



## wwPDB EM Validation Summary Report ⓘ

Dec 30, 2024 – 10:35 AM EST

PDB ID : 8C83  
EMDB ID : EMD-16470  
Title : Cryo-EM structure of in vitro reconstituted Otu2-bound Ub-40S complex  
Authors : Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.  
Deposited on : 2023-01-18  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

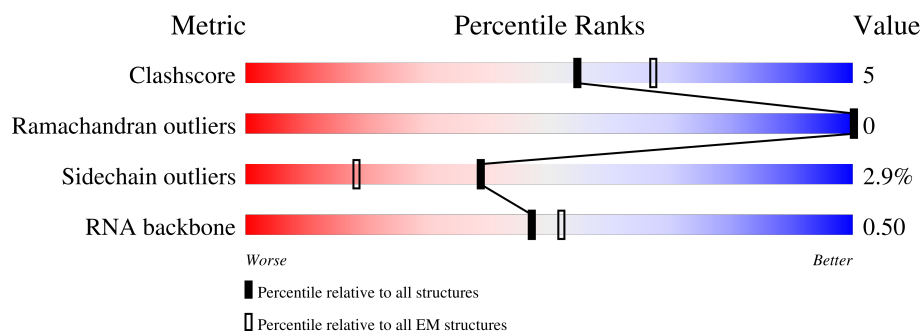
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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




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

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

Mol	Chain	Length	Quality of chain
1	x	307	
2	y	76	
3	2	1800	
4	P	252	
5	R	254	
6	S	261	
7	T	236	

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Mol	Chain	Length	Quality of chain
8	U	190	
9	V	200	
10	W	197	
11	X	156	
12	Y	151	
13	a	87	
14	b	130	
15	c	145	
16	d	135	
17	f	82	
18	g	63	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 45803 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	259	Total	C	N	O	S	0	0
			1509	917	298	292	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	178	SER	CYS	engineered mutation	UNP P38747

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	y	76	Total	C	N	O	0	0
			374	222	76	76		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	19	PRO	SER	conflict	UNP P05759
y	24	GLU	ASP	conflict	UNP P05759
y	28	ALA	SER	conflict	UNP P05759

- Molecule 3 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	1177	Total	C	N	O	P	0	0
			25088	11220	4455	8236	1177		

- Molecule 4 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	U	184	Total	C	N	O	0	0
			1473	946	263	264		

- Molecule 9 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 13 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 15 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	f	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

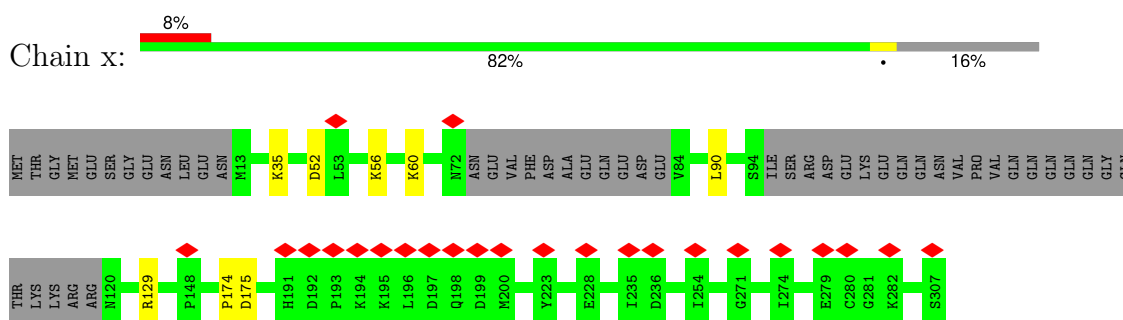
- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

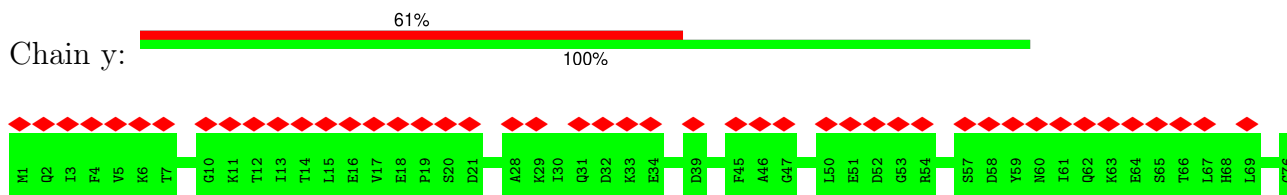
### 3 Residue-property plots [i](#)

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.

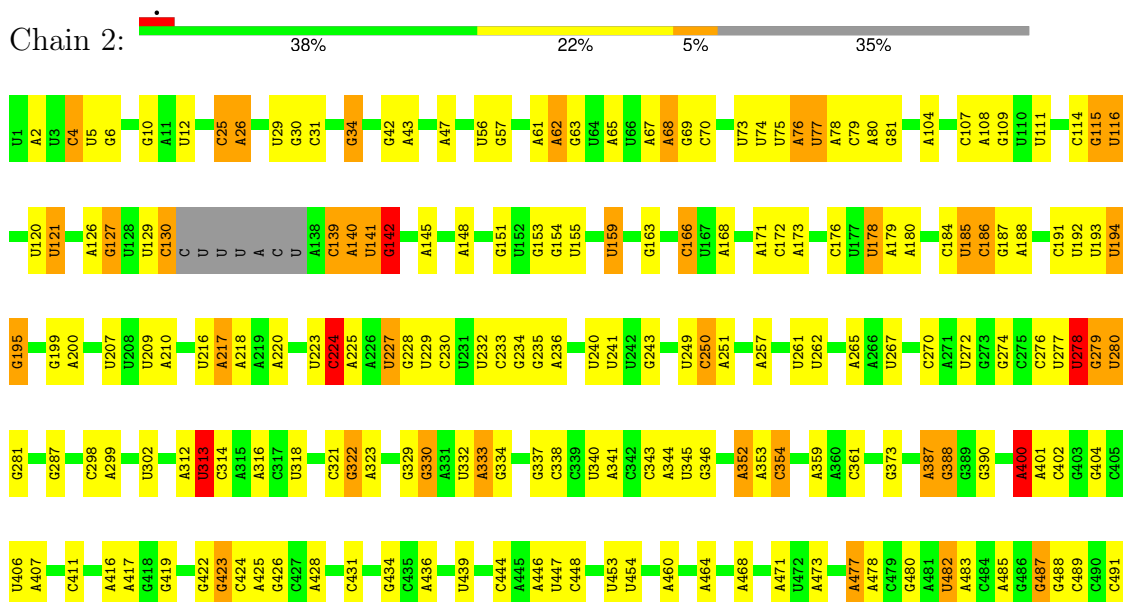
#### • Molecule 1: OTU domain-containing protein 2



#### • Molecule 2: Ubiquitin

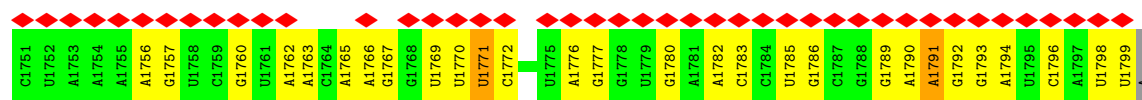


#### • Molecule 3: 18S ribosomal RNA

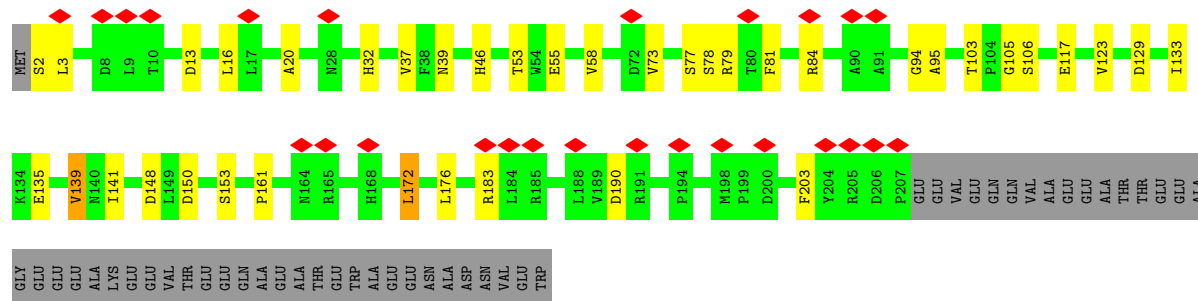




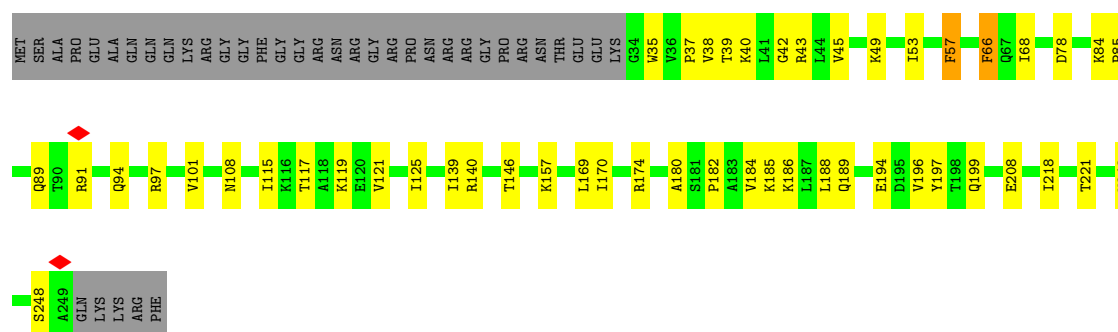




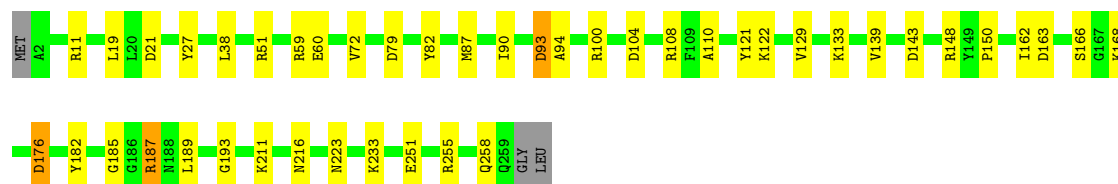
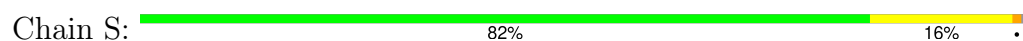
• Molecule 4: 40S ribosomal protein S0-A



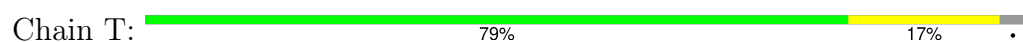
• Molecule 5: 40S ribosomal protein S2



• Molecule 6: 40S ribosomal protein S4-A



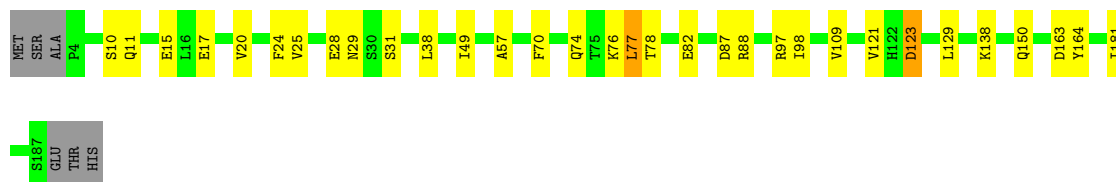
• Molecule 7: 40S ribosomal protein S6-A





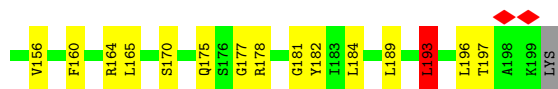
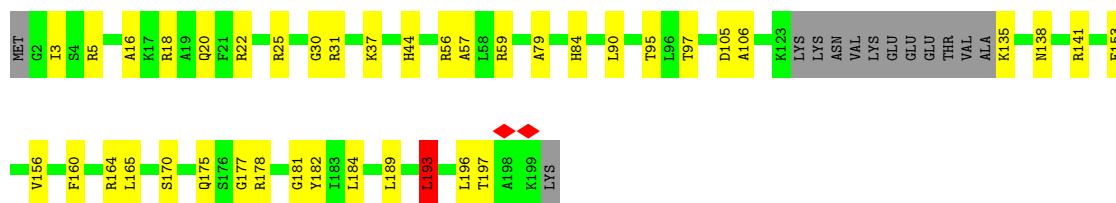
- Molecule 8: 40S ribosomal protein S7-A

Chain U: 80% 16%



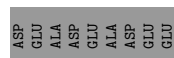
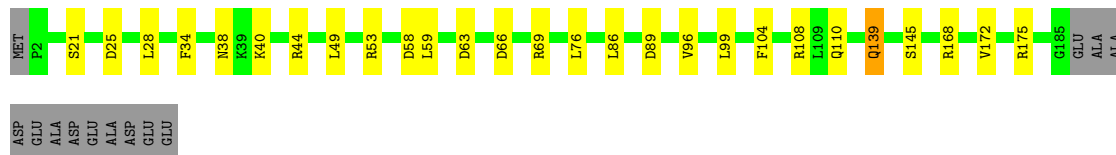
- Molecule 9: 40S ribosomal protein S8-B

Chain V: 74% 20% 6%



- Molecule 10: 40S ribosomal protein S9-A

Chain W: 80% 13% 7%



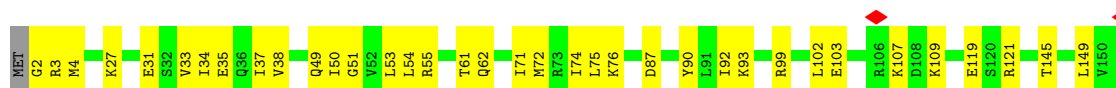
- Molecule 11: 40S ribosomal protein S11-A

Chain X: 77% 14% 9%



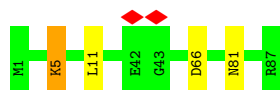
- Molecule 12: 40S ribosomal protein S13

Chain Y: 75% 24%



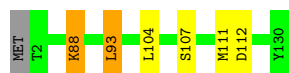
- Molecule 13: 40S ribosomal protein S21-A

Chain a:  95%



- Molecule 14: 40S ribosomal protein S22-A

Chain b:  95%



- Molecule 15: 40S ribosomal protein S23-A

Chain c:  98%



- Molecule 16: 40S ribosomal protein S24-A

Chain d:  95%



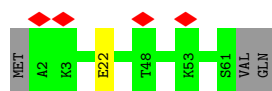
- Molecule 17: 40S ribosomal protein S27-A

Chain f:  96%



- Molecule 18: 40S ribosomal protein S30-A

Chain g:  94% 5%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.178	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	x	0.29	0/1514	0.58	4/2075 (0.2%)
2	y	0.24	0/373	0.48	0/517
3	2	0.45	0/28062	1.06	142/43713 (0.3%)
4	P	0.31	0/1644	0.75	5/2249 (0.2%)
5	R	0.39	0/1656	0.82	3/2251 (0.1%)
6	S	0.34	0/2097	0.75	4/2823 (0.1%)
7	T	0.30	0/1839	0.61	0/2460
8	U	0.31	0/1498	0.66	2/2019 (0.1%)
9	V	0.32	0/1501	0.78	3/2006 (0.1%)
10	W	0.33	0/1504	0.71	2/2016 (0.1%)
11	X	0.35	0/1168	0.71	2/1575 (0.1%)
12	Y	0.36	0/1215	0.71	1/1638 (0.1%)
13	a	0.39	0/682	0.87	2/921 (0.2%)
14	b	0.36	0/1038	0.72	3/1395 (0.2%)
15	c	0.34	0/1139	0.67	0/1518
16	d	0.38	0/1087	0.81	2/1449 (0.1%)
17	f	0.31	0/620	0.71	1/838 (0.1%)
18	g	0.37	0/480	0.73	0/639
All	All	0.40	0/49117	0.94	176/72102 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	P	0	1

There are no bond length outliers.

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	105	ASP	CB-CG-OD1	11.16	128.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	85	PRO	CA-N-CD	-10.94	96.19	111.50
9	V	193	LEU	CA-CB-CG	10.56	139.60	115.30
6	S	93	ASP	CB-CG-OD2	9.66	126.99	118.30
3	2	653	C	N1-C2-O2	9.58	124.65	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P	94	GLY	Peptide

## 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	x	1509	0	997	0	0
2	y	374	0	163	0	0
3	2	25088	0	12624	138	0
4	P	1603	0	1610	18	0
5	R	1626	0	1715	30	0
6	S	2056	0	2140	23	0
7	T	1815	0	1894	29	0
8	U	1473	0	1555	18	0
9	V	1476	0	1501	25	0
10	W	1479	0	1556	14	0
11	X	1142	0	1209	12	0
12	Y	1192	0	1255	26	0
13	a	673	0	662	0	0
14	b	1021	0	1060	0	0
15	c	1121	0	1196	0	0
16	d	1073	0	1132	0	0
17	f	610	0	633	0	0
18	g	472	0	521	0	0
All	All	45803	0	33423	291	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 5.

The worst 5 of 291 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)
3:2:1697:G:H1	3:2:1704:U:H3	1.08	0.90
3:2:1688:U:H3	3:2:1713:G:H1	1.28	0.81
3:2:699:U:H3	3:2:739:G:H1	1.26	0.81
3:2:480:G:H1	3:2:508:U:H3	1.40	0.68
8:U:70:PHE:O	8:U:74:GLN:HB2	1.94	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	x	253/307 (82%)	249 (98%)	4 (2%)	0	100	100
2	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
4	P	204/252 (81%)	182 (89%)	22 (11%)	0	100	100
5	R	214/254 (84%)	201 (94%)	13 (6%)	0	100	100
6	S	256/261 (98%)	238 (93%)	18 (7%)	0	100	100
7	T	226/236 (96%)	214 (95%)	12 (5%)	0	100	100
8	U	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
9	V	183/200 (92%)	172 (94%)	11 (6%)	0	100	100
10	W	182/197 (92%)	172 (94%)	10 (6%)	0	100	100
11	X	140/156 (90%)	131 (94%)	9 (6%)	0	100	100
12	Y	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
13	a	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
14	b	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
15	c	142/145 (98%)	131 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	d	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
17	f	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
18	g	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
All	All	2685/2922 (92%)	2521 (94%)	164 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	x	62/282 (22%)	58 (94%)	4 (6%)	14	43
4	P	170/210 (81%)	167 (98%)	3 (2%)	54	80
5	R	175/205 (85%)	171 (98%)	4 (2%)	45	75
6	S	220/222 (99%)	211 (96%)	9 (4%)	26	60
7	T	189/201 (94%)	185 (98%)	4 (2%)	48	77
8	U	163/170 (96%)	157 (96%)	6 (4%)	29	63
9	V	148/161 (92%)	144 (97%)	4 (3%)	40	71
10	W	156/166 (94%)	152 (97%)	4 (3%)	41	72
11	X	126/137 (92%)	125 (99%)	1 (1%)	79	90
12	Y	127/128 (99%)	124 (98%)	3 (2%)	44	74
13	a	71/74 (96%)	68 (96%)	3 (4%)	25	59
14	b	110/111 (99%)	105 (96%)	5 (4%)	23	57
15	c	119/120 (99%)	117 (98%)	2 (2%)	56	81
16	d	112/113 (99%)	107 (96%)	5 (4%)	23	57
17	f	70/71 (99%)	69 (99%)	1 (1%)	62	83
18	g	50/54 (93%)	49 (98%)	1 (2%)	50	78
All	All	2068/2425 (85%)	2009 (97%)	59 (3%)	39	70



5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	U	123	ASP
16	d	63	GLN
10	W	89	ASP
16	d	53	ASP
14	b	111	MET

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

Mol	Chain	Res	Type
10	W	139	GLN
13	a	7	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	1170/1800 (65%)	319 (27%)	26 (2%)

5 of 319 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	2	A
3	2	4	C
3	2	25	C
3	2	26	A
3	2	34	G

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	2	555	A
3	2	640	U
3	2	1742	U
3	2	639	U
3	2	705	U

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

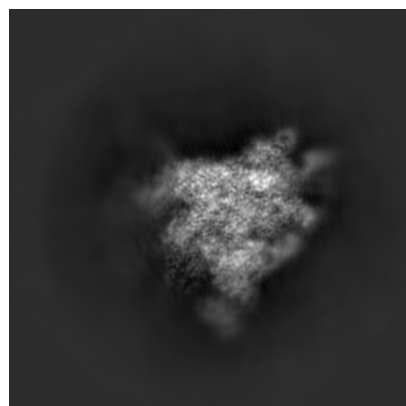
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16470. These allow visual inspection of the internal detail of the map and identification of artifacts.

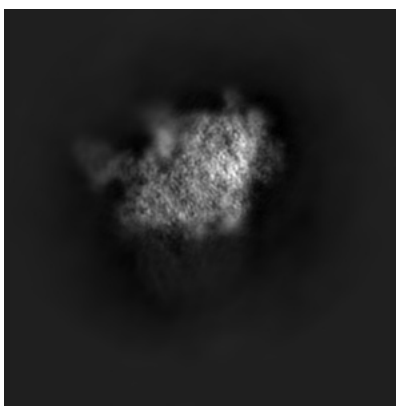
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

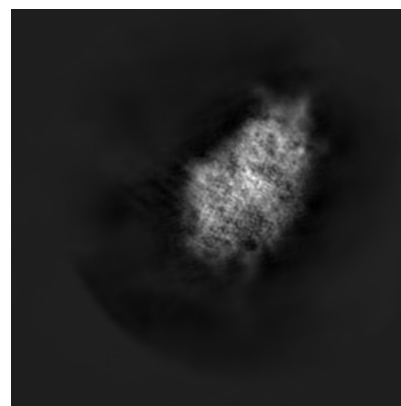
#### 6.1.1 Primary map



X

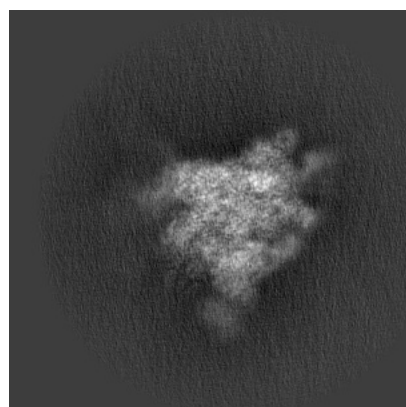


Y

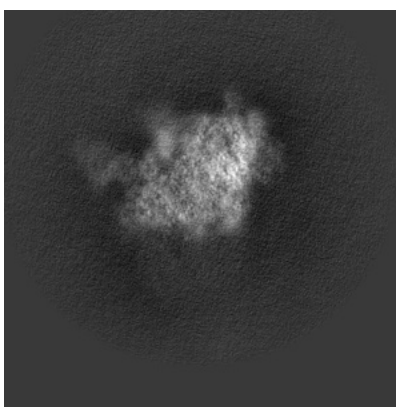


Z

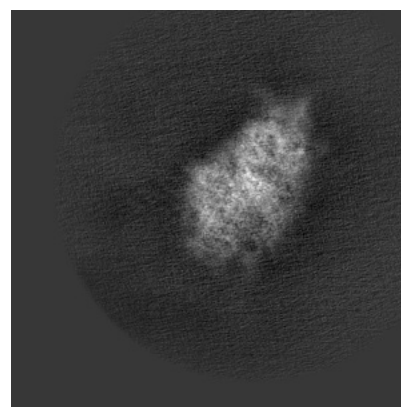
#### 6.1.2 Raw map



X



Y

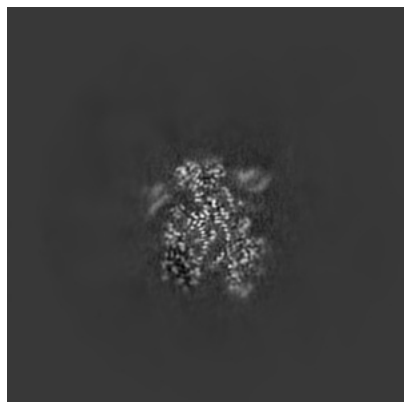


Z

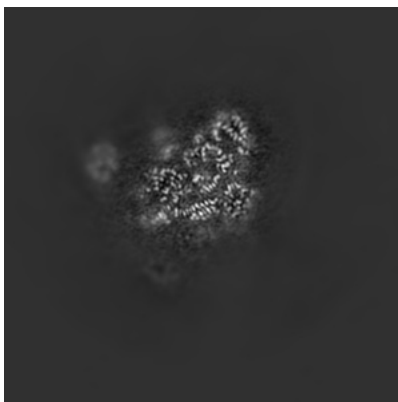
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

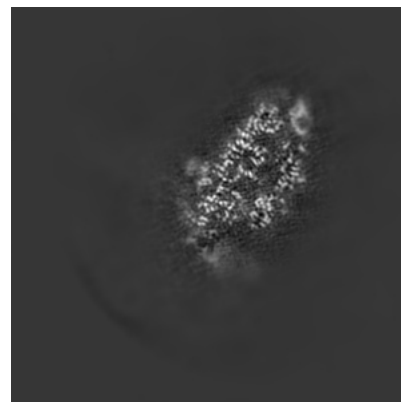
### 6.2.1 Primary map



X Index: 180

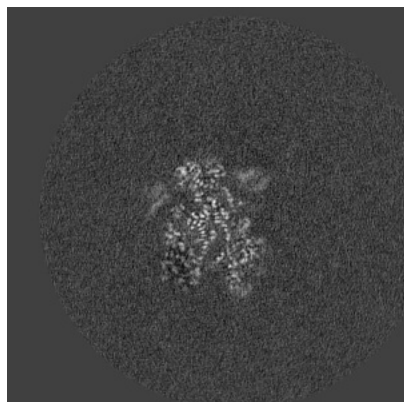


Y Index: 180

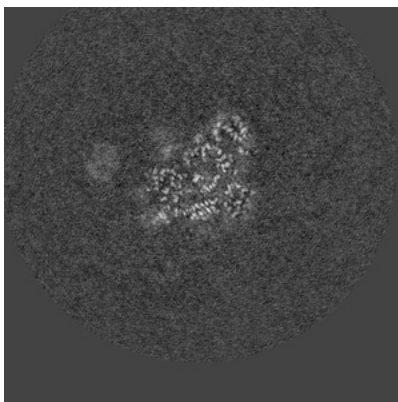


Z Index: 180

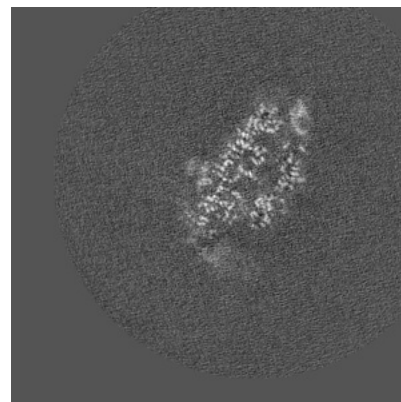
### 6.2.2 Raw map



X Index: 180



Y Index: 180

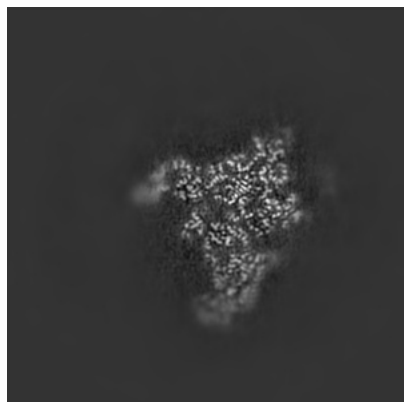


Z Index: 180

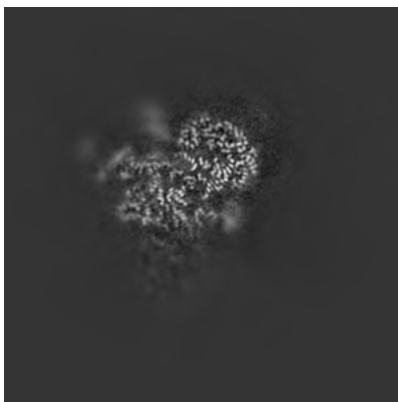
The images above show central slices of the map in three orthogonal directions.

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

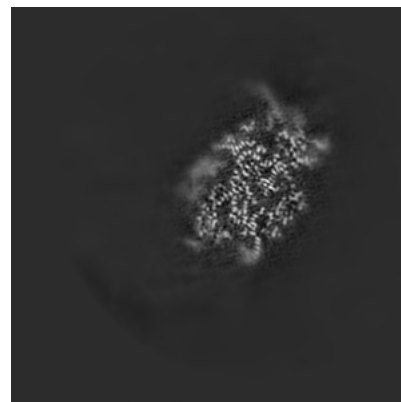
### 6.3.1 Primary map



X Index: 213

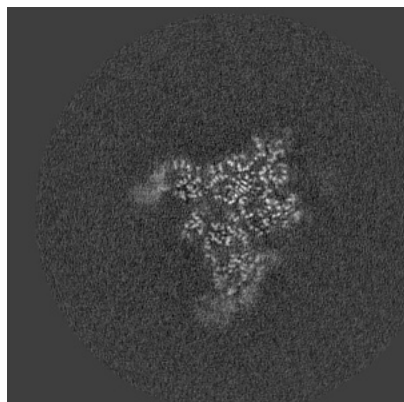


Y Index: 207

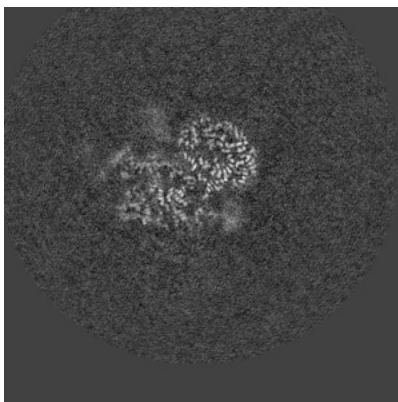


Z Index: 207

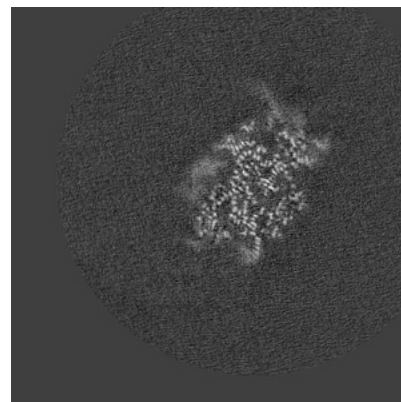
### 6.3.2 Raw map



X Index: 213



Y Index: 207

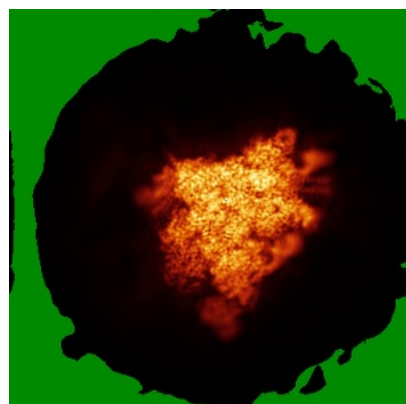


Z Index: 207

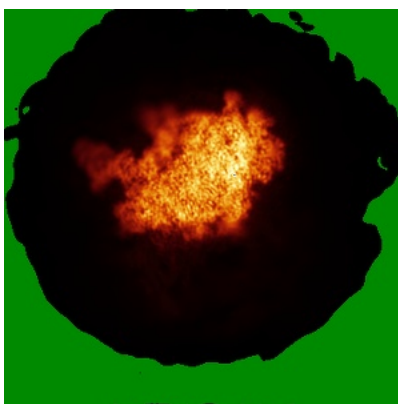
The images above show the largest variance slices of the map in three orthogonal directions.

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

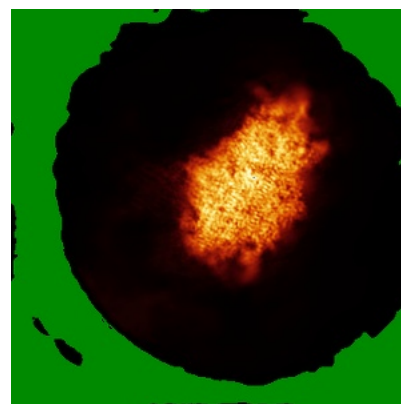
### 6.4.1 Primary map



X

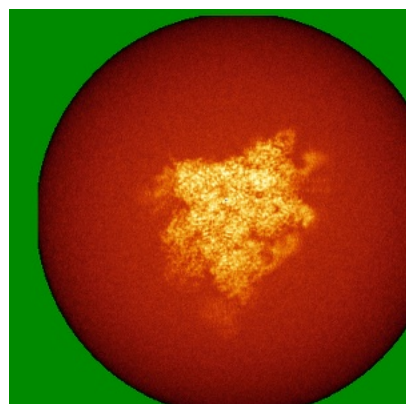


Y

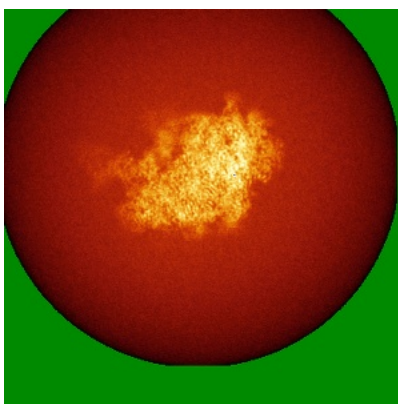


Z

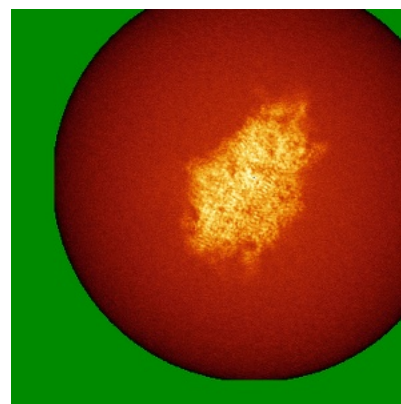
### 6.4.2 Raw map



X



Y



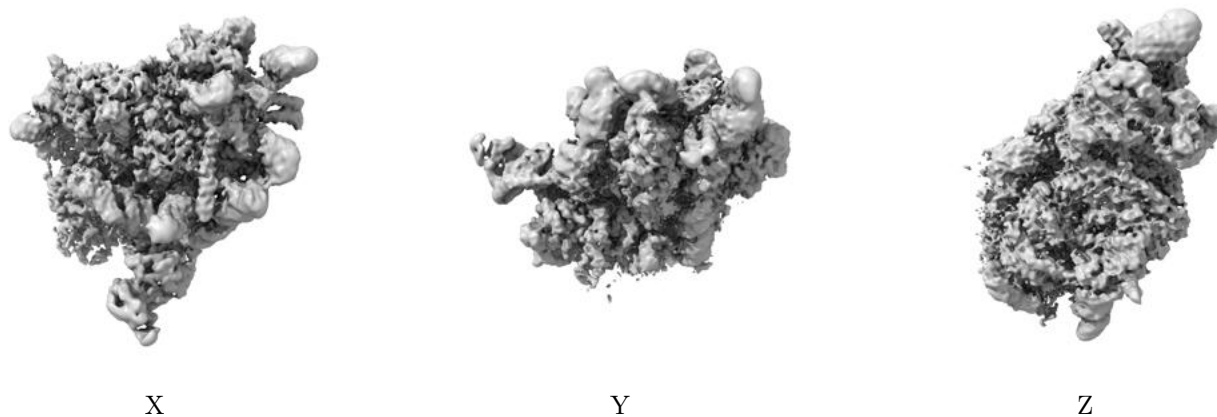
Z

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.



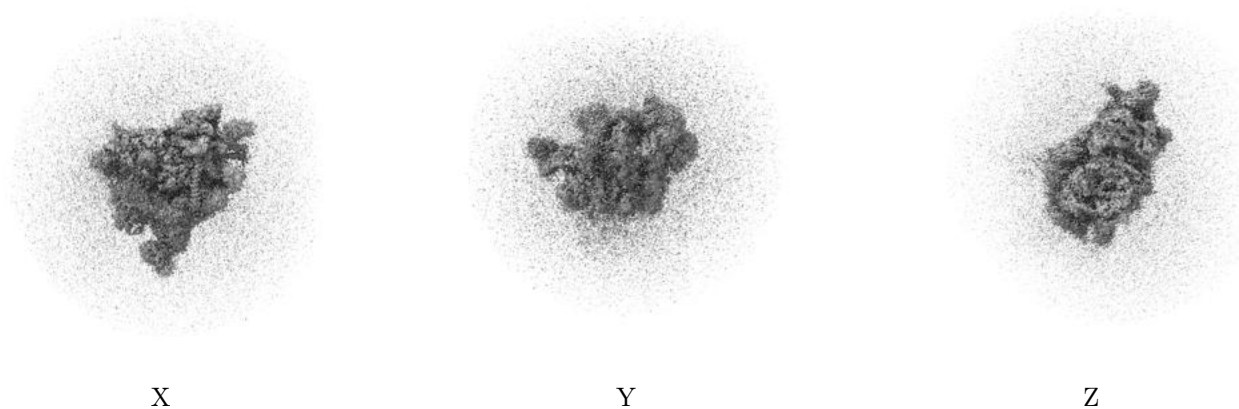
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.019. 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.

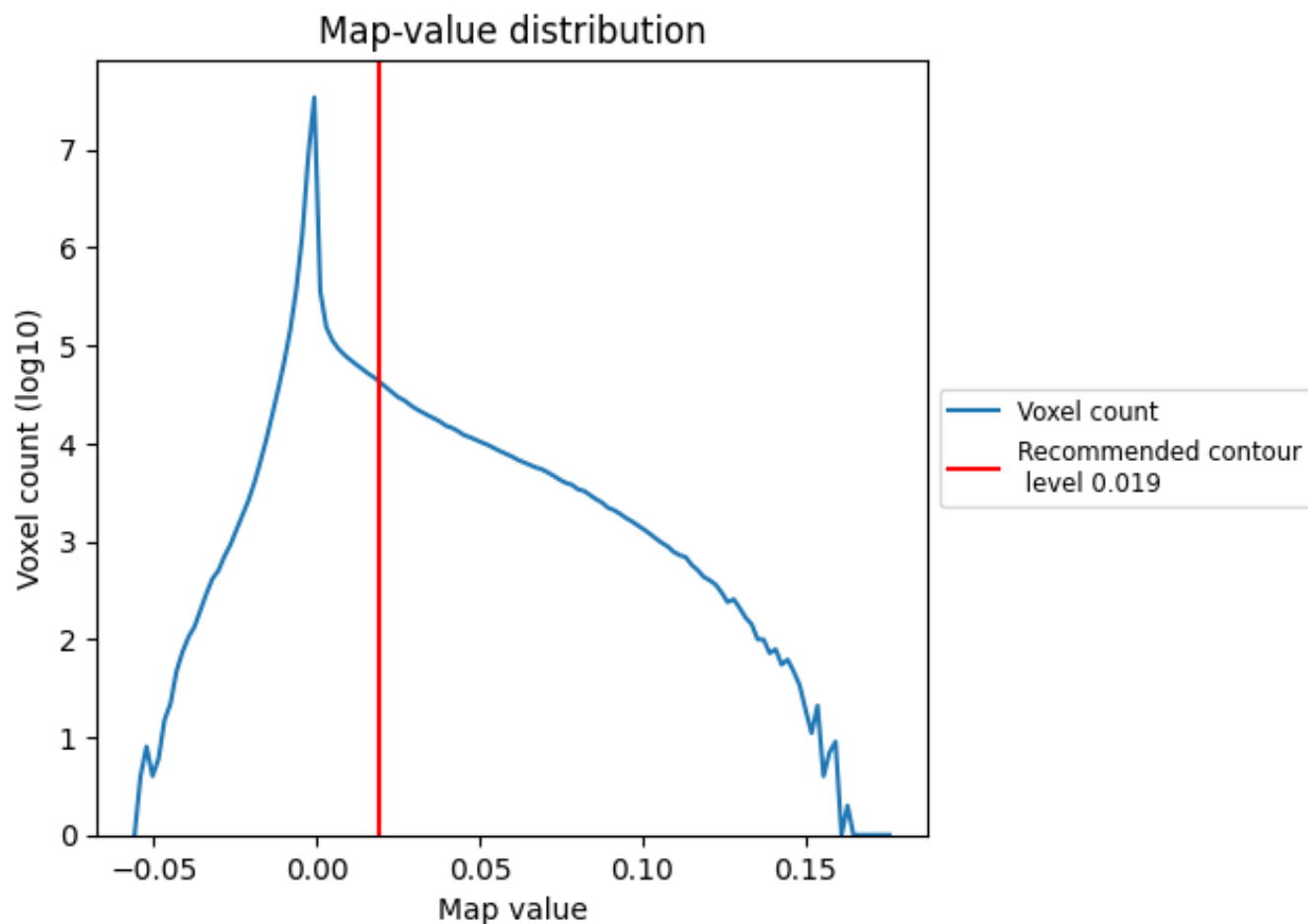
## 6.6 Mask visualisation [i](#)

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.

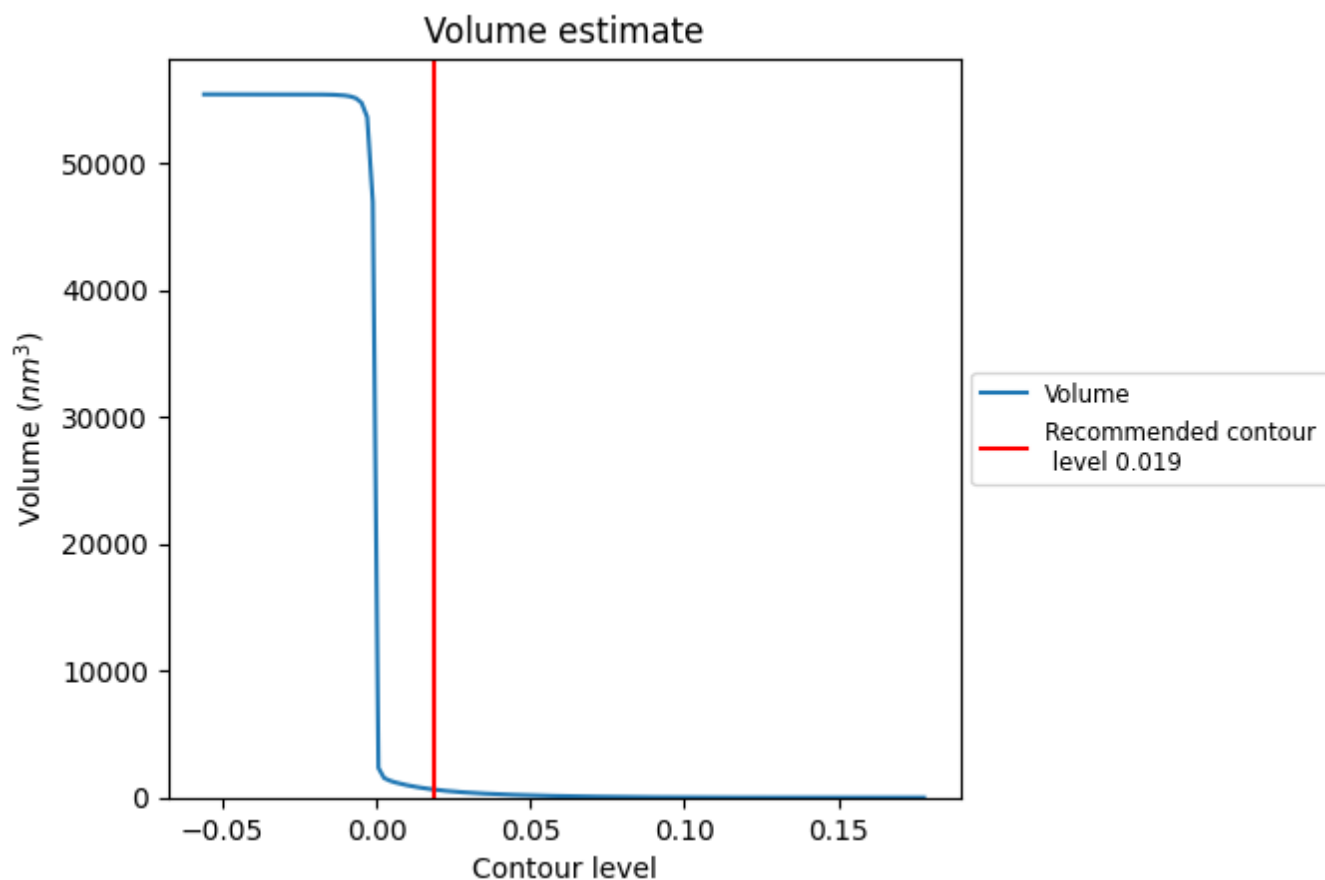
### 7.1 Map-value distribution [i](#)



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.



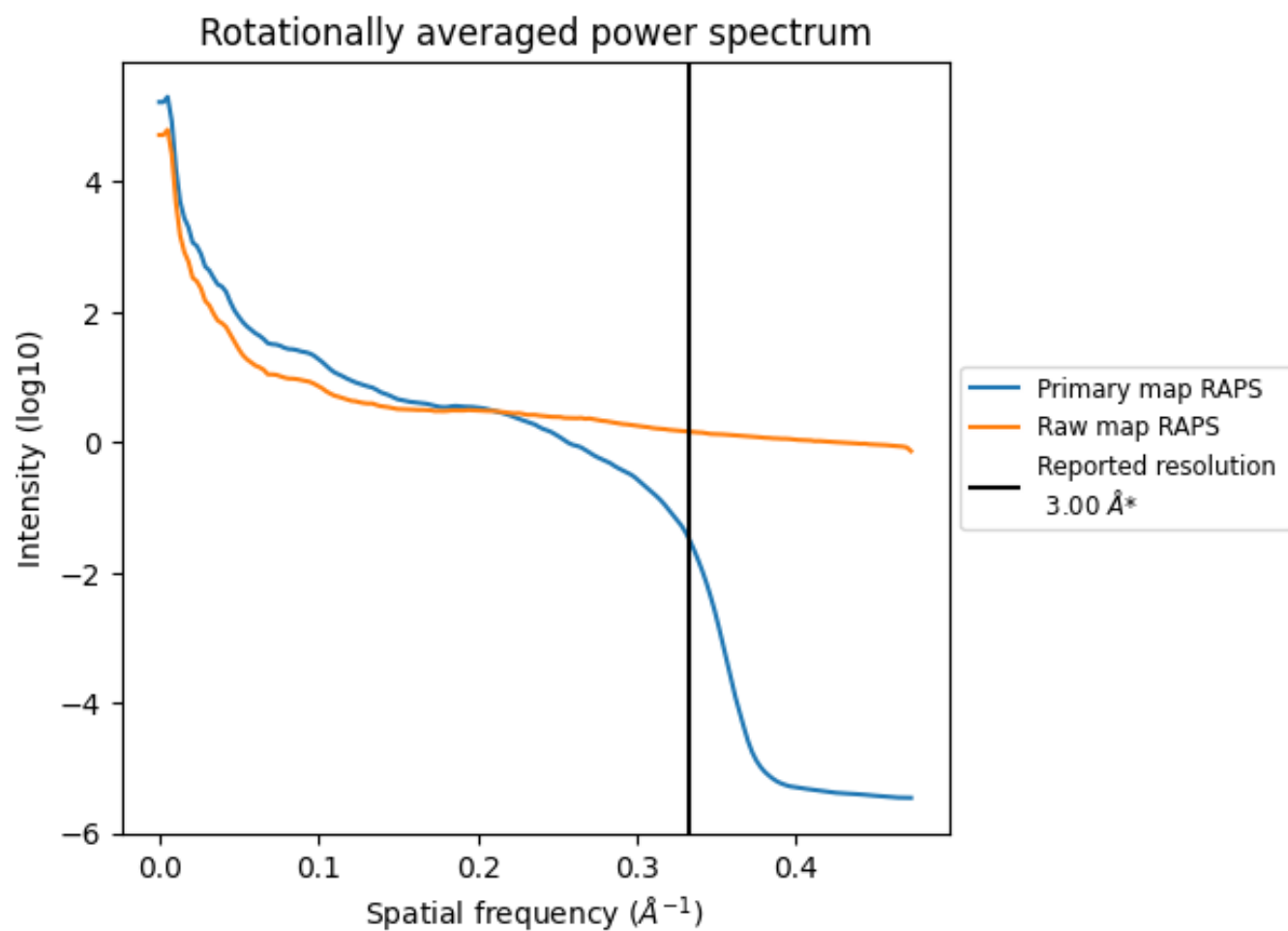
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 624  $\text{nm}^3$ ; this corresponds to an approximate mass of 564 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 ⓘ

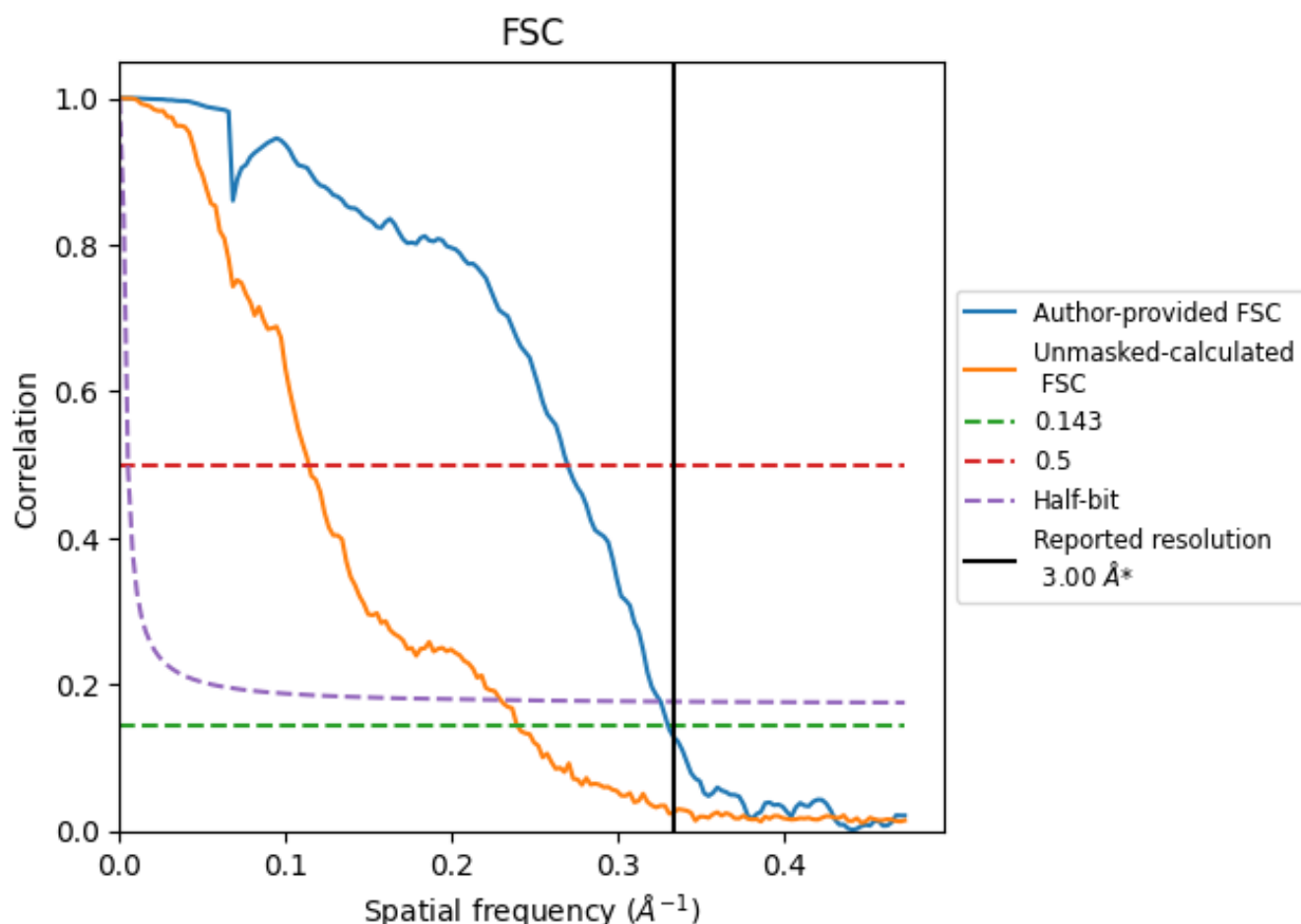


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

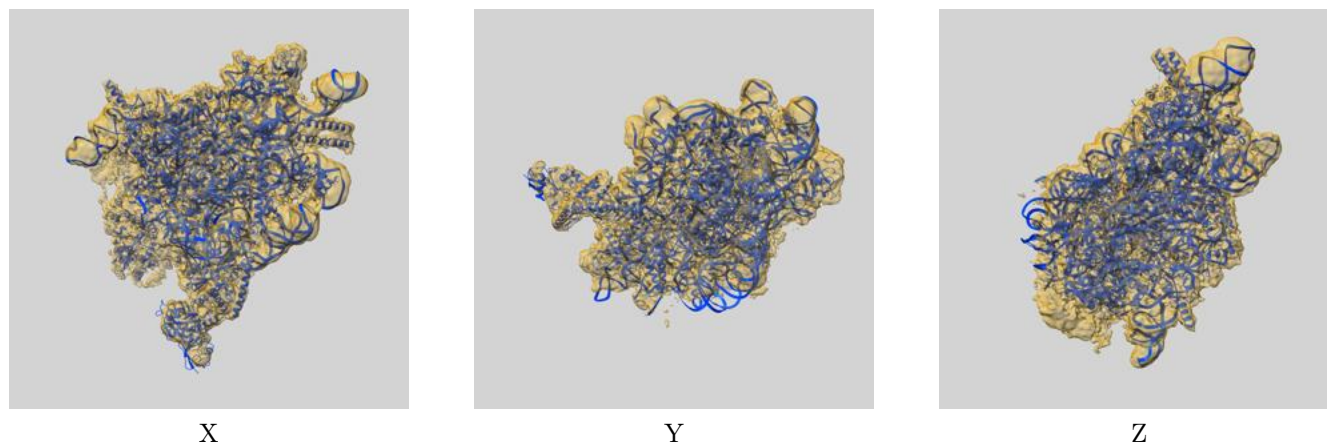
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.71	3.07
Unmasked-calculated*	4.18	8.80	4.36

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.0 by more than 10 %

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

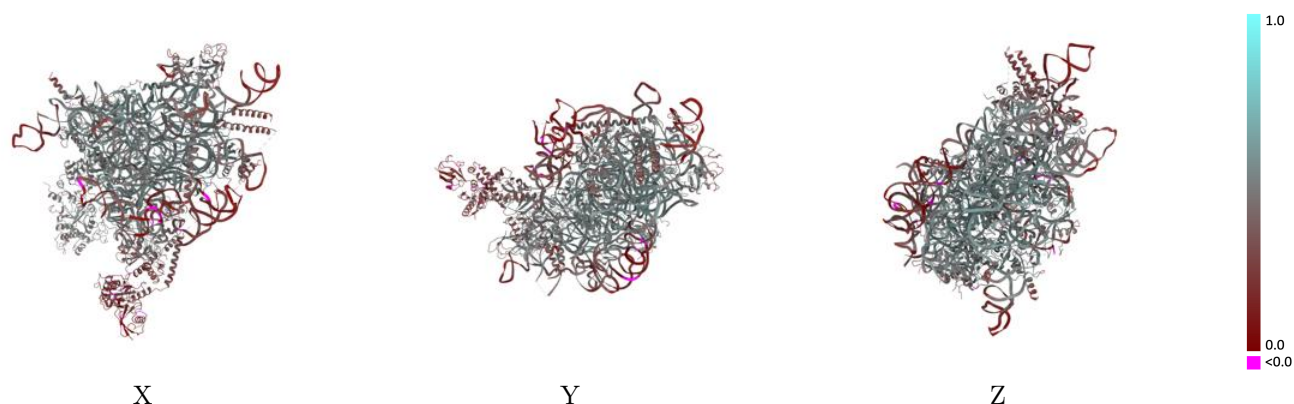
This section contains information regarding the fit between EMDB map EMD-16470 and PDB model 8C83. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



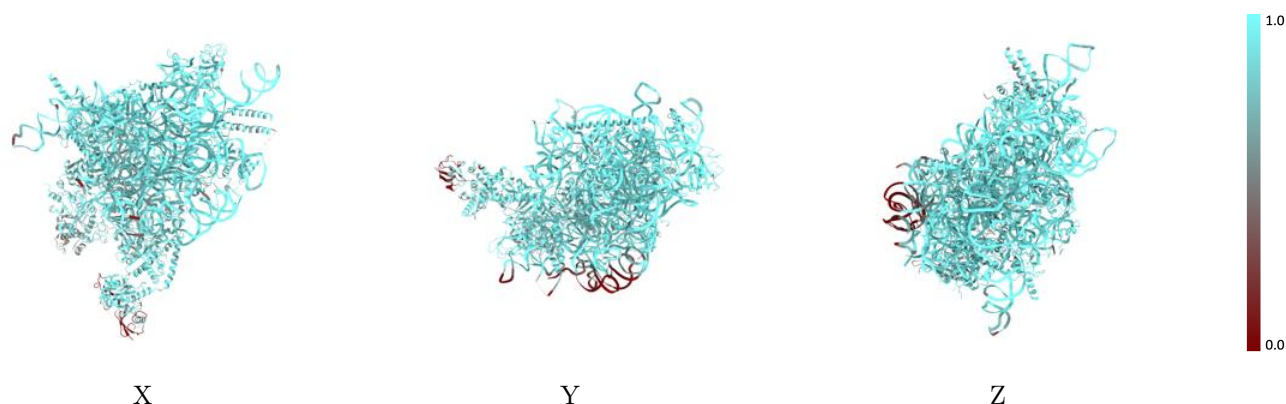
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



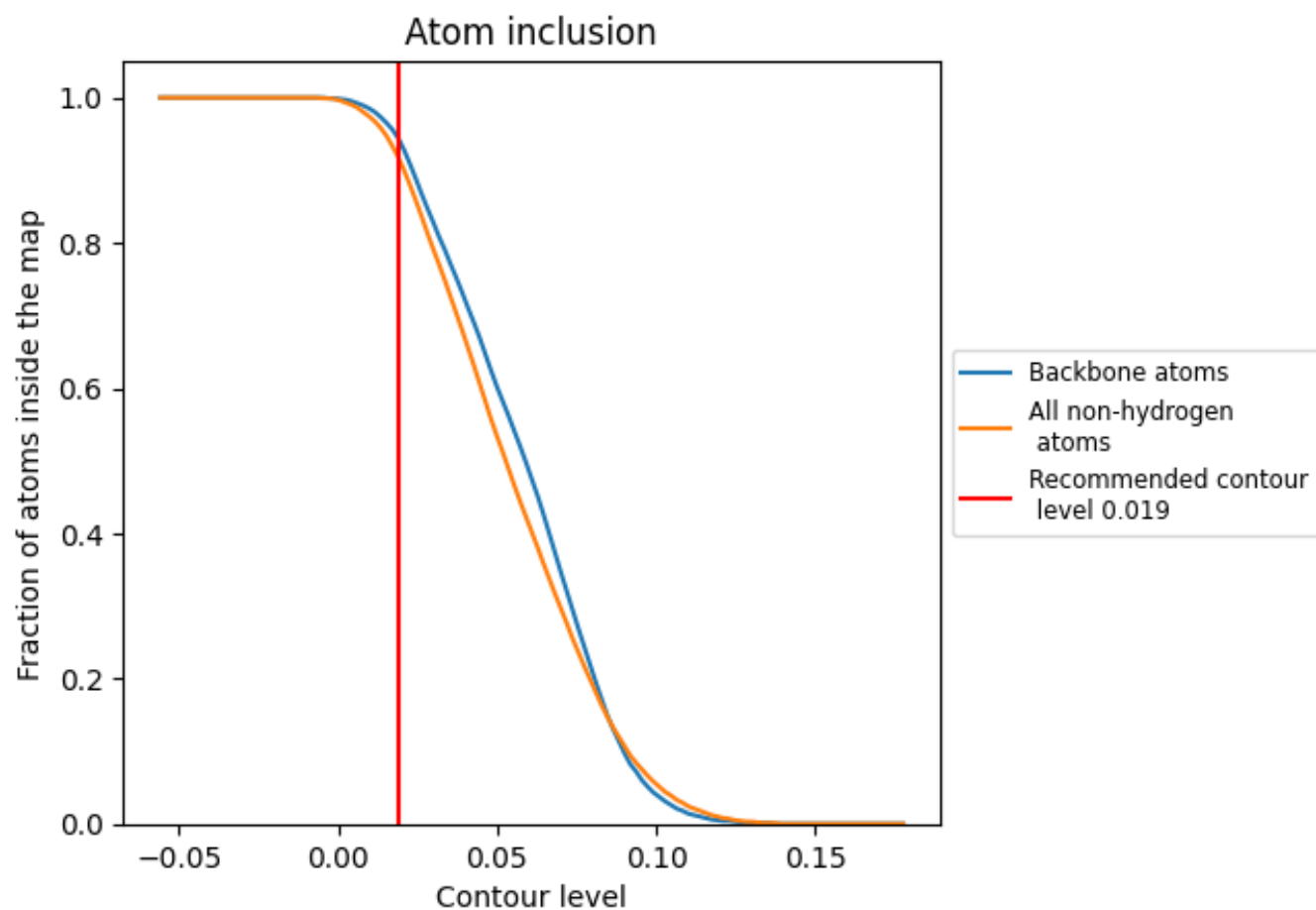
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.4410
2	 0.9220	 0.4290
P	 0.7100	 0.4460
R	 0.9300	 0.4900
S	 0.9690	 0.5140
T	 0.9600	 0.4410
U	 0.9310	 0.3960
V	 0.9750	 0.4910
W	 0.9570	 0.4980
X	 0.9520	 0.5270
Y	 0.9130	 0.4180
a	 0.9110	 0.4770
b	 0.9740	 0.5300
c	 0.9800	 0.5270
d	 0.9460	 0.4810
f	 0.9700	 0.4580
g	 0.9190	 0.4420
x	 0.8130	 0.2800
y	 0.3960	 0.1370

