%
20	t	93	 84% 12%
21	u	86	 97%
22	c	277	 77% 5% 18%
23	x	11	 91% 9%
24	w	264	 12% 93%

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 54459 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1515	32521	14485	5945	10576	1515	0	0

- Molecule 2 is a protein called 30S ribosomal protein bS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	b	154	1193	758	198	237	0	0

- Molecule 3 is a protein called 30S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	v	31	271	166	69	35	1	0	0

- Molecule 4 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	207	1656	1034	321	297	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	200	1641	1028	316	295	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	168	1223	769	230	220	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	96	771	486	138	145	2	0	0

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	153	1207	751	235	219	2	0	0

- Molecule 9 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	131	1010	633	189	187	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	j	126	994	630	194	170	0	0

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	80	645	409	119	115	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	115	855	528	170	156	1	0	0

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	121	949	588	195	164	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	116	Total	C	N	O	S	0	0
			935	572	191	169	3		

- Molecule 15 is a protein called 30S ribosomal protein S14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 16 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	p	88	Total	C	N	O	0	0
			720	449	147	124		

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	q	113	Total	C	N	O	0	0
			891	570	162	159		

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	94	Total	C	N	O	S	0	0
			748	469	142	135	2		

- Molecule 19 is a protein called 30S ribosomal protein S18B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	65	Total	C	N	O	S	0	0
			513	318	102	90	3		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	82	Total	C	N	O	S	0	0
			662	425	124	112	1		

- Molecule 21 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	u	85	Total	C	N	O	0	0
			660	402	139	119		

- Molecule 22 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	228	Total	C	N	O	S	0	0
			1793	1132	322	330	9		

- Molecule 23 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	x	11	Total	C	N	O	0	0
			94	59	21	14		

- Molecule 24 is a protein called Ribosome hibernation promotion factor RaffH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	255	Total	C	N	O	S	0	0
			2030	1273	387	364	6		

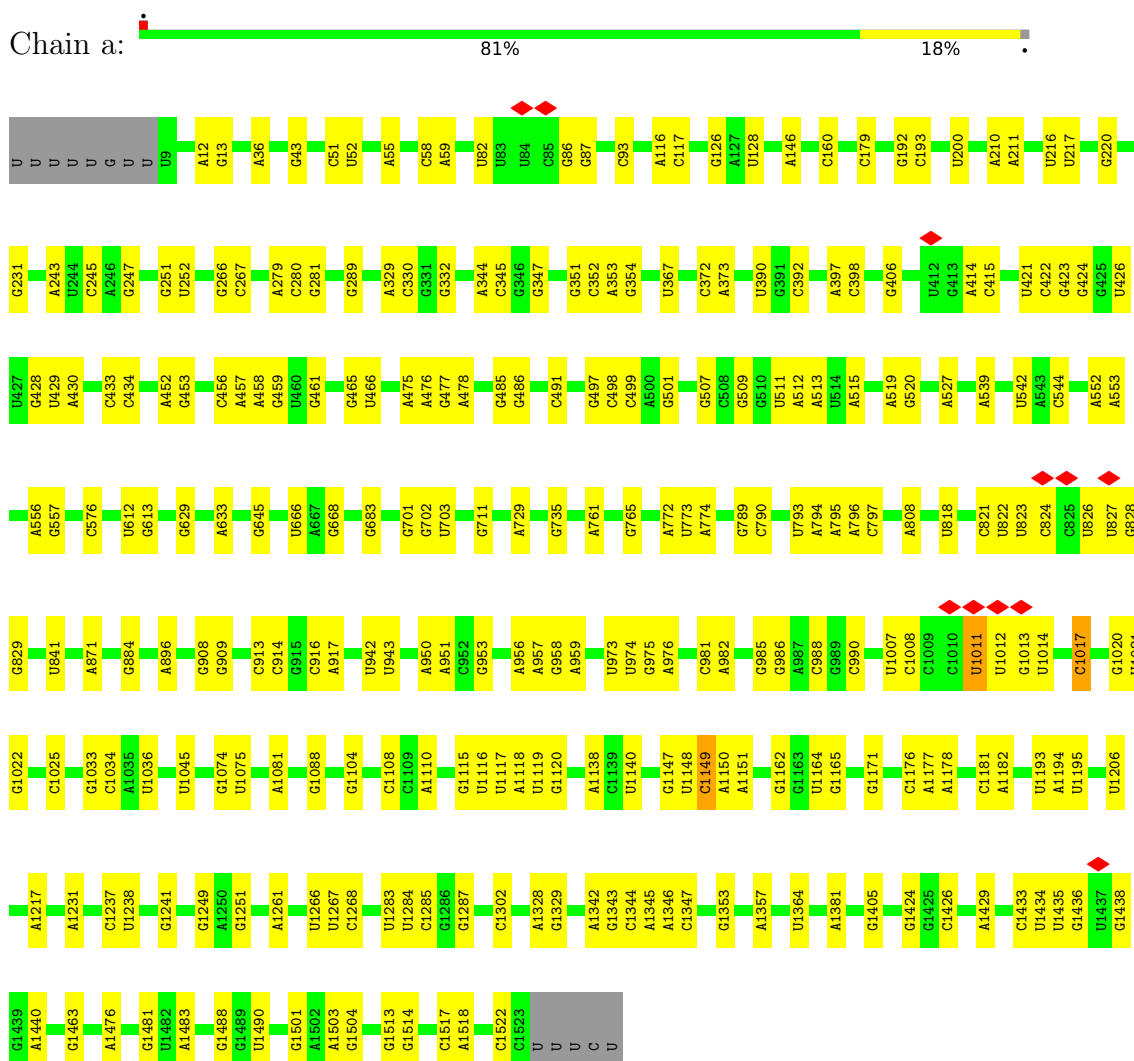
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	259	HIS	-	expression tag	UNP A0QZ86
w	260	HIS	-	expression tag	UNP A0QZ86
w	261	HIS	-	expression tag	UNP A0QZ86
w	262	HIS	-	expression tag	UNP A0QZ86
w	263	HIS	-	expression tag	UNP A0QZ86
w	264	HIS	-	expression tag	UNP A0QZ86

3 Residue-property plots [i](#)

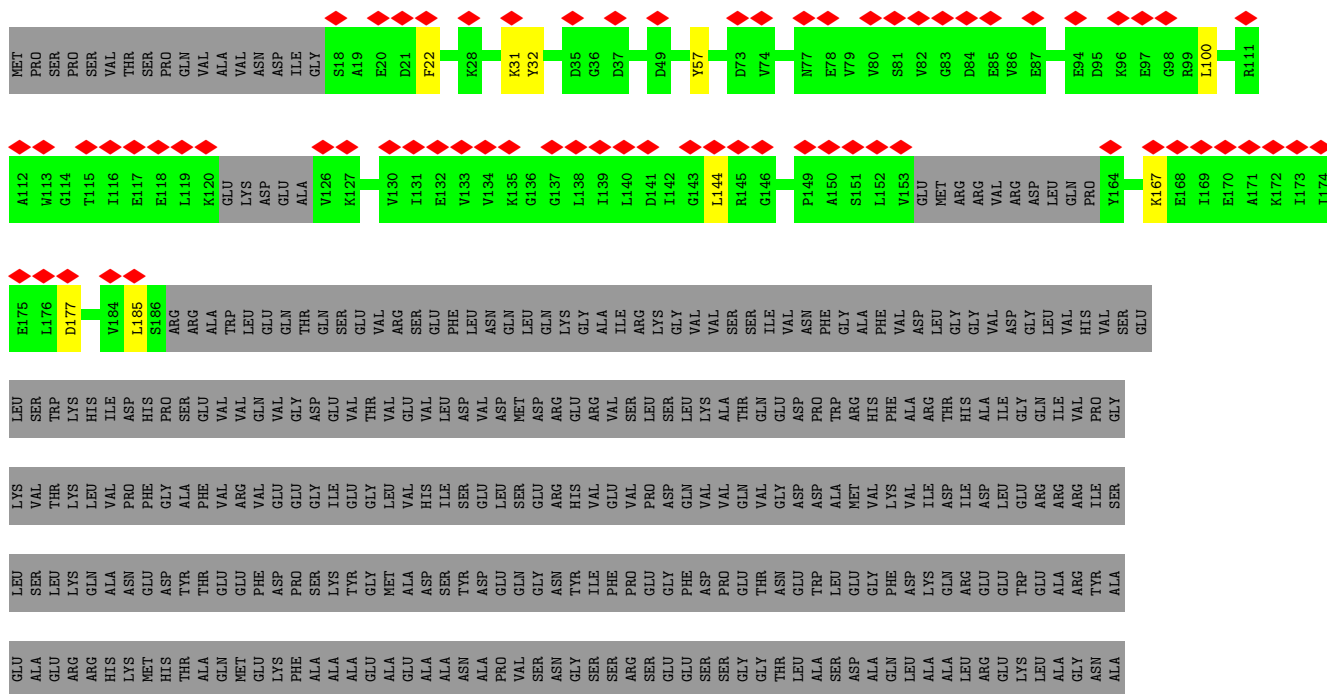
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

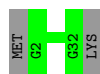


• Molecule 2: 30S ribosomal protein bS1

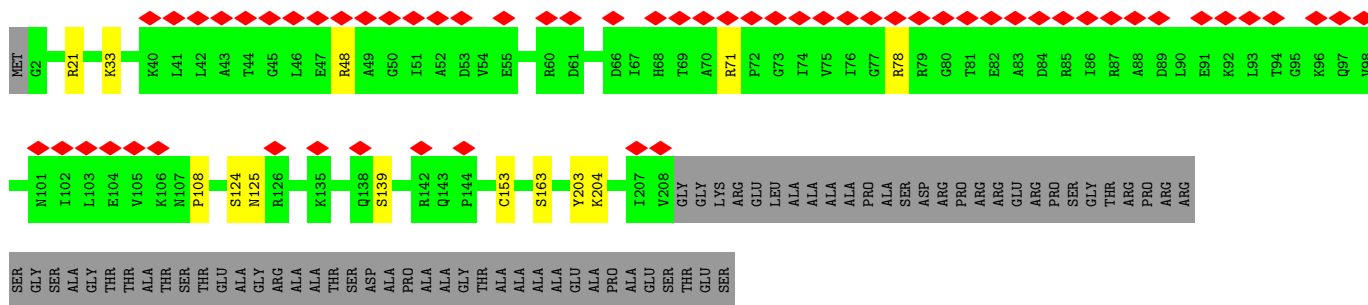




• Molecule 3: 30S ribosomal protein S22




• Molecule 4: 30S ribosomal protein S3

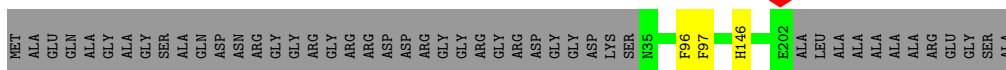


• Molecule 5: 30S ribosomal protein S4



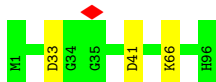
• Molecule 6: 30S ribosomal protein S5

Chain f:  77% 21%



• Molecule 7: 30S ribosomal protein S6

Chain g:  97%



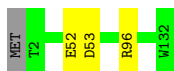
• Molecule 8: 30S ribosomal protein S7

Chain h:  95%




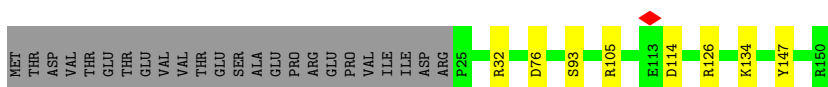
• Molecule 9: 30S ribosomal protein S8

Chain i:  97%




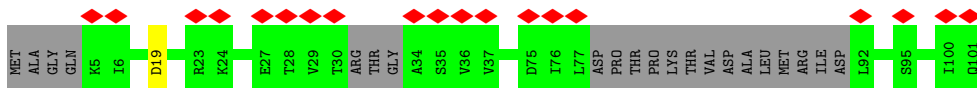
• Molecule 10: 30S ribosomal protein S9

Chain j:  79% 5% 16%




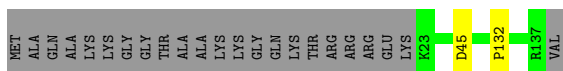
• Molecule 11: 30S ribosomal protein S10

Chain k:  19% 78% 21%



• Molecule 12: 30S ribosomal protein S11

Chain l:  82% 17%




- Molecule 13: 30S ribosomal protein S12

Chain m:  97%




- Molecule 14: 30S ribosomal protein S13

Chain n:  88% 6% 6%



- Molecule 15: 30S ribosomal protein S14A

Chain o:  89% 10%



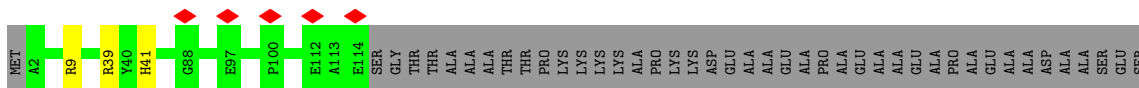
- Molecule 16: 30S ribosomal protein S15

Chain p:  98%



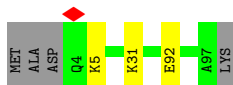
- Molecule 17: 30S ribosomal protein S16

Chain q:  71% 28%



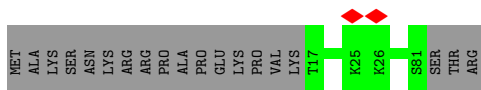
- Molecule 18: 30S ribosomal protein S17

Chain r:  93%

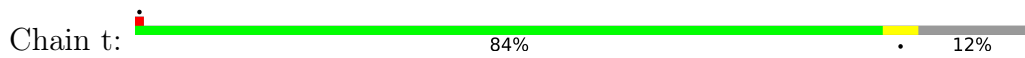


- Molecule 19: 30S ribosomal protein S18B

Chain s:  77% 23%



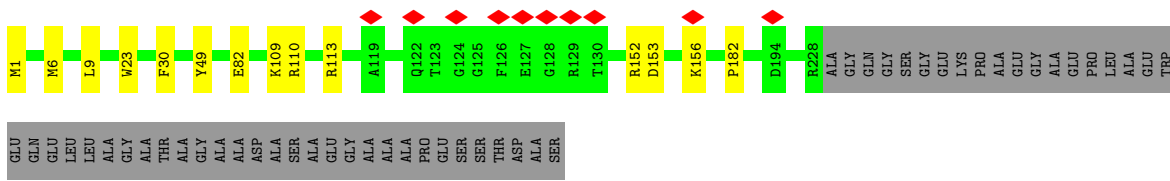
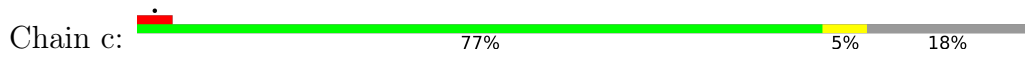
• Molecule 20: 30S ribosomal protein S19



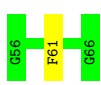
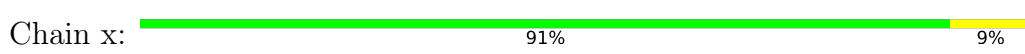
• Molecule 21: 30S ribosomal protein S20



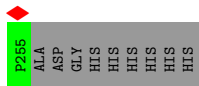
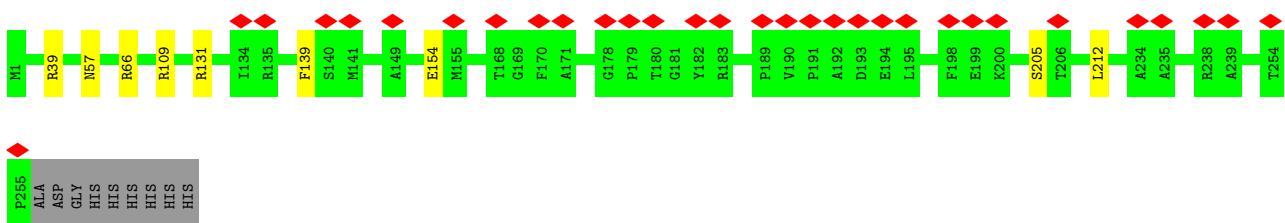
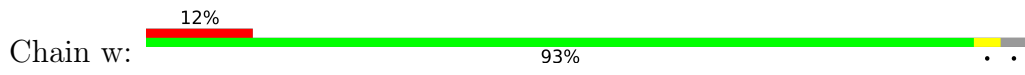
• Molecule 22: 30S ribosomal protein S2



• Molecule 23: 50S ribosomal protein L31



• Molecule 24: Ribosome hibernation promotion factor Raff



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110934	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE; CTF correction in RELION 3.1.4	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.34	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.196	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.24	0/36400	0.78	16/56798 (0.0%)
2	b	0.26	0/1201	0.61	2/1615 (0.1%)
3	v	0.23	0/271	0.64	0/348
4	d	0.26	0/1680	0.59	1/2256 (0.0%)
5	e	0.26	0/1672	0.56	0/2251
6	f	0.26	0/1239	0.53	0/1673
7	g	0.27	0/782	0.57	0/1059
8	h	0.25	0/1225	0.59	1/1653 (0.1%)
9	i	0.26	0/1025	0.54	0/1385
10	j	0.27	0/1012	0.62	1/1362 (0.1%)
11	k	0.26	0/655	0.57	0/883
12	l	0.29	0/873	0.55	0/1180
13	m	0.25	0/960	0.56	0/1283
14	n	0.26	0/942	0.68	0/1260
15	o	0.25	0/488	0.56	0/650
16	p	0.25	0/729	0.54	0/977
17	q	0.27	0/908	0.56	0/1226
18	r	0.27	0/759	0.57	0/1016
19	s	0.26	0/518	0.56	0/693
20	t	0.26	0/680	0.58	1/915 (0.1%)
21	u	0.26	0/663	0.58	0/882
22	c	0.26	0/1822	0.56	1/2457 (0.0%)
23	x	0.28	0/95	0.76	0/123
24	w	0.25	0/2078	0.56	0/2816
All	All	0.25	0/58677	0.72	23/86761 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1017	C	N3-C2-O2	-7.73	116.49	121.90
22	c	182	PRO	CA-N-CD	-7.71	100.70	111.50
8	h	58	PRO	CA-N-CD	-7.69	100.73	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1206	U	C2-N1-C1'	7.36	126.53	117.70
1	a	179	C	C2-N1-C1'	7.01	126.51	118.80
1	a	179	C	N1-C2-O2	6.95	123.07	118.90
4	d	108	PRO	CA-N-CD	-6.51	102.38	111.50
1	a	1017	C	N1-C2-O2	6.40	122.74	118.90
1	a	1011	U	C2-N1-C1'	5.99	124.89	117.70
10	j	76	ASP	CB-CG-OD1	5.69	123.42	118.30
1	a	415	C	C2-N1-C1'	5.61	124.97	118.80
1	a	1149	C	P-O3'-C3'	5.56	126.37	119.70
20	t	53	ASP	CB-CG-OD1	5.48	123.23	118.30
1	a	179	C	N3-C2-O2	-5.44	118.09	121.90
1	a	1206	U	N1-C2-O2	5.39	126.57	122.80
1	a	1206	U	N3-C2-O2	-5.27	118.51	122.20
2	b	185	LEU	CA-CB-CG	5.22	127.30	115.30
2	b	144	LEU	CA-CB-CG	5.21	127.29	115.30
1	a	1206	U	C6-N1-C1'	-5.20	113.92	121.20
1	a	985	G	N1-C6-O6	-5.18	116.79	119.90
1	a	790	C	N1-C2-O2	5.13	121.98	118.90
1	a	986	G	N3-C4-N9	-5.04	122.98	126.00
1	a	179	C	C6-N1-C1'	-5.03	114.77	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32521	0	16366	0	0
2	b	1193	0	1238	0	0
3	v	271	0	329	0	0
4	d	1656	0	1704	0	0
5	e	1641	0	1668	0	0
6	f	1223	0	1287	0	0
7	g	771	0	797	0	0
8	h	1207	0	1259	0	0
9	i	1010	0	1046	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	j	994	0	1050	0	0
11	k	645	0	672	0	0
12	l	855	0	863	0	0
13	m	949	0	1032	0	0
14	n	935	0	986	0	0
15	o	477	0	503	0	0
16	p	720	0	760	0	0
17	q	891	0	935	0	0
18	r	748	0	795	0	0
19	s	513	0	540	0	0
20	t	662	0	677	0	0
21	u	660	0	712	0	0
22	c	1793	0	1839	0	0
23	x	94	0	95	0	0
24	w	2030	0	2023	0	0
All	All	54459	0	39176	0	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 10.

There are no clashes within the asymmetric unit.

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	
2	b	148/479 (31%)	143 (97%)	5 (3%)	0	100	100
3	v	29/33 (88%)	29 (100%)	0	0	100	100
4	d	205/275 (74%)	195 (95%)	10 (5%)	0	100	100
5	e	198/201 (98%)	189 (96%)	9 (4%)	0	100	100
6	f	166/214 (78%)	162 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
8	h	151/156 (97%)	148 (98%)	3 (2%)	0	100	100
9	i	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
10	j	124/150 (83%)	116 (94%)	8 (6%)	0	100	100
11	k	74/101 (73%)	71 (96%)	3 (4%)	0	100	100
12	l	113/138 (82%)	107 (95%)	6 (5%)	0	100	100
13	m	119/124 (96%)	112 (94%)	7 (6%)	0	100	100
14	n	114/124 (92%)	110 (96%)	4 (4%)	0	100	100
15	o	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
16	p	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
17	q	111/156 (71%)	105 (95%)	6 (5%)	0	100	100
18	r	92/98 (94%)	89 (97%)	3 (3%)	0	100	100
19	s	63/84 (75%)	61 (97%)	2 (3%)	0	100	100
20	t	80/93 (86%)	77 (96%)	3 (4%)	0	100	100
21	u	83/86 (96%)	83 (100%)	0	0	100	100
22	c	226/277 (82%)	211 (93%)	15 (7%)	0	100	100
23	x	9/11 (82%)	9 (100%)	0	0	100	100
24	w	253/264 (96%)	240 (95%)	13 (5%)	0	100	100
All	All	2725/3442 (79%)	2610 (96%)	115 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	132/407 (32%)	125 (95%)	7 (5%)	22	55
3	v	29/31 (94%)	29 (100%)	0	100	100
4	d	170/212 (80%)	158 (93%)	12 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	175/176 (99%)	170 (97%)	5 (3%)	42	71
6	f	123/147 (84%)	120 (98%)	3 (2%)	49	76
7	g	85/85 (100%)	82 (96%)	3 (4%)	36	67
8	h	129/132 (98%)	125 (97%)	4 (3%)	40	70
9	i	107/108 (99%)	104 (97%)	3 (3%)	43	72
10	j	102/125 (82%)	95 (93%)	7 (7%)	15	47
11	k	73/90 (81%)	72 (99%)	1 (1%)	67	85
12	l	89/105 (85%)	87 (98%)	2 (2%)	52	78
13	m	102/105 (97%)	101 (99%)	1 (1%)	76	88
14	n	99/104 (95%)	92 (93%)	7 (7%)	14	46
15	o	49/50 (98%)	43 (88%)	6 (12%)	5	23
16	p	76/77 (99%)	75 (99%)	1 (1%)	69	86
17	q	92/118 (78%)	89 (97%)	3 (3%)	38	68
18	r	80/83 (96%)	77 (96%)	3 (4%)	33	65
19	s	55/72 (76%)	55 (100%)	0	100	100
20	t	73/84 (87%)	70 (96%)	3 (4%)	30	63
21	u	69/70 (99%)	67 (97%)	2 (3%)	42	71
22	c	191/218 (88%)	178 (93%)	13 (7%)	16	48
23	x	8/8 (100%)	7 (88%)	1 (12%)	4	23
24	w	208/215 (97%)	199 (96%)	9 (4%)	29	62
All	All	2316/2822 (82%)	2220 (96%)	96 (4%)	34	63

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	22	PHE
2	b	31	LYS
2	b	32	TYR
2	b	57	TYR
2	b	100	LEU
2	b	167	LYS
2	b	177	ASP
4	d	21	ARG
4	d	33	LYS
4	d	48	ARG

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Mol	Chain	Res	Type
4	d	71	ARG
4	d	78	ARG
4	d	124	SER
4	d	125	ASN
4	d	139	SER
4	d	153	CYS
4	d	163	SER
4	d	203	TYR
4	d	204	LYS
5	e	80	LYS
5	e	108	MET
5	e	139	ASP
5	e	141	LYS
5	e	160	ARG
6	f	96	PHE
6	f	97	PHE
6	f	146	HIS
7	g	33	ASP
7	g	41	ASP
7	g	66	LYS
8	h	10	ARG
8	h	90	GLU
8	h	112	ARG
8	h	136	LYS
9	i	52	GLU
9	i	53	ASP
9	i	96	ARG
10	j	32	ARG
10	j	93	SER
10	j	105	ARG
10	j	114	ASP
10	j	126	ARG
10	j	134	LYS
10	j	147	TYR
11	k	19	ASP
12	l	45	ASP
12	l	132	PRO
13	m	110	ARG
14	n	46	LYS
14	n	51	ASP
14	n	75	GLN
14	n	79	ARG

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Mol	Chain	Res	Type
14	n	91	ARG
14	n	101	GLN
14	n	102	ARG
15	o	19	ARG
15	o	21	TYR
15	o	29	ARG
15	o	36	LYS
15	o	41	ARG
15	o	61	TRP
16	p	83	GLU
17	q	9	ARG
17	q	39	ARG
17	q	41	HIS
18	r	5	LYS
18	r	31	LYS
18	r	92	GLU
20	t	17	LYS
20	t	20	ASP
20	t	25	LYS
21	u	45	ASP
21	u	49	GLU
22	c	1	MET
22	c	6	MET
22	c	9	LEU
22	c	23	TRP
22	c	30	PHE
22	c	49	TYR
22	c	82	GLU
22	c	109	LYS
22	c	110	ARG
22	c	113	ARG
22	c	152	ARG
22	c	153	ASP
22	c	156	LYS
23	x	61	PHE
24	w	39	ARG
24	w	57	ASN
24	w	66	ARG
24	w	109	ARG
24	w	131	ARG
24	w	139	PHE
24	w	154	GLU

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Mol	Chain	Res	Type
24	w	205	SER
24	w	212	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
17	q	107	ASN
24	w	161	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1514/1528 (99%)	266 (17%)	0

All (266) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	12	A
1	a	13	G
1	a	36	A
1	a	43	G
1	a	51	C
1	a	52	U
1	a	55	A
1	a	58	C
1	a	59	A
1	a	82	U
1	a	86	G
1	a	87	G
1	a	93	C
1	a	116	A
1	a	117	C
1	a	126	G
1	a	128	U
1	a	146	A
1	a	160	C
1	a	192	G
1	a	193	C
1	a	200	U
1	a	210	A

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Mol	Chain	Res	Type
1	a	211	A
1	a	216	U
1	a	217	U
1	a	220	G
1	a	231	G
1	a	243	A
1	a	245	C
1	a	247	G
1	a	251	G
1	a	252	U
1	a	266	G
1	a	267	C
1	a	279	A
1	a	280	C
1	a	281	G
1	a	289	G
1	a	329	A
1	a	330	C
1	a	332	G
1	a	344	A
1	a	345	C
1	a	347	G
1	a	351	G
1	a	352	C
1	a	353	A
1	a	354	G
1	a	367	U
1	a	372	C
1	a	373	A
1	a	390	U
1	a	392	C
1	a	397	A
1	a	398	C
1	a	406	G
1	a	414	A
1	a	421	U
1	a	422	C
1	a	423	G
1	a	424	G
1	a	426	U
1	a	428	G
1	a	429	U

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Mol	Chain	Res	Type
1	a	430	A
1	a	433	C
1	a	434	C
1	a	452	A
1	a	453	G
1	a	456	C
1	a	457	A
1	a	458	A
1	a	459	G
1	a	461	G
1	a	465	G
1	a	466	U
1	a	475	A
1	a	476	A
1	a	477	G
1	a	478	A
1	a	485	G
1	a	486	G
1	a	491	C
1	a	497	G
1	a	498	C
1	a	499	C
1	a	501	G
1	a	507	G
1	a	509	G
1	a	511	U
1	a	512	A
1	a	513	A
1	a	515	A
1	a	519	A
1	a	520	G
1	a	527	A
1	a	539	A
1	a	542	U
1	a	544	C
1	a	552	A
1	a	553	A
1	a	556	A
1	a	557	G
1	a	576	C
1	a	612	U
1	a	613	G

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Mol	Chain	Res	Type
1	a	629	G
1	a	633	A
1	a	645	G
1	a	666	U
1	a	668	G
1	a	683	G
1	a	701	G
1	a	702	G
1	a	703	U
1	a	711	G
1	a	729	A
1	a	735	G
1	a	761	A
1	a	765	G
1	a	772	A
1	a	773	U
1	a	774	A
1	a	789	G
1	a	793	U
1	a	794	A
1	a	795	A
1	a	796	A
1	a	797	C
1	a	808	A
1	a	818	U
1	a	821	C
1	a	822	U
1	a	823	U
1	a	824	C
1	a	826	U
1	a	827	U
1	a	828	G
1	a	829	G
1	a	841	U
1	a	871	A
1	a	884	G
1	a	896	A
1	a	908	G
1	a	909	G
1	a	913	C
1	a	914	C
1	a	916	C

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Mol	Chain	Res	Type
1	a	917	A
1	a	942	U
1	a	943	U
1	a	950	A
1	a	951	A
1	a	953	G
1	a	956	A
1	a	957	A
1	a	958	G
1	a	959	A
1	a	973	U
1	a	974	U
1	a	975	G
1	a	976	A
1	a	981	C
1	a	982	A
1	a	988	C
1	a	990	C
1	a	1007	U
1	a	1008	C
1	a	1011	U
1	a	1012	U
1	a	1013	G
1	a	1014	U
1	a	1017	C
1	a	1020	G
1	a	1021	U
1	a	1022	G
1	a	1025	C
1	a	1033	G
1	a	1034	C
1	a	1036	U
1	a	1045	U
1	a	1074	G
1	a	1075	U
1	a	1081	A
1	a	1088	G
1	a	1104	G
1	a	1108	C
1	a	1110	A
1	a	1115	G
1	a	1116	U

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Mol	Chain	Res	Type
1	a	1117	U
1	a	1118	A
1	a	1119	U
1	a	1120	G
1	a	1138	A
1	a	1140	U
1	a	1147	G
1	a	1148	U
1	a	1149	C
1	a	1150	A
1	a	1151	A
1	a	1162	G
1	a	1164	U
1	a	1165	G
1	a	1171	G
1	a	1176	C
1	a	1177	A
1	a	1178	A
1	a	1181	C
1	a	1182	A
1	a	1193	U
1	a	1194	A
1	a	1195	U
1	a	1217	A
1	a	1231	A
1	a	1237	C
1	a	1238	U
1	a	1241	G
1	a	1249	G
1	a	1251	G
1	a	1261	A
1	a	1266	U
1	a	1267	U
1	a	1268	C
1	a	1283	U
1	a	1284	U
1	a	1285	C
1	a	1287	G
1	a	1302	C
1	a	1328	A
1	a	1329	G
1	a	1342	A

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Mol	Chain	Res	Type
1	a	1343	G
1	a	1344	C
1	a	1345	A
1	a	1346	A
1	a	1347	C
1	a	1353	G
1	a	1357	A
1	a	1364	U
1	a	1381	A
1	a	1405	G
1	a	1424	G
1	a	1426	C
1	a	1429	A
1	a	1433	C
1	a	1434	U
1	a	1435	U
1	a	1436	G
1	a	1438	G
1	a	1440	A
1	a	1463	G
1	a	1476	A
1	a	1481	G
1	a	1483	A
1	a	1488	G
1	a	1490	U
1	a	1501	G
1	a	1503	A
1	a	1504	G
1	a	1513	G
1	a	1514	G
1	a	1517	C
1	a	1518	A
1	a	1522	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

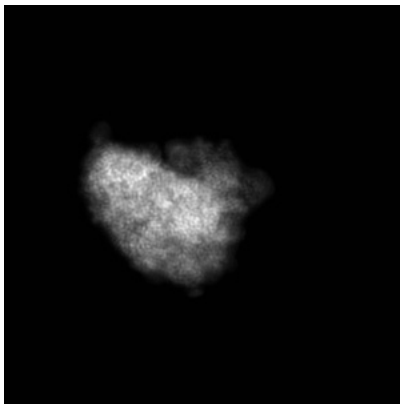
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37561. These allow visual inspection of the internal detail of the map and identification of artifacts.

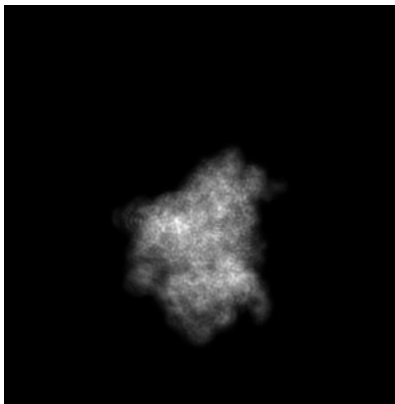
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

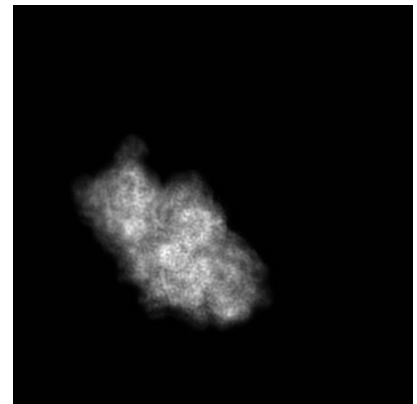
6.1.1 Primary map



X

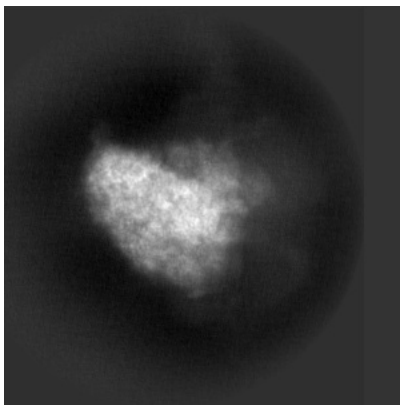


Y

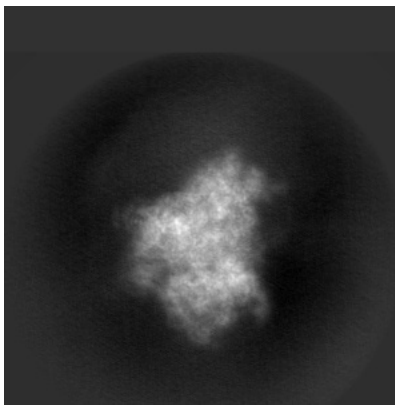


Z

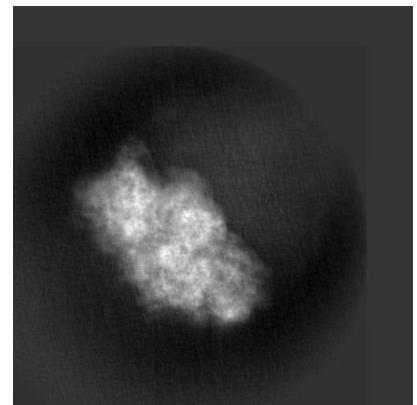
6.1.2 Raw map



X



Y

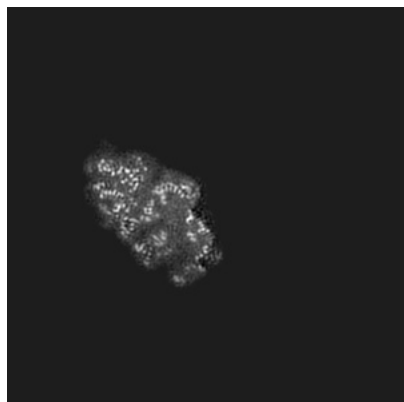


Z

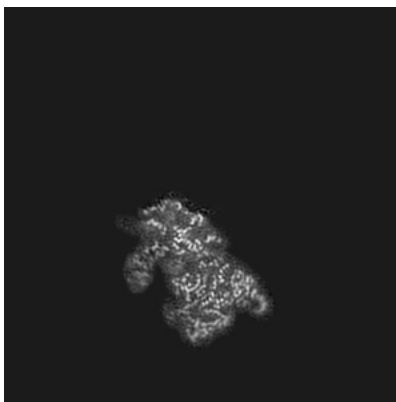
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

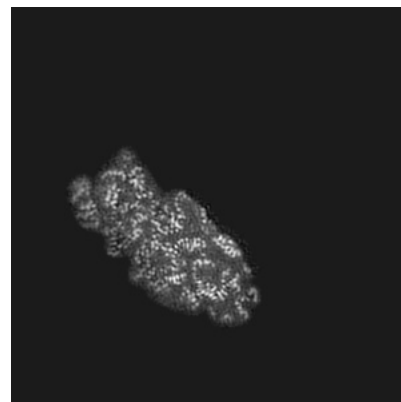
6.2.1 Primary map



X Index: 190

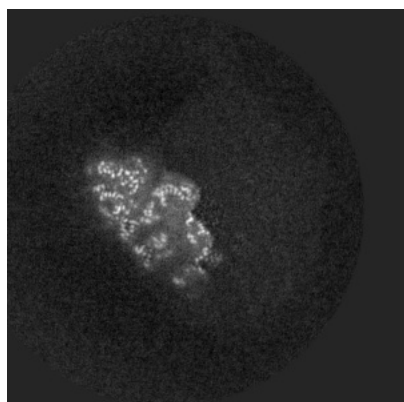


Y Index: 190

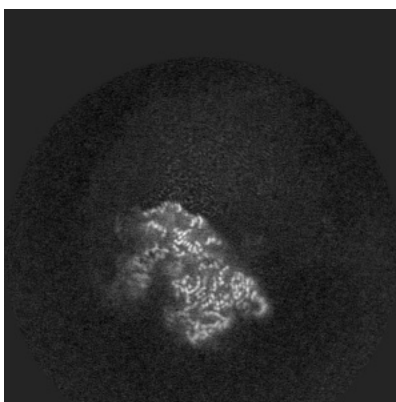


Z Index: 190

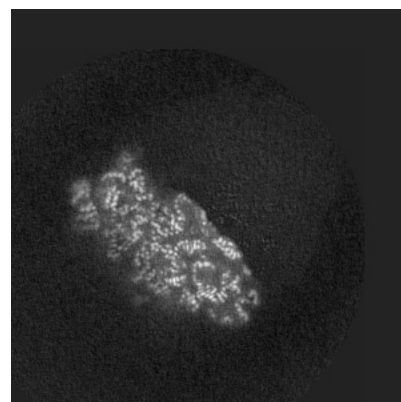
6.2.2 Raw map



X Index: 190



Y Index: 190

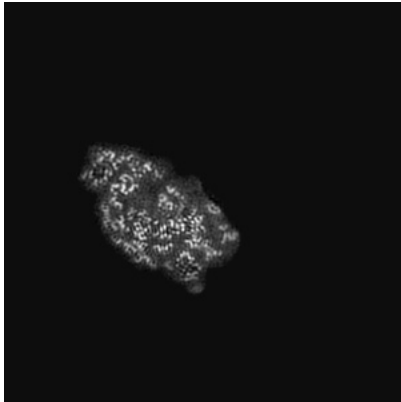


Z Index: 190

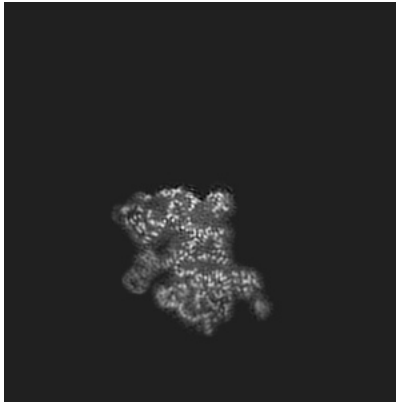
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

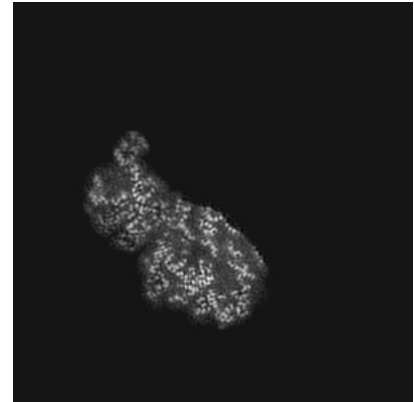
6.3.1 Primary map



X Index: 171

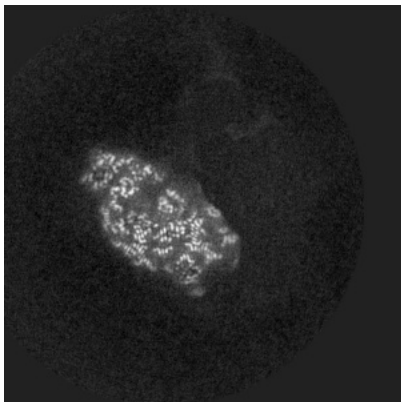


Y Index: 174

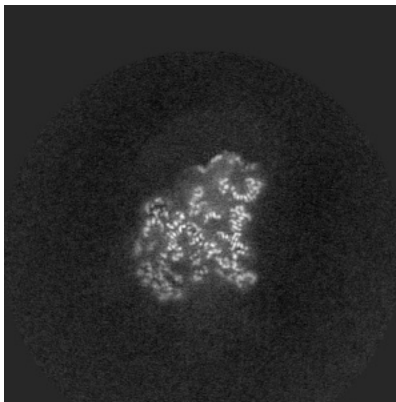


Z Index: 204

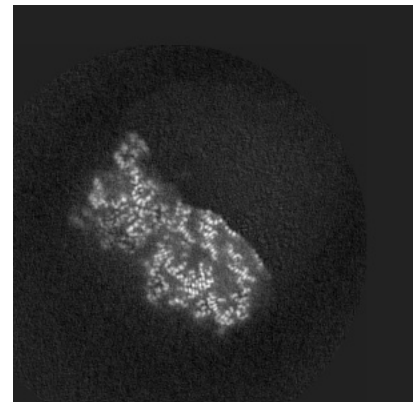
6.3.2 Raw map



X Index: 171



Y Index: 133

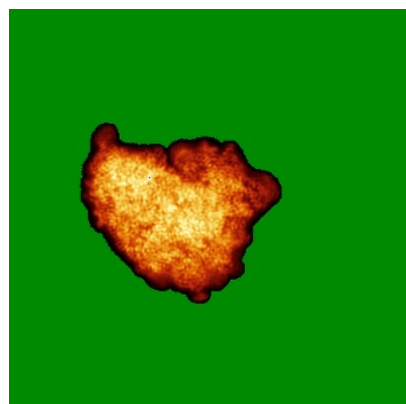


Z Index: 204

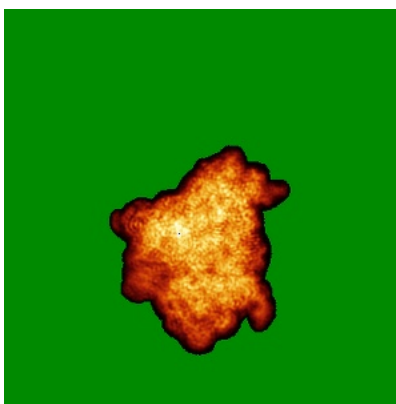
The images above show the largest variance slices of the map in three orthogonal directions.

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

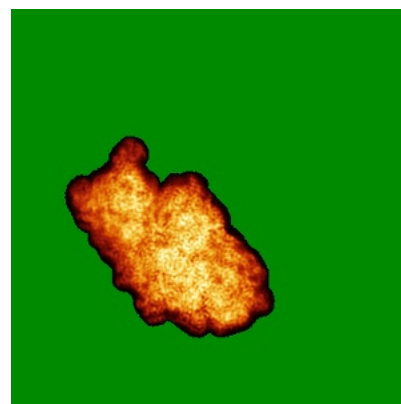
6.4.1 Primary map



X

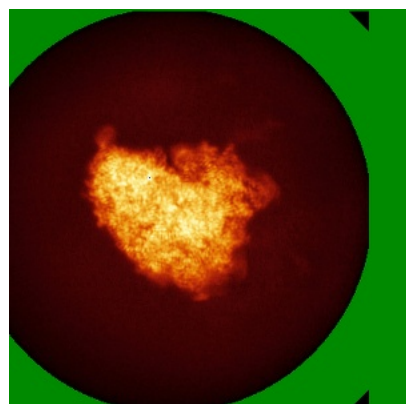


Y

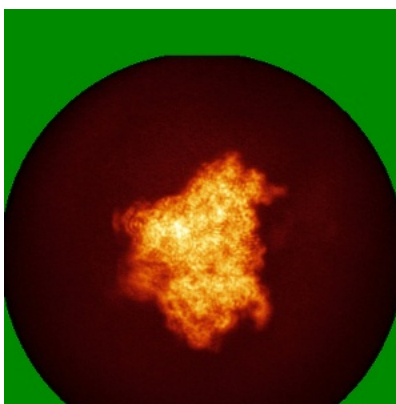


Z

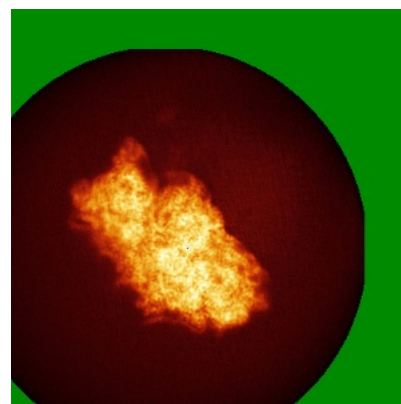
6.4.2 Raw map



X



Y

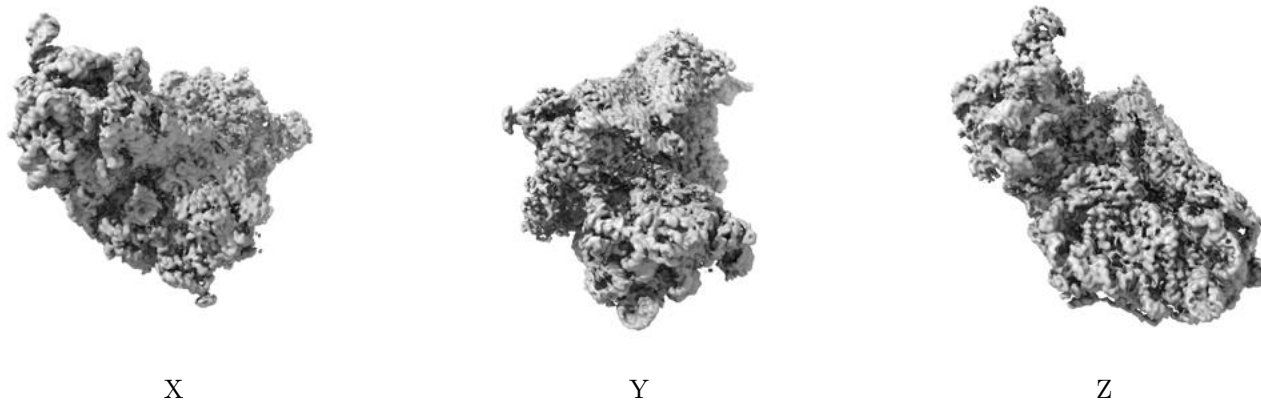


Z

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.

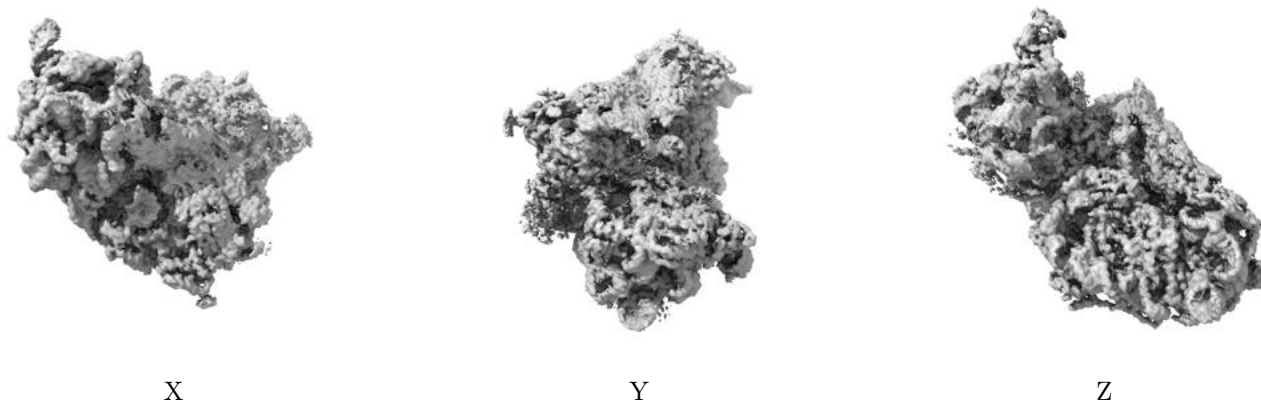
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

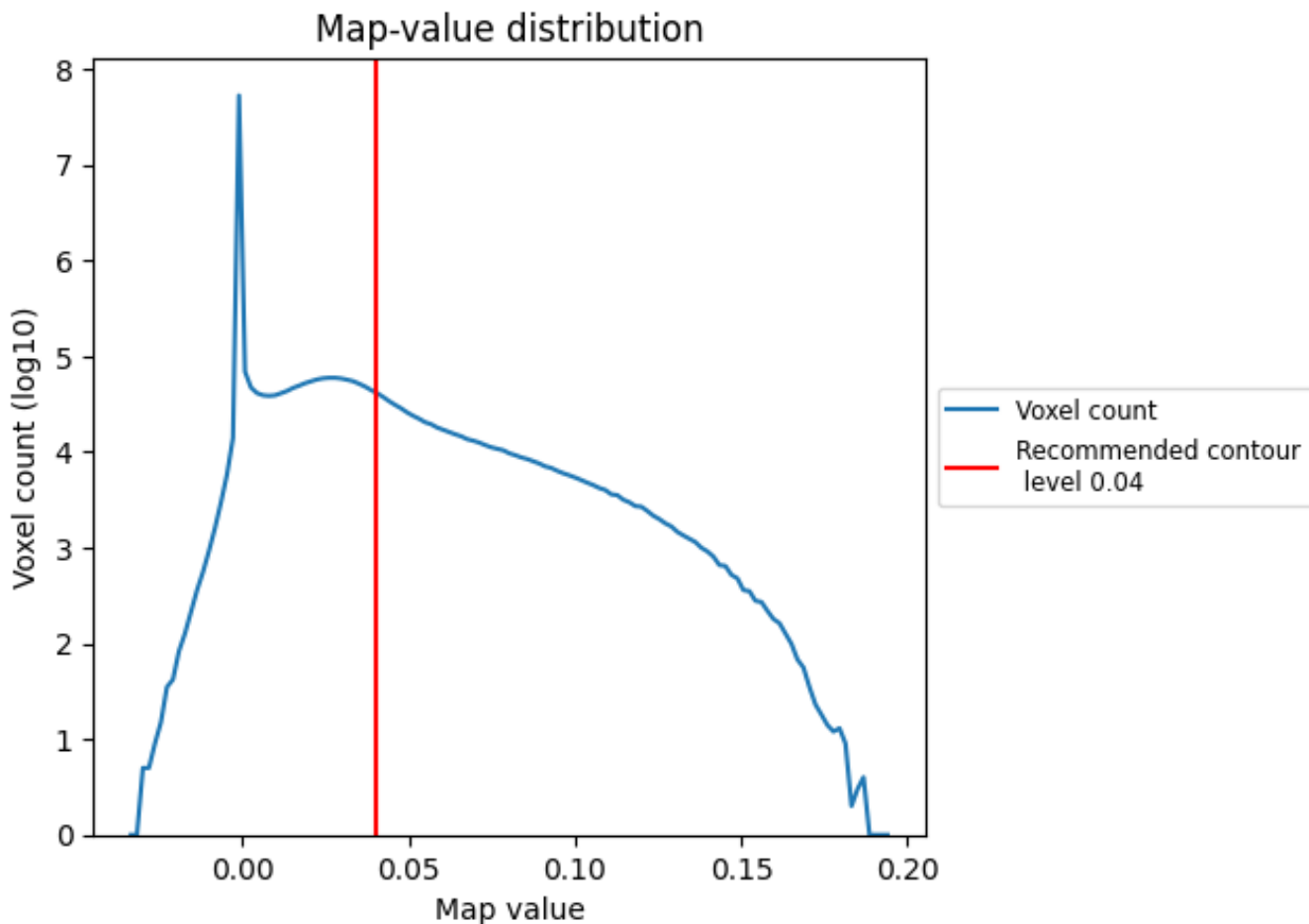
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

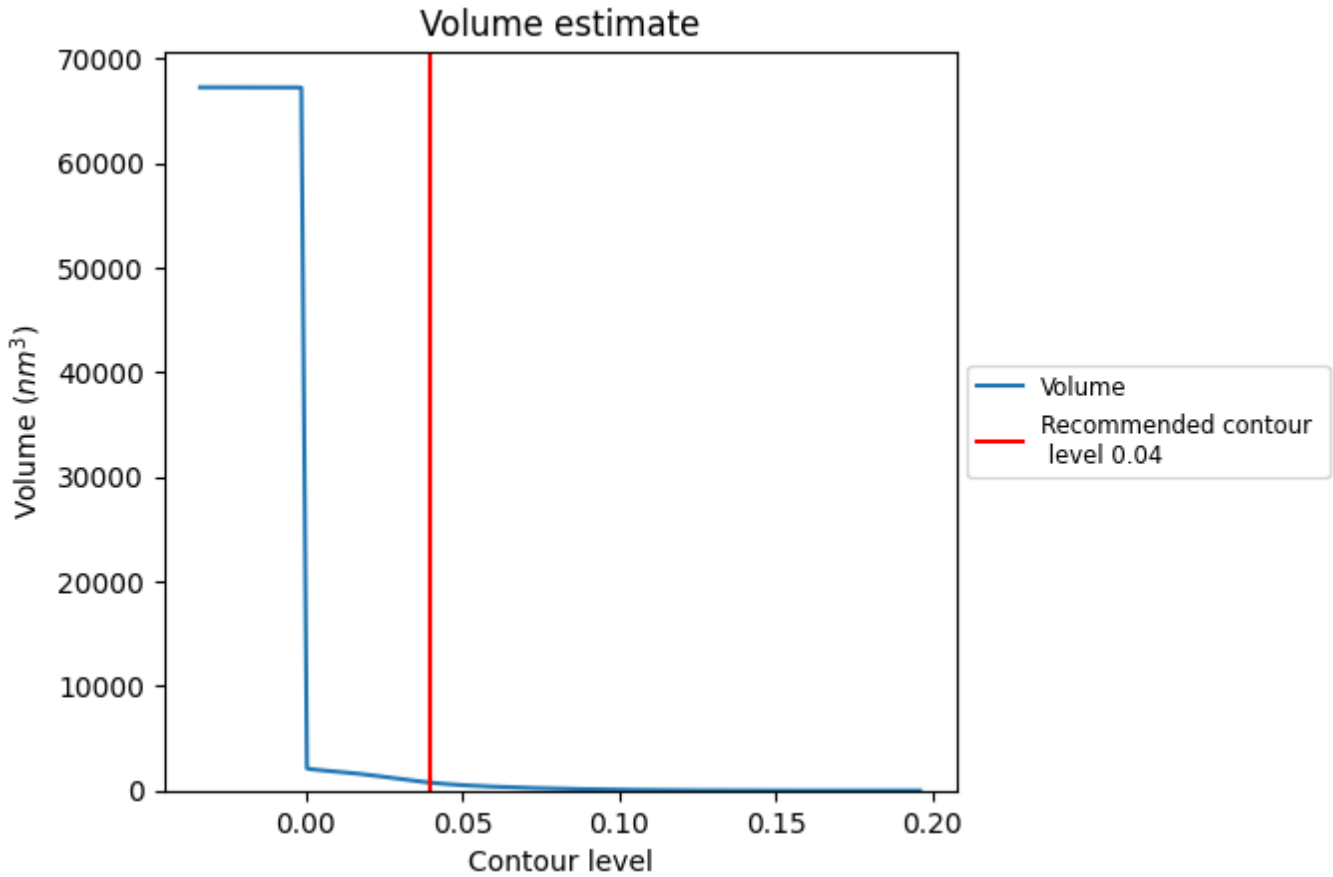
This section contains the results of statistical analysis of the map.

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.

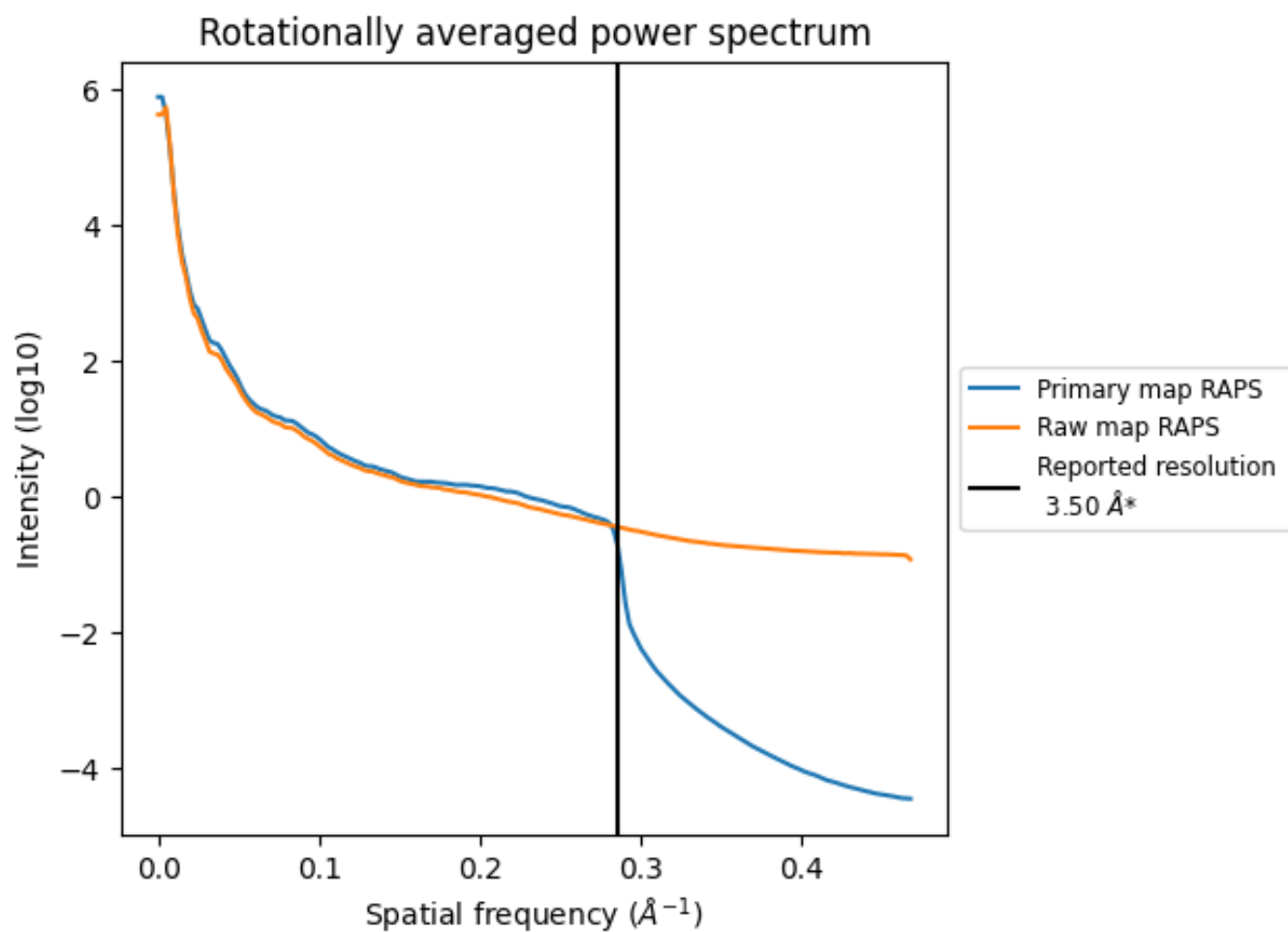
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 753 nm³; this corresponds to an approximate mass of 681 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

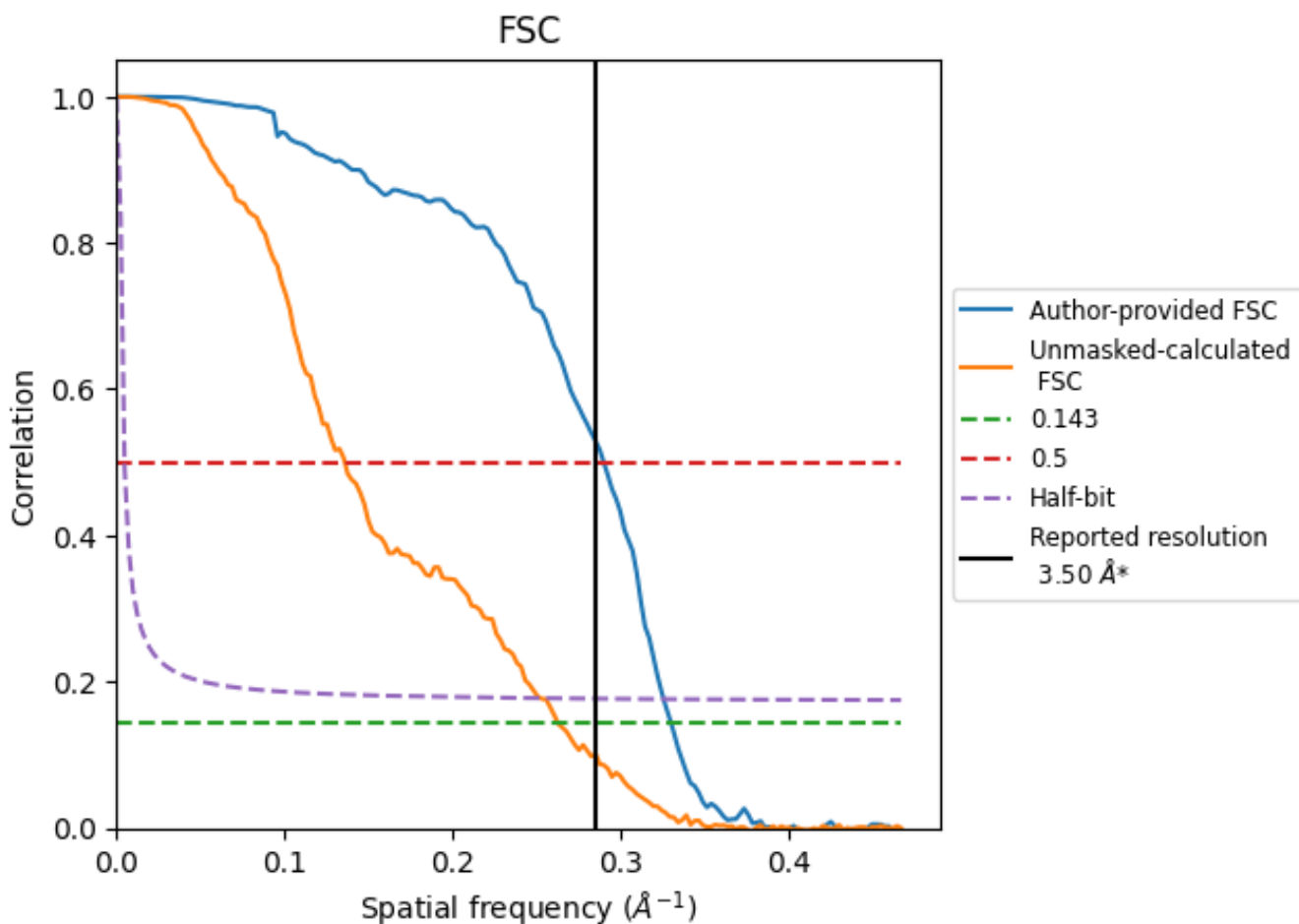


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

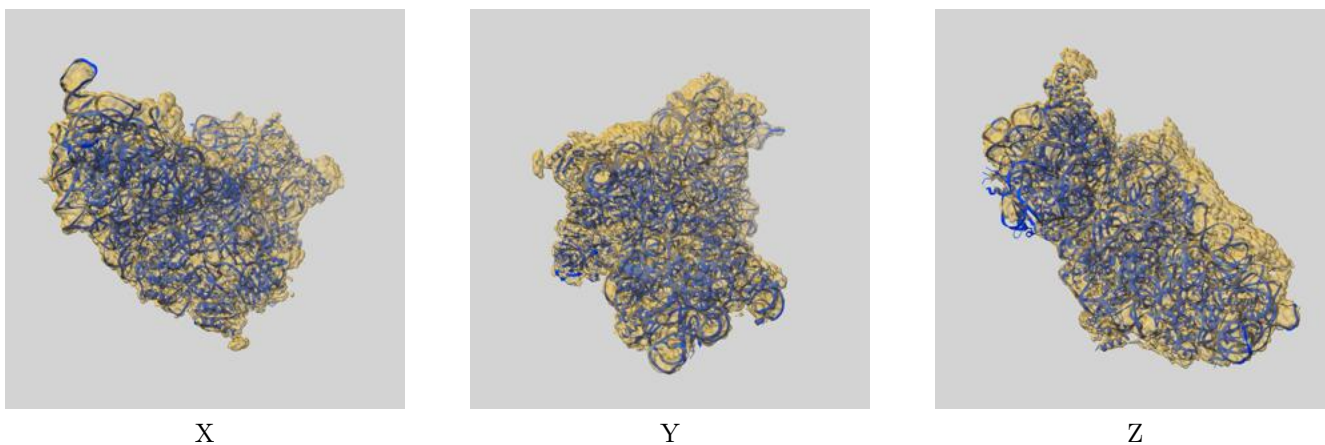
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.50
Author-provided FSC curve	3.03	3.45	3.07	-
Unmasked-calculated*	3.80	7.35	3.96	-

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

9 Map-model fit [i](#)

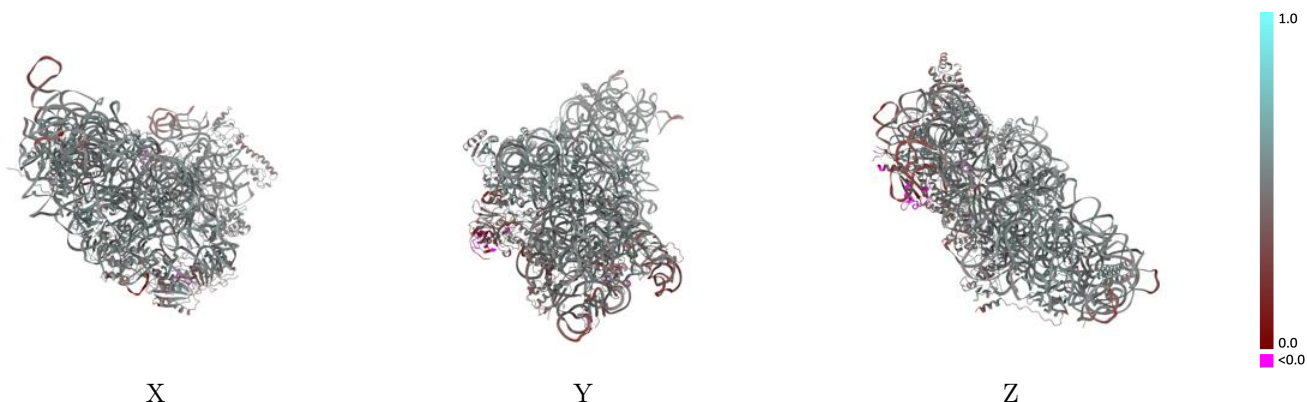
This section contains information regarding the fit between EMDB map EMD-37561 and PDB model 8WI9. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



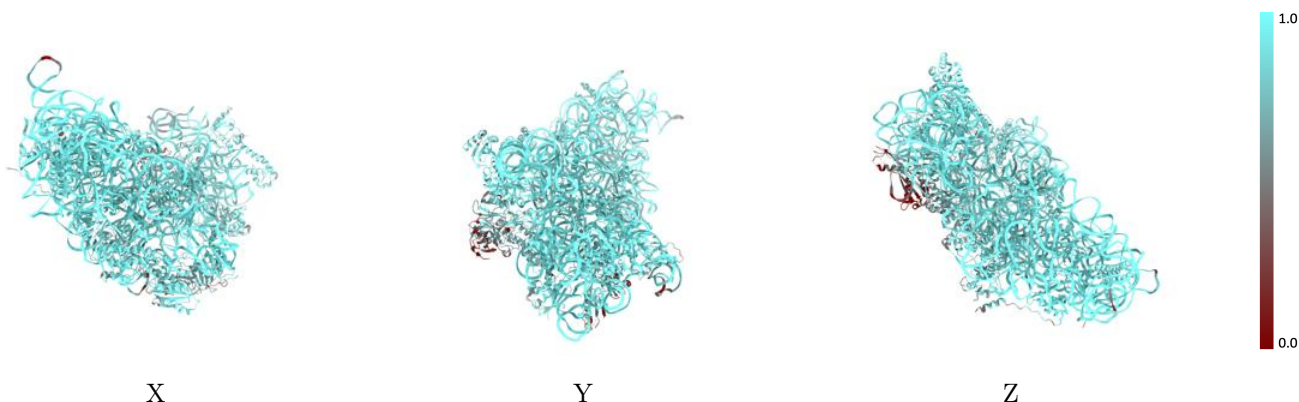
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



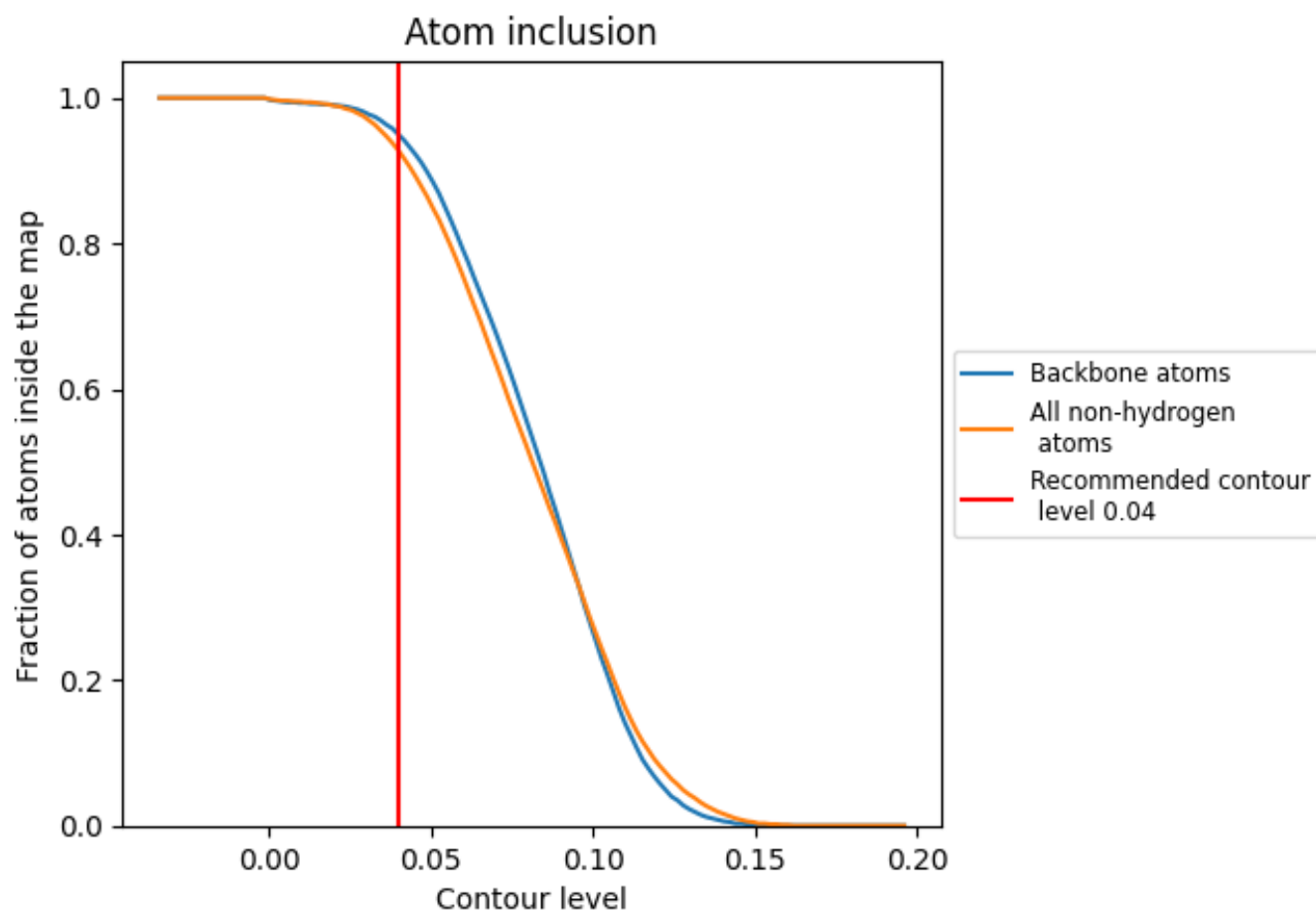
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9280	 0.4770
a	 0.9830	 0.4880
b	 0.4490	 0.2600
c	 0.8170	 0.4180
d	 0.5850	 0.3930
e	 0.9080	 0.4940
f	 0.9170	 0.5110
g	 0.9000	 0.4860
h	 0.9090	 0.4780
i	 0.9610	 0.5240
j	 0.8870	 0.4630
k	 0.6900	 0.4280
l	 0.9510	 0.5100
m	 0.9610	 0.5300
n	 0.9360	 0.4660
o	 0.8750	 0.4840
p	 0.9450	 0.5040
q	 0.9040	 0.5030
r	 0.9590	 0.5180
s	 0.9290	 0.4890
t	 0.9020	 0.4800
u	 0.9580	 0.5090
v	 0.9920	 0.5000
w	 0.7770	 0.4190
x	 0.7700	 0.3980

