



## wwPDB EM Validation Summary Report ⓘ

Jul 3, 2024 – 07:07 pm BST

PDB ID : 8BYV  
EMDB ID : EMD-16334  
Title : Cryo-EM structure of a Staphylococcus aureus 30S-RbfA complex  
Authors : Bikmullin, A.G.; Fatkhullin, B.; Stetsenko, A.; Guskov, A.; Yusupov, M.  
Deposited on : 2022-12-14  
Resolution : 2.89 Å(reported)

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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.dev92  
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) : 2.37.1

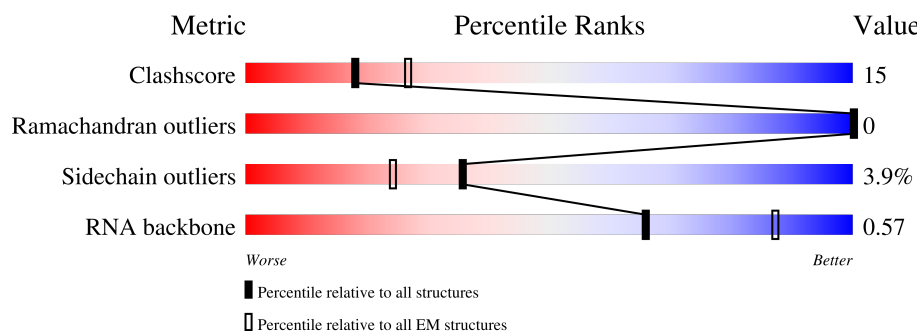
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.89 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  $\geq 3$ , 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	a	1547	
2	b	255	
3	c	217	
4	d	200	
5	e	166	
6	f	98	
7	g	156	

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Mol	Chain	Length	Quality of chain
8	h	132	
9	i	132	
10	j	102	
11	k	129	
12	l	137	
13	m	121	
14	n	61	
15	o	89	
16	p	91	
17	q	87	
18	r	80	
19	s	92	
20	t	83	
21	A	116	

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 51866 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1533	Total	C	N	O	P	0	0
			32835	14659	5988	10655	1533		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	222	Total	C	N	O	S	0	0
			1774	1128	312	327	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	204	Total	C	N	O	S	0	0
			1609	1012	302	293	2		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	197	Total	C	N	O	S	0	0
			1600	1009	300	289	2		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	154	Total	C	N	O	S	0	0
			1154	725	211	216	2		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	94	Total	C	N	O	S	0	0
			781	494	137	147	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	140	Total	C	N	O	S	0	0
			1120	700	210	206	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	128	Total	C	N	O	S	0	0
			1017	629	203	184	1		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	99	Total	C	N	O	S	0	0
			791	498	144	147	2		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	118	Total	C	N	O	S	0	0
			880	543	169	165	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	110	Total	C	N	O	S	0	0
			877	537	175	164	1		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	85	Total	C	N	O	S	0	0
			698	441	125	131	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	58	Total	C	N	O	S	0	0
			478	303	90	83	2		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	82	Total	C	N	O	S	0	0
			661	426	118	115	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

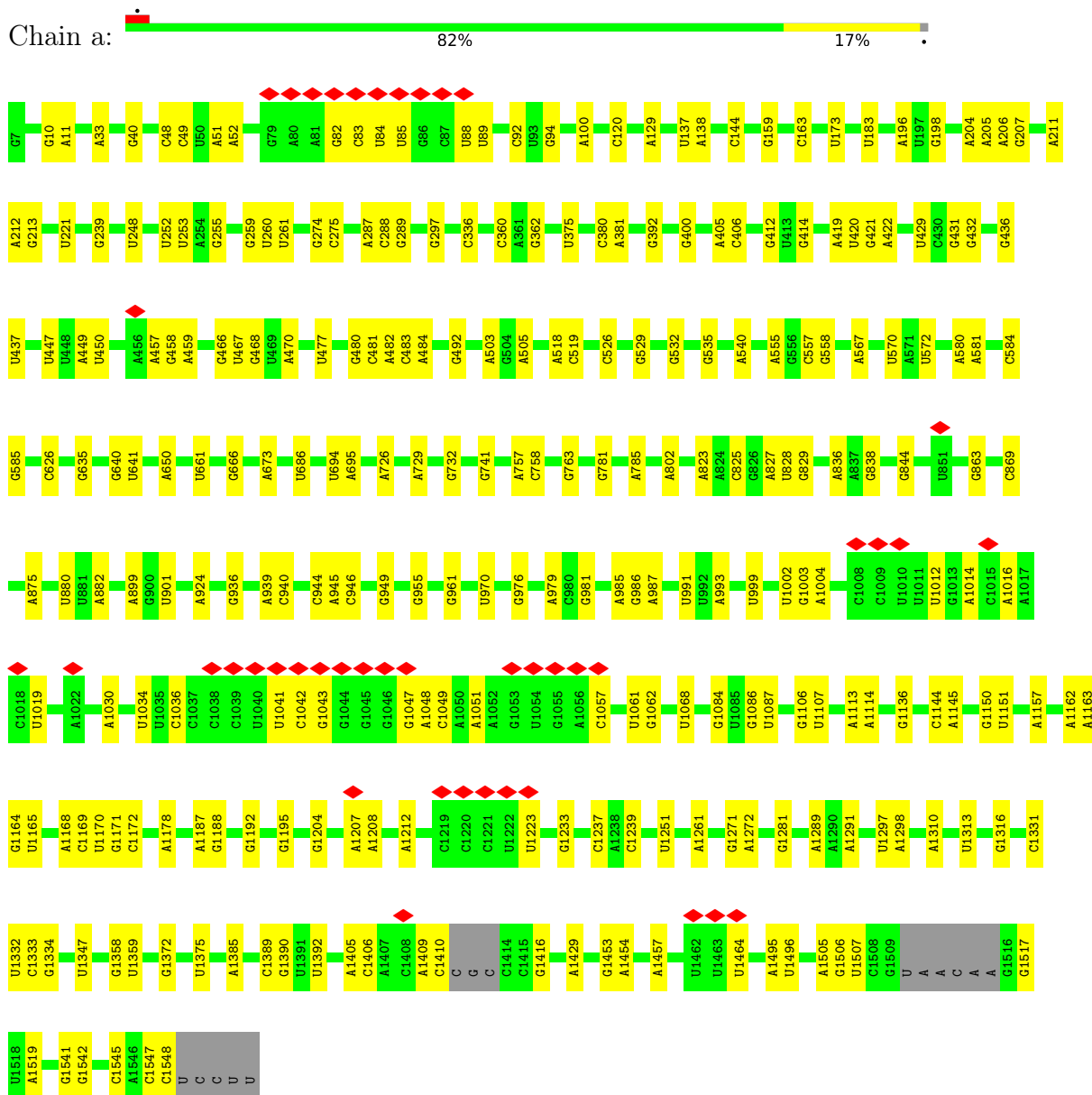
- Molecule 21 is a protein called Ribosome-binding factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	116	Total	C	N	O	S	0	0
			943	590	165	180	8		

### 3 Residue-property plots

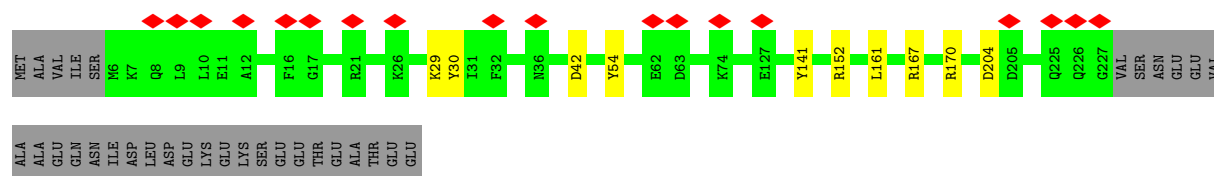
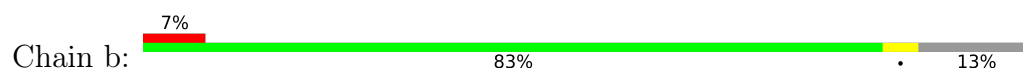
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

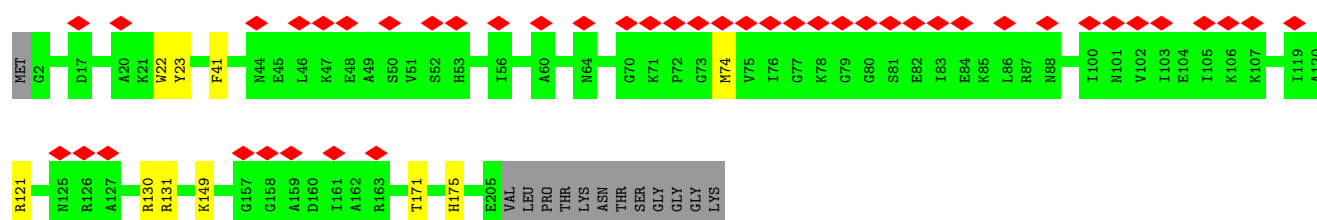
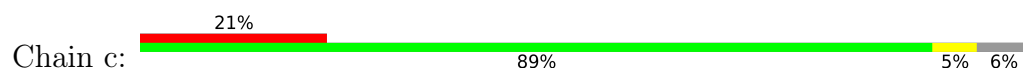


#### • Molecule 2: 30S ribosomal protein S2

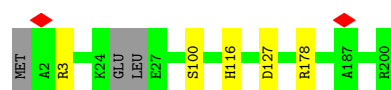




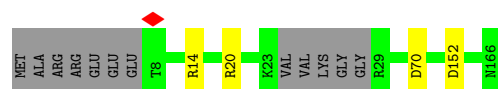
- Molecule 3: 30S ribosomal protein S3



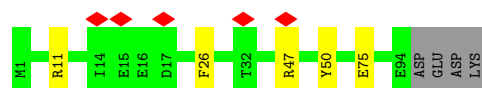
- Molecule 4: 30S ribosomal protein S4



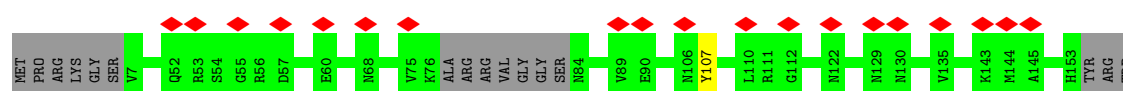
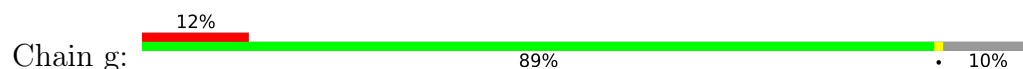
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

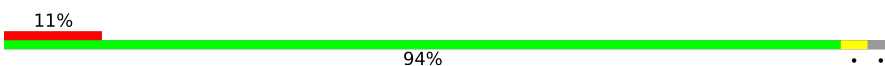


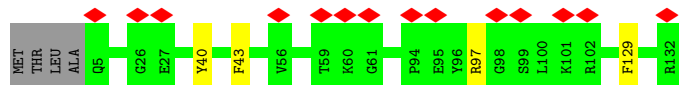
- Molecule 8: 30S ribosomal protein S8

Chain h:  97%

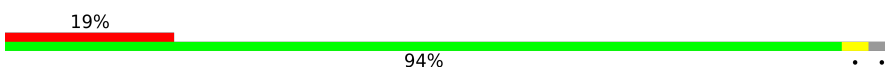


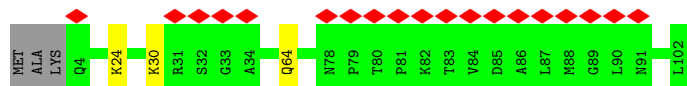
- Molecule 9: 30S ribosomal protein S9

Chain i:  11% 94%

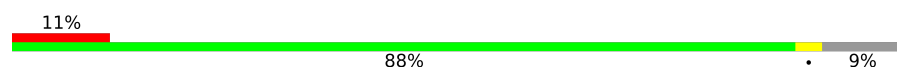


- Molecule 10: 30S ribosomal protein S10

Chain j:  19% 94%



- Molecule 11: 30S ribosomal protein S11

Chain k:  11% 88% 9%

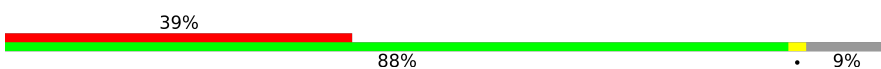


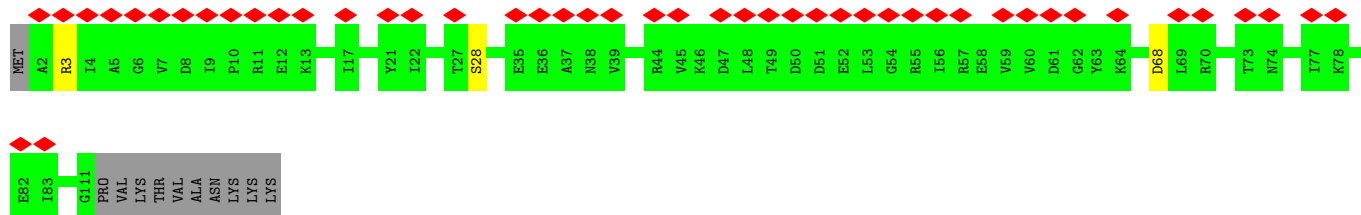
- Molecule 12: 30S ribosomal protein S12

Chain l:  95%



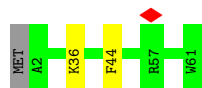
- Molecule 13: 30S ribosomal protein S13

Chain m:  39% 88% 9%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain n:  95%



- Molecule 15: 30S ribosomal protein S15

Chain o:  97%




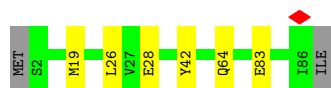
- Molecule 16: 30S ribosomal protein S16

Chain p:  97%



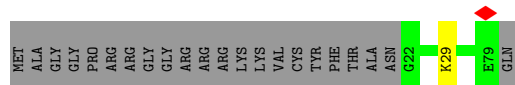
- Molecule 17: 30S ribosomal protein S17

Chain q:  91% 7%




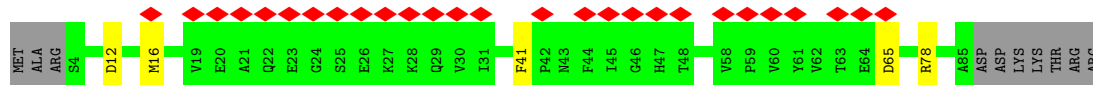
- Molecule 18: 30S ribosomal protein S18

Chain r:  71% 28%



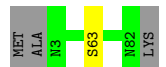
- Molecule 19: 30S ribosomal protein S19

Chain s:  29% 84% 5% 11%

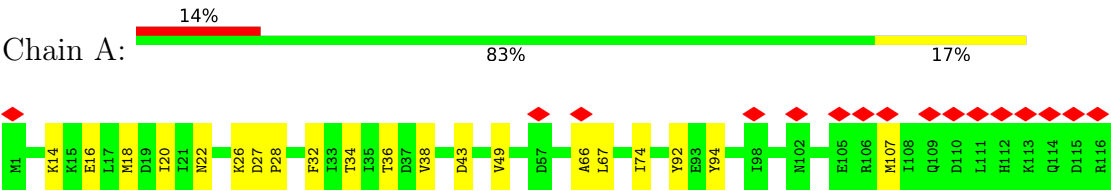


- Molecule 20: 30S ribosomal protein S20

Chain t:  95%



● Molecule 21: Ribosome-binding factor A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81421	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	53.3	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.124	Depositor
Minimum map value	-0.326	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	378.13998, 378.13998, 378.13998	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.022, 1.022, 1.022	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	a	0.33	0/36760	0.78	0/57322
2	b	0.26	0/1800	0.53	0/2414
3	c	0.25	0/1631	0.54	0/2190
4	d	0.30	0/1629	0.56	0/2185
5	e	0.29	0/1167	0.58	0/1572
6	f	0.28	0/792	0.62	0/1062
7	g	0.24	0/1135	0.58	0/1528
8	h	0.29	0/1044	0.57	0/1401
9	i	0.25	0/1033	0.58	0/1386
10	j	0.24	0/803	0.55	0/1082
11	k	0.26	0/895	0.56	0/1207
12	l	0.29	0/1075	0.58	0/1439
13	m	0.23	0/883	0.60	0/1182
14	n	0.24	0/512	0.57	0/678
15	o	0.27	0/747	0.56	0/996
16	p	0.31	0/723	0.54	0/971
17	q	0.29	0/706	0.55	0/944
18	r	0.26	0/485	0.57	0/648
19	s	0.25	0/679	0.52	0/912
20	t	0.24	0/606	0.45	0/810
21	A	0.26	0/952	0.58	0/1268
All	All	0.31	0/56057	0.72	0/83197

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

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	32835	0	16531	0	0
2	b	1774	0	1822	0	0
3	c	1609	0	1668	0	0
4	d	1600	0	1628	0	0
5	e	1154	0	1211	0	0
6	f	781	0	784	0	0
7	g	1120	0	1150	0	0
8	h	1032	0	1082	0	0
9	i	1017	0	1039	0	0
10	j	791	0	829	0	0
11	k	880	0	899	0	0
12	l	1058	0	1130	0	0
13	m	877	0	919	0	0
14	n	502	0	527	0	0
15	o	738	0	769	0	0
16	p	712	0	744	0	0
17	q	698	0	738	0	0
18	r	478	0	510	0	0
19	s	661	0	664	0	0
20	t	606	0	650	0	0
21	A	943	0	974	11	0
All	All	51866	0	36268	11	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 15.

The worst 5 of 11 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)
21:A:28:PRO:HB3	21:A:66:ALA:HB1	1.72	0.70
21:A:18:MET:HE1	21:A:22:ASN:ND2	2.14	0.62
21:A:38:VAL:HG22	21:A:49:VAL:HG13	1.83	0.59
21:A:26:LYS:HG3	21:A:27:ASP:N	2.18	0.58
21:A:74:ILE:HD13	21:A:92:TYR:OH	2.05	0.56

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	
2	b	220/255 (86%)	210 (96%)	10 (4%)	0	100	100
3	c	202/217 (93%)	196 (97%)	6 (3%)	0	100	100
4	d	193/200 (96%)	182 (94%)	11 (6%)	0	100	100
5	e	150/166 (90%)	145 (97%)	5 (3%)	0	100	100
6	f	92/98 (94%)	86 (94%)	6 (6%)	0	100	100
7	g	136/156 (87%)	133 (98%)	3 (2%)	0	100	100
8	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
9	i	126/132 (96%)	118 (94%)	8 (6%)	0	100	100
10	j	97/102 (95%)	93 (96%)	4 (4%)	0	100	100
11	k	116/129 (90%)	110 (95%)	6 (5%)	0	100	100
12	l	133/137 (97%)	125 (94%)	8 (6%)	0	100	100
13	m	108/121 (89%)	102 (94%)	6 (6%)	0	100	100
14	n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	p	88/91 (97%)	83 (94%)	5 (6%)	0	100	100
17	q	83/87 (95%)	76 (92%)	7 (8%)	0	100	100
18	r	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
19	s	80/92 (87%)	77 (96%)	3 (4%)	0	100	100
20	t	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
21	A	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
All	All	2345/2544 (92%)	2247 (96%)	98 (4%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	188/221 (85%)	178 (95%)	10 (5%)	22	54
3	c	165/175 (94%)	155 (94%)	10 (6%)	18	48
4	d	172/175 (98%)	167 (97%)	5 (3%)	42	76
5	e	122/131 (93%)	118 (97%)	4 (3%)	38	72
6	f	82/86 (95%)	77 (94%)	5 (6%)	18	48
7	g	120/132 (91%)	119 (99%)	1 (1%)	81	94
8	h	112/113 (99%)	109 (97%)	3 (3%)	44	77
9	i	106/109 (97%)	102 (96%)	4 (4%)	33	67
10	j	89/91 (98%)	86 (97%)	3 (3%)	37	71
11	k	94/104 (90%)	90 (96%)	4 (4%)	29	62
12	l	117/119 (98%)	112 (96%)	5 (4%)	29	62
13	m	94/104 (90%)	91 (97%)	3 (3%)	39	73
14	n	52/53 (98%)	50 (96%)	2 (4%)	33	67
15	o	80/81 (99%)	78 (98%)	2 (2%)	47	78
16	p	76/77 (99%)	74 (97%)	2 (3%)	46	77
17	q	80/82 (98%)	74 (92%)	6 (8%)	13	37
18	r	52/68 (76%)	51 (98%)	1 (2%)	57	84
19	s	71/80 (89%)	66 (93%)	5 (7%)	15	41
20	t	67/69 (97%)	66 (98%)	1 (2%)	65	87
21	A	106/106 (100%)	103 (97%)	3 (3%)	43	76
All	All	2045/2176 (94%)	1966 (96%)	79 (4%)	36	66

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	n	36	LYS
19	s	16	MET
15	o	14	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
17	q	28	GLU
20	t	63	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
17	q	5	ASN
20	t	77	GLN
21	A	22	ASN
3	c	151	GLN
7	g	28	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1530/1547 (98%)	266 (17%)	0

5 of 266 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	G
1	a	11	A
1	a	33	A
1	a	40	G
1	a	48	C

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [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.

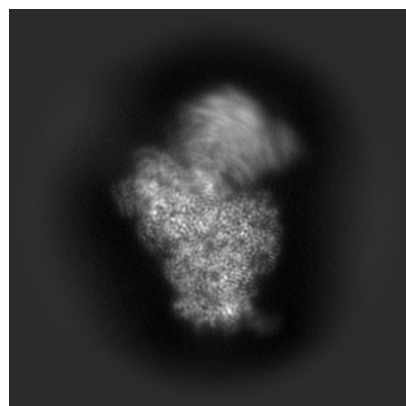
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16334. These allow visual inspection of the internal detail of the map and identification of artifacts.

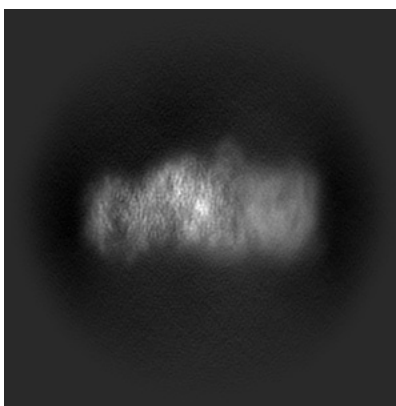
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

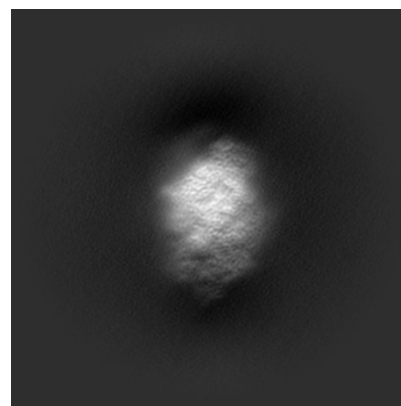
#### 6.1.1 Primary map



X

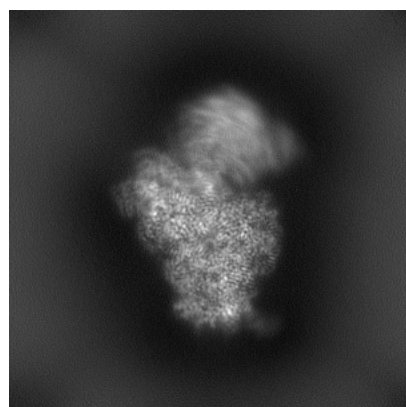


Y

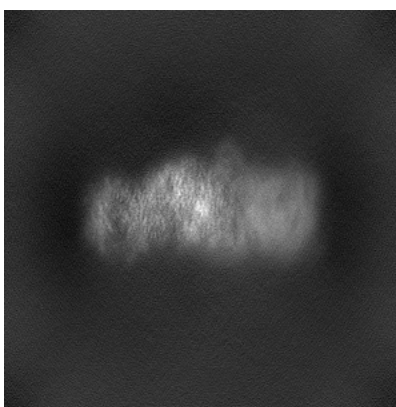


Z

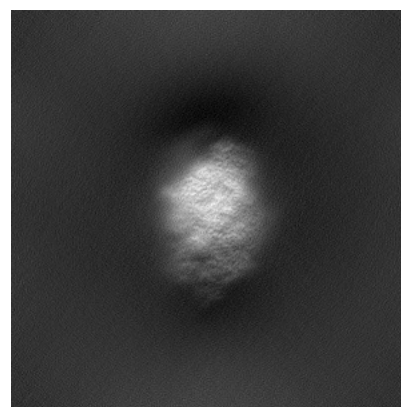
#### 6.1.2 Raw map



X



Y

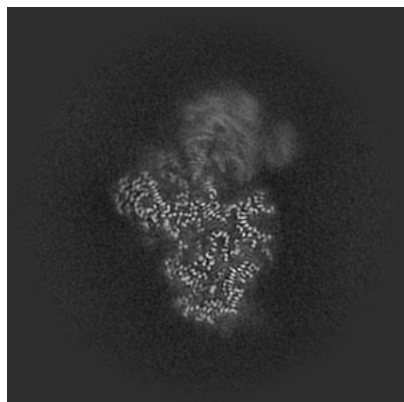


Z

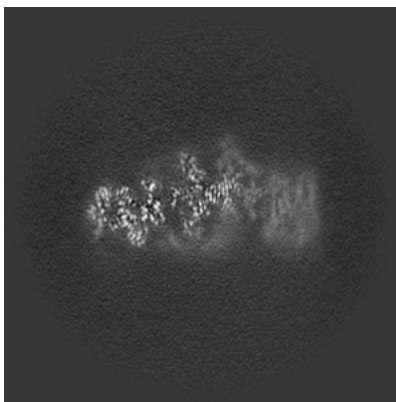
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

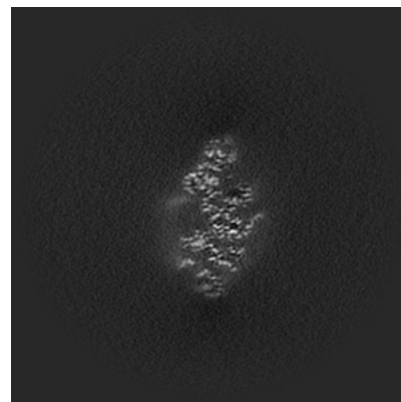
### 6.2.1 Primary map



X Index: 185

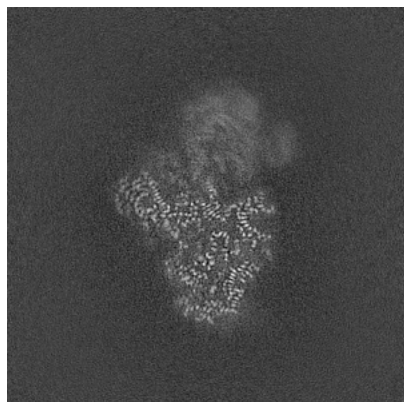


Y Index: 185

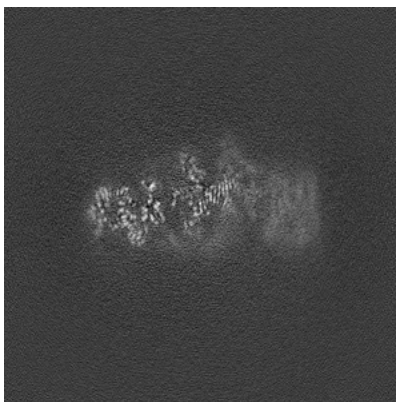


Z Index: 185

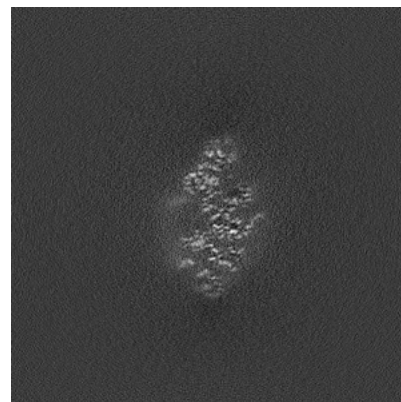
### 6.2.2 Raw map



X Index: 185



Y Index: 185

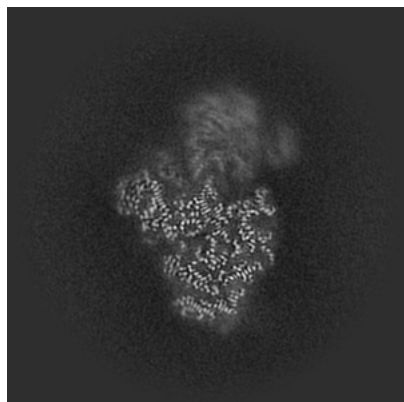


Z Index: 185

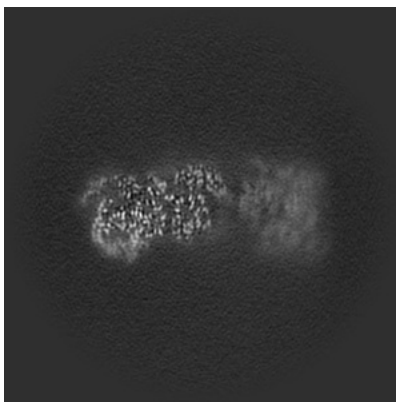
The images above show central slices of the map in three orthogonal directions.

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

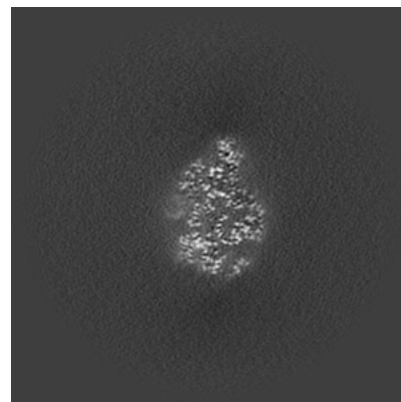
### 6.3.1 Primary map



X Index: 188



Y Index: 199

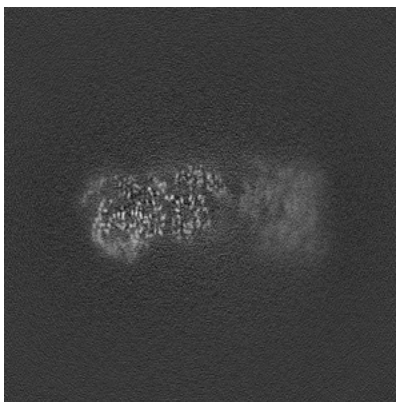


Z Index: 175

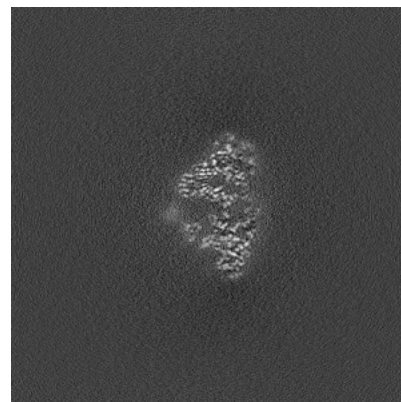
### 6.3.2 Raw map



X Index: 188



Y Index: 199



Z Index: 161

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

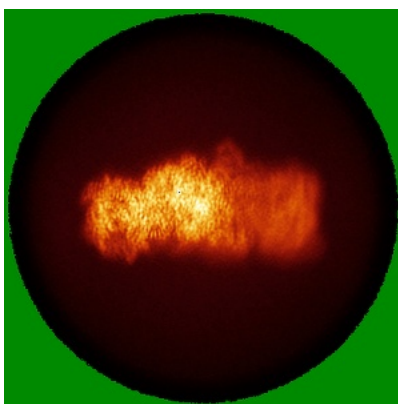


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

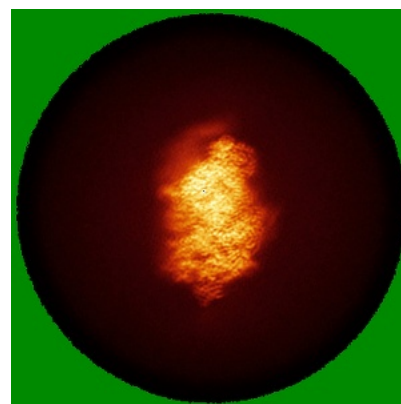
### 6.4.1 Primary map



X



Y

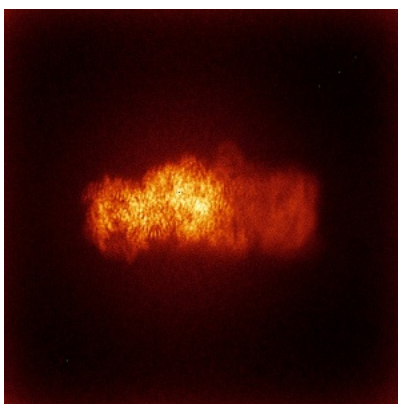


Z

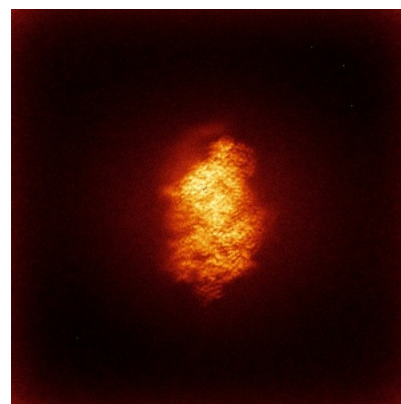
### 6.4.2 Raw map



X



Y

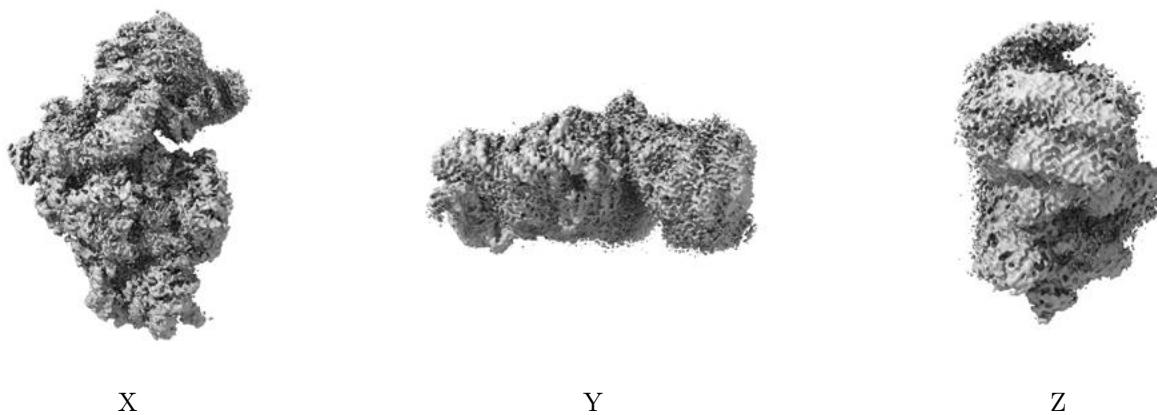


Z

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.

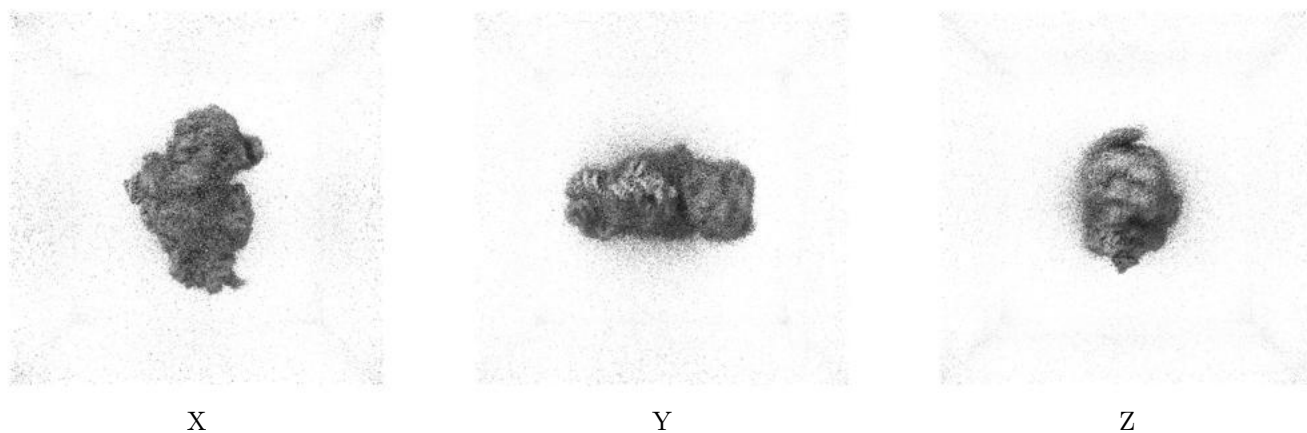
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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](#)

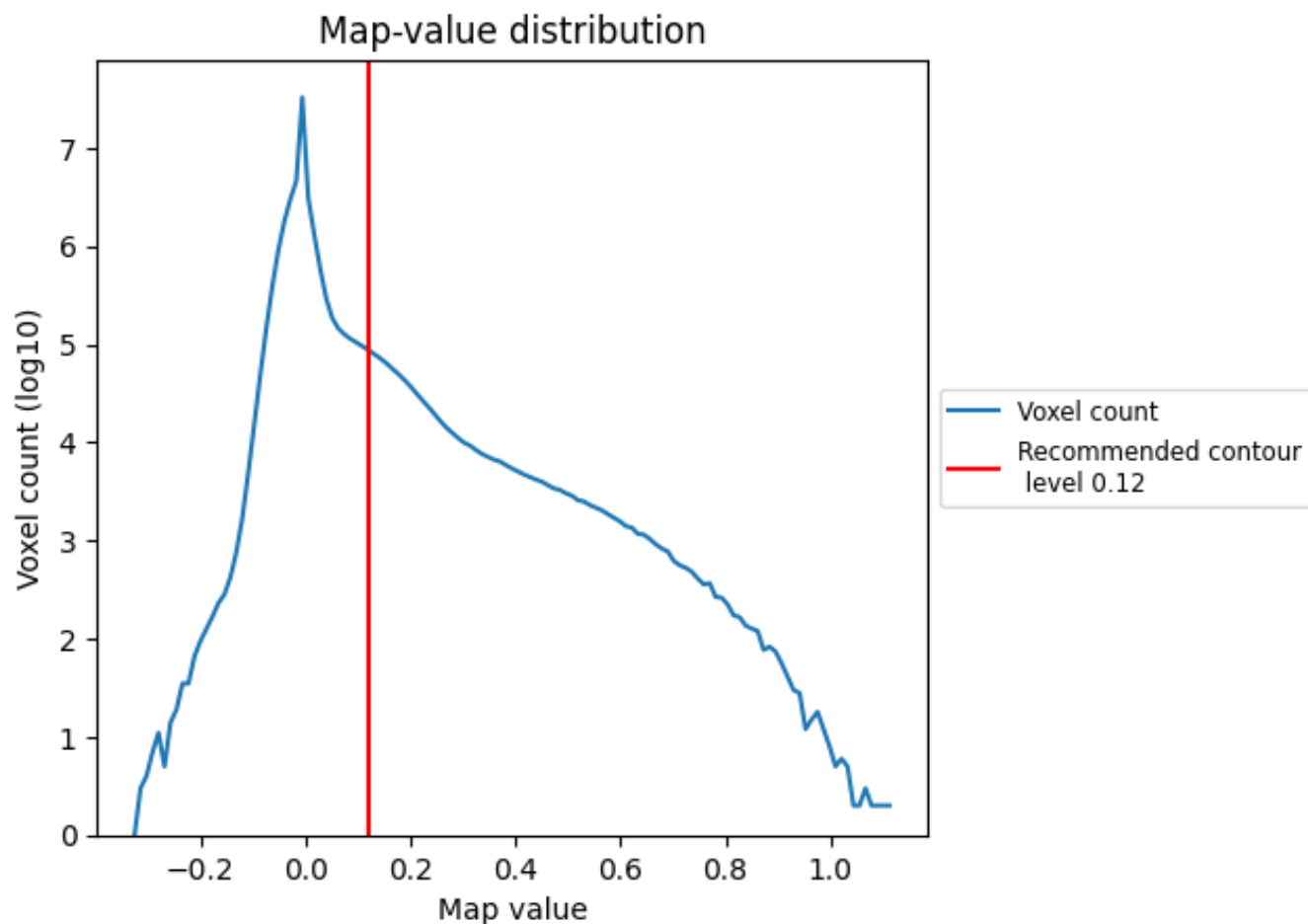
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

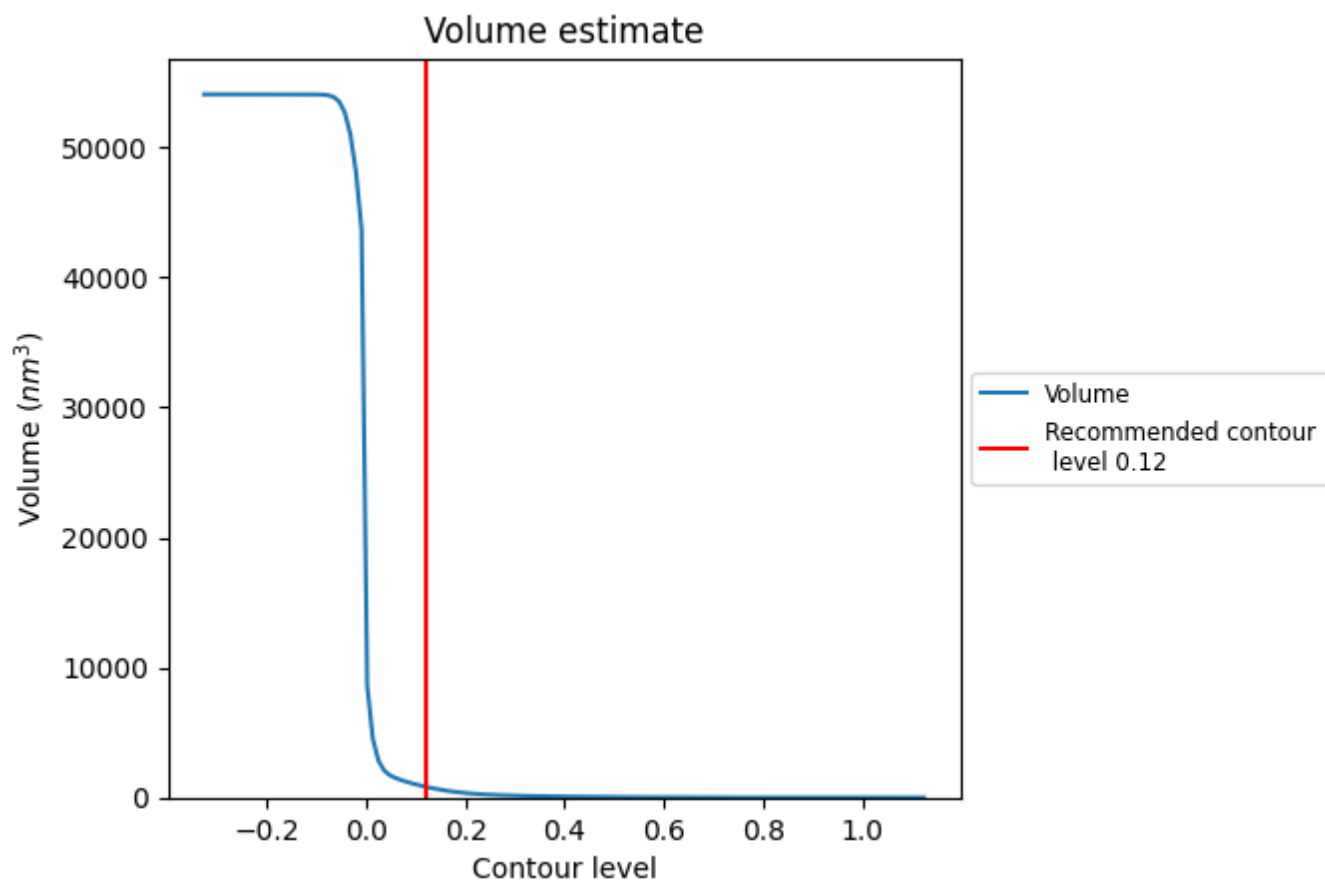
This section contains the results of statistical analysis of the map.

### 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.

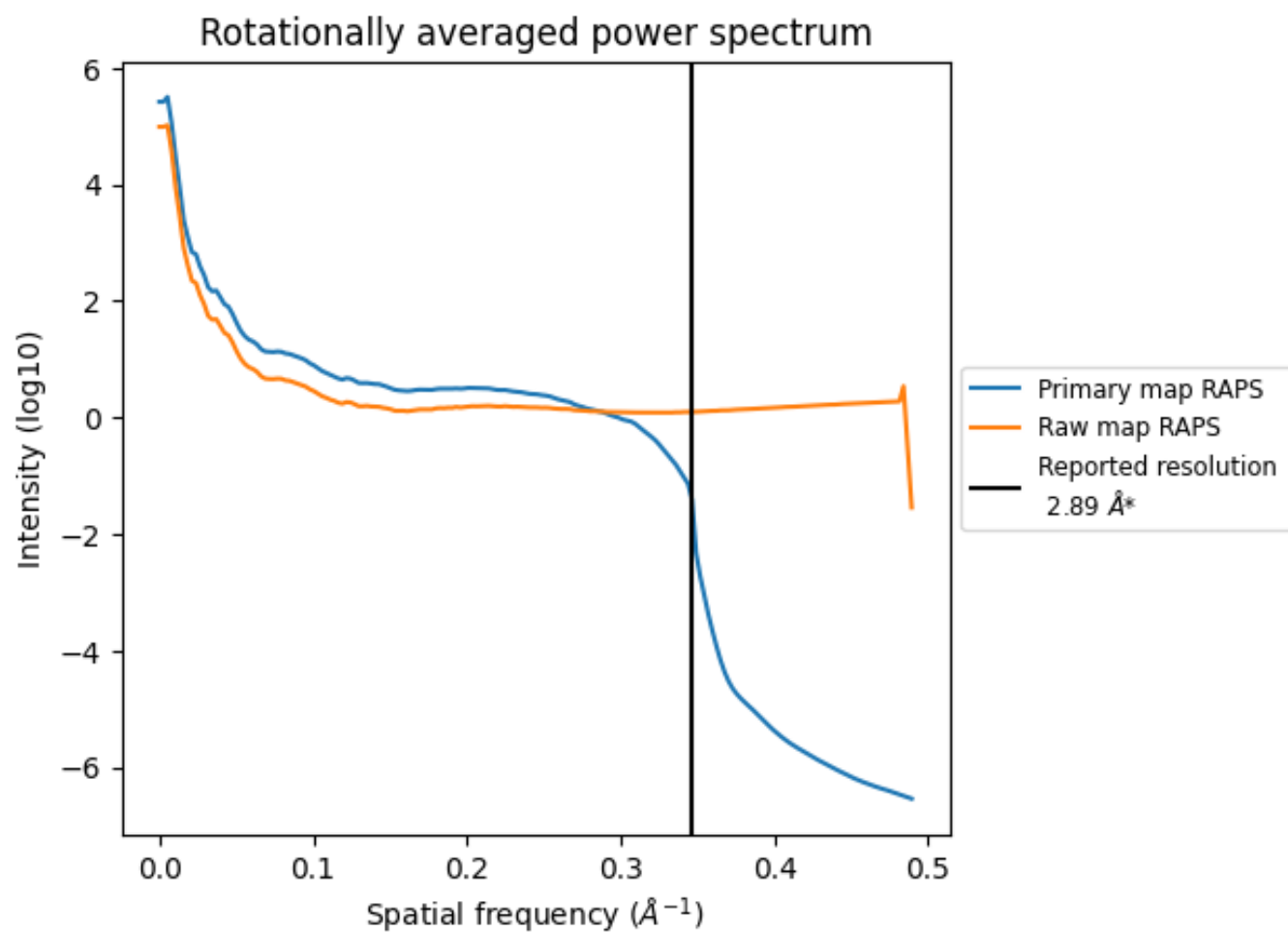
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 833 nm<sup>3</sup>; this corresponds to an approximate mass of 752 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 ⓘ

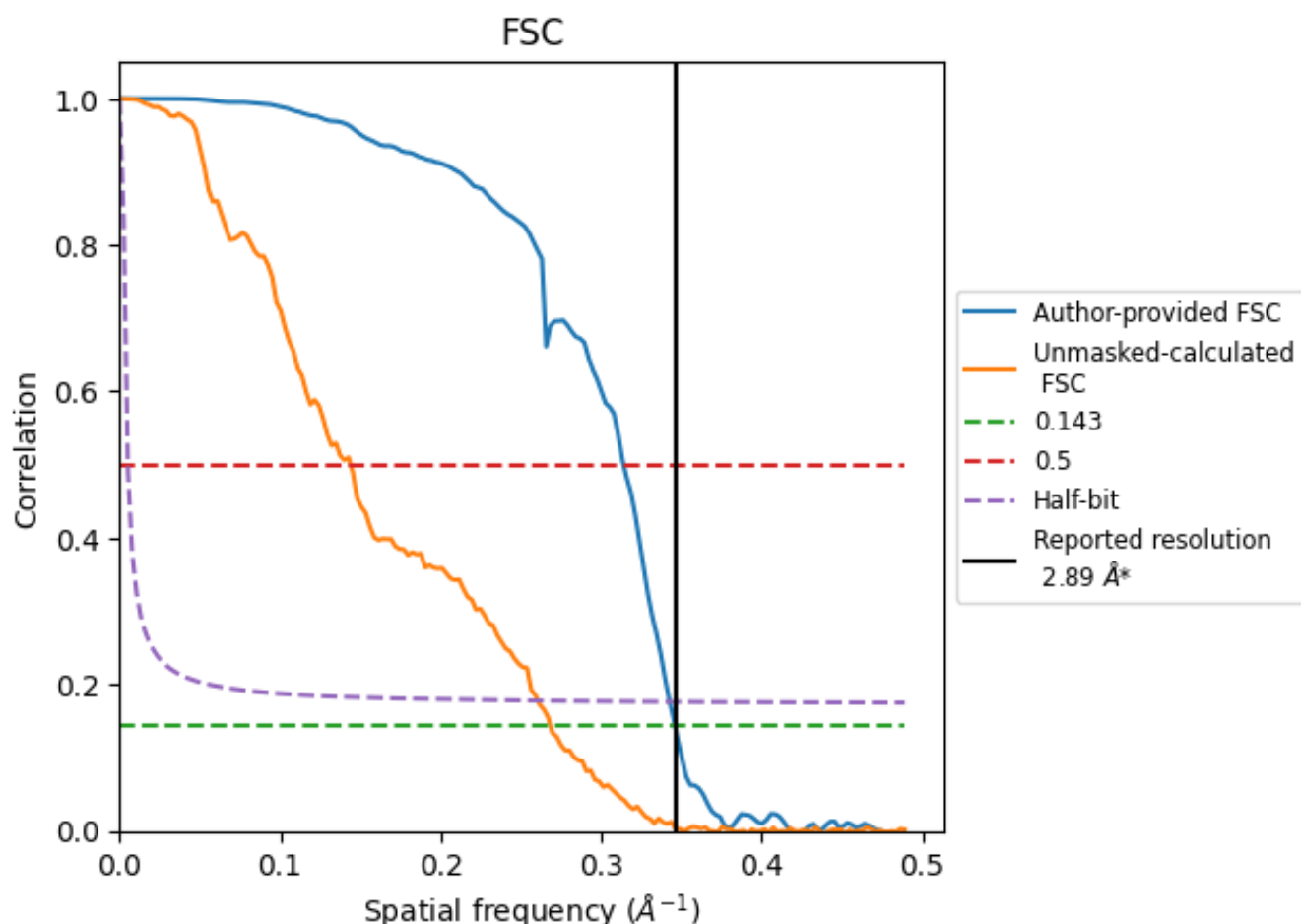


\*Reported resolution corresponds to spatial frequency of 0.346  $\text{\AA}^{-1}$

## 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 0.346 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

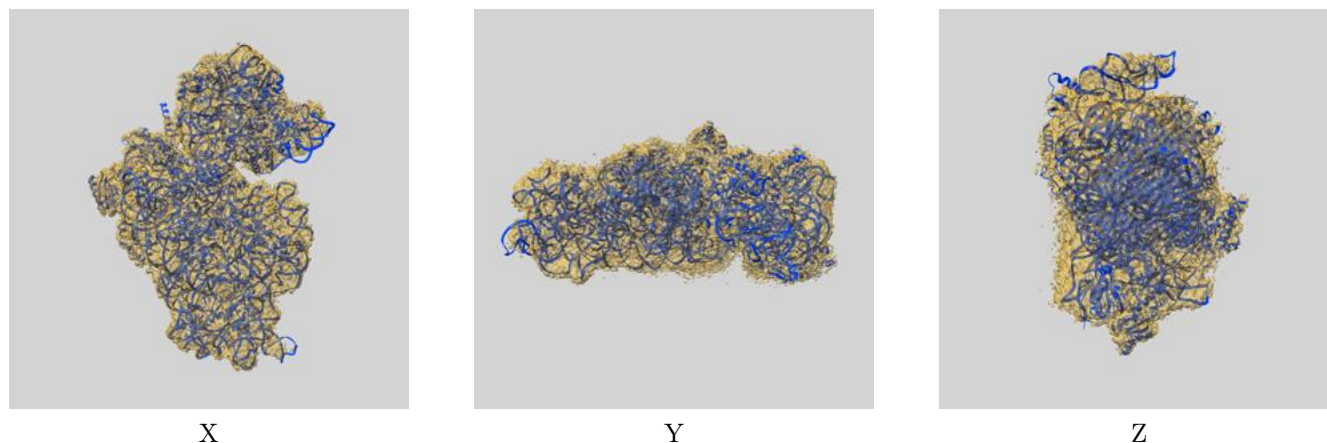
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.18	2.92
Unmasked-calculated*	3.72	6.94	3.84

\*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 3.72 differs from the reported value 2.89 by more than 10 %

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

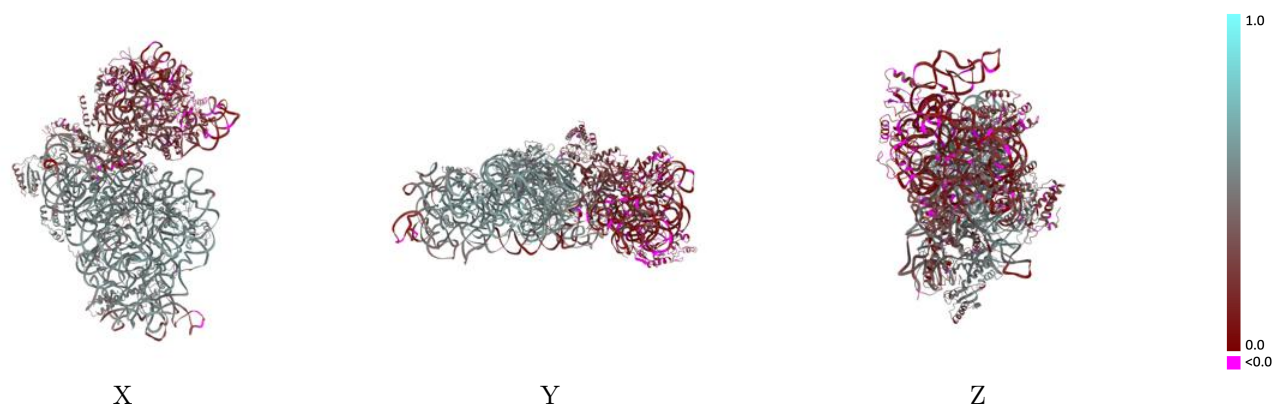
This section contains information regarding the fit between EMDB map EMD-16334 and PDB model 8BYV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



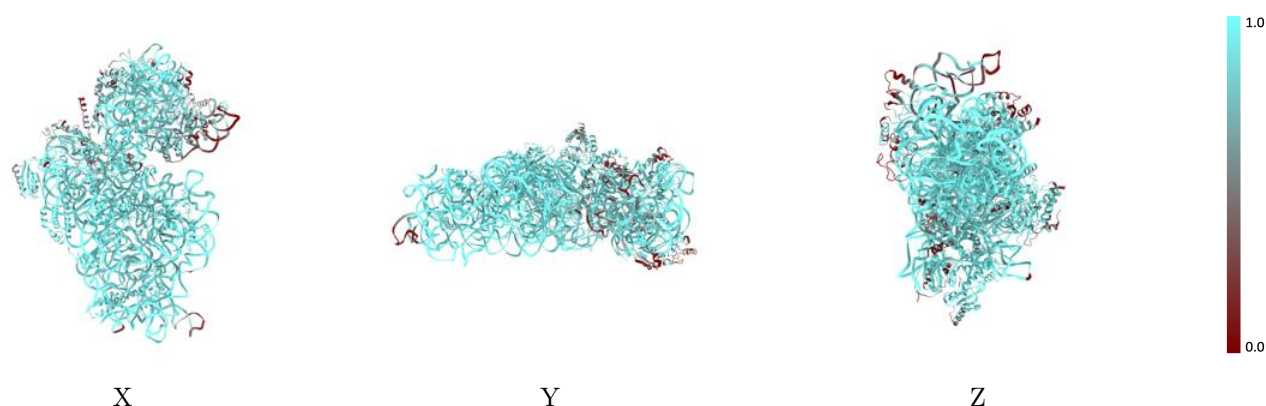
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



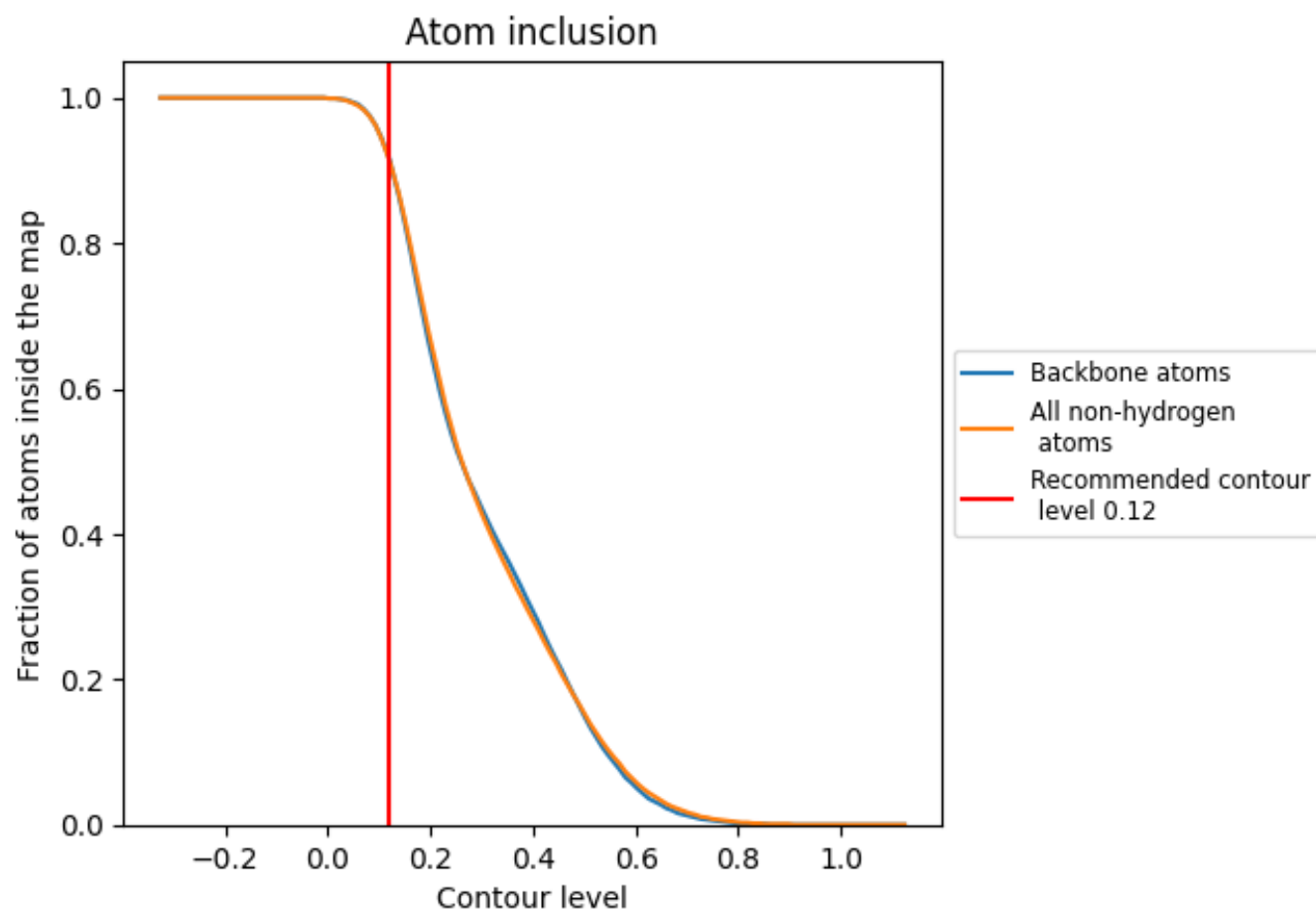
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion ⓘ















































At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.3830
A	 0.7660	 0.3510
a	 0.9530	 0.3990
b	 0.8050	 0.2660
c	 0.6860	 0.2170
d	 0.9840	 0.5230
e	 0.9580	 0.5100
f	 0.8520	 0.4110
g	 0.7470	 0.2050
h	 0.9900	 0.5360
i	 0.8450	 0.1870
j	 0.7850	 0.1600
k	 0.7670	 0.3270
l	 0.9870	 0.5420
m	 0.5240	 0.1110
n	 0.9040	 0.1390
o	 0.9550	 0.5160
p	 0.9730	 0.5200
q	 0.9650	 0.5050
r	 0.9740	 0.4860
s	 0.6050	 0.0980
t	 0.9770	 0.5080

