



## wwPDB EM Validation Summary Report ⓘ

Jul 8, 2024 – 03:25 am BST

PDB ID : 7OQB  
EMDB ID : EMD-13028  
Title : The U2 part of *Saccharomyces cerevisiae* spliceosomal pre-A complex (delta BS-A ACT1)  
Authors : Zhang, Z.; Rigo, N.; Dybkov, O.; Fourmann, J.; Will, C.L.; Kumar, V.; Urlaub, H.; Stark, H.; Luehrmann, R.  
Deposited on : 2021-06-03  
Resolution : 9.00 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>.

---

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

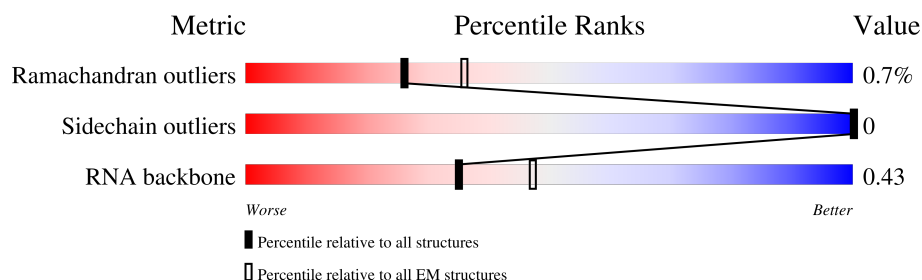
EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 9.00 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)
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	O	971	<div> <div>12%</div> <div>80%</div> <div>16%</div> </div>
2	I	318	<div> <div>93%</div> </div>
3	U	282	<div> <div>37%</div> <div>66%</div> <div>33%</div> </div>
4	V	280	<div> <div>13%</div> <div>36%</div> <div>63%</div> </div>
5	T	530	<div> <div>19%</div> <div>87%</div> <div>13%</div> </div>
6	S	107	<div> <div>21%</div> <div>86%</div> <div>14%</div> </div>
7	Q	436	<div> <div>20%</div> <div>50%</div> <div>50%</div> </div>
8	P	1361	<div> <div>8%</div> <div>86%</div> <div>13%</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
9	R	213	
10	Z	84	
11	W	238	
12	Y	111	
13	s	196	
14	t	146	
15	u	110	
16	v	101	
17	w	93	
18	x	86	
19	y	77	
20	p	849	
21	2	1175	

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 26426 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 U2 snRNP component HSH155.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	O	812	Total	C	N	O	0	0
			4108	2484	812	812		

- Molecule 2 is a RNA chain called ACT1 pre-mRNA (delta-BS-A).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	23	Total	C	N	O	P	0	0
			480	216	78	163	23		

- Molecule 3 is a protein called Pre-mRNA-splicing factor PRP11.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	U	188	Total	C	N	O	0	0
			943	567	188	188		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	121	UNK	-	insertion	UNP Q07350
U	122	UNK	-	insertion	UNP Q07350
U	123	UNK	-	insertion	UNP Q07350
U	124	UNK	-	insertion	UNP Q07350
U	125	UNK	-	insertion	UNP Q07350
U	126	UNK	-	insertion	UNP Q07350
U	127	UNK	-	insertion	UNP Q07350
U	128	UNK	-	insertion	UNP Q07350
U	129	UNK	-	insertion	UNP Q07350
U	130	UNK	-	insertion	UNP Q07350
U	131	UNK	-	insertion	UNP Q07350
U	132	UNK	-	insertion	UNP Q07350
U	133	UNK	-	insertion	UNP Q07350
U	134	UNK	-	insertion	UNP Q07350
U	135	UNK	-	insertion	UNP Q07350

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
U	136	UNK	-	insertion	UNP Q07350

- Molecule 4 is a protein called Pre-mRNA-splicing factor PRP21.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	V	103	Total	C	N	O	0	0
			515	309	103	103		

- Molecule 5 is a protein called Pre-mRNA-splicing factor PRP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	T	462	Total	C	N	O	0	0
			2318	1394	462	462		

- Molecule 6 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 7 is a protein called Cold sensitive U2 snRNA suppressor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	220	Total	C	N	O	0	0
			1122	682	220	220		

- Molecule 8 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	1186	Total	C	N	O	0	0
			5972	3600	1186	1186		

- Molecule 9 is a protein called Protein HSH49.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	173	Total	C	N	O	0	0
			868	522	173	173		

- Molecule 10 is a protein called RDS3 complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	83	Total	C	N	O	0	0
			412	246	83	83		

- Molecule 11 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	W	170	Total	C	N	O	0	0
			862	522	170	170		

- Molecule 12 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	84	Total	C	N	O	0	0
			418	250	84	84		

- Molecule 13 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	s	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	t	72	Total	C	N	O	0	0
			363	219	72	72		

- Molecule 15 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	u	92	Total	C	N	O	0	0
			463	279	92	92		

- Molecule 16 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	v	82	Total	C	N	O	0	0
			412	248	82	82		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	w	77	Total	C	N	O	0	0
			389	235	77	77		

- Molecule 18 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	x	73	Total	C	N	O	0	0
			365	219	73	73		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	y	75	Total	C	N	O	0	0
			373	223	75	75		

- Molecule 20 is a protein called Pre-mRNA-processing ATP-dependent RNA helicase PRP5.

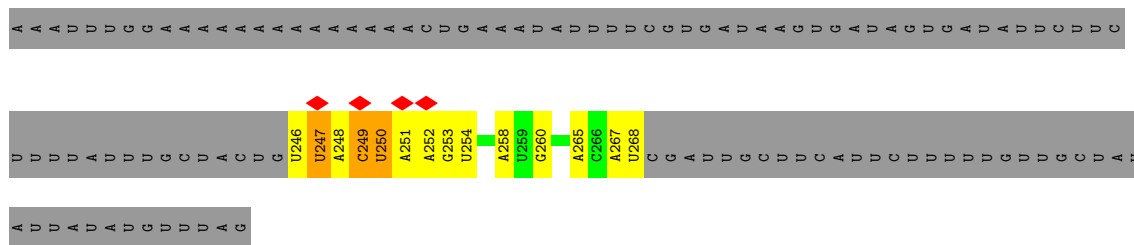
Mol	Chain	Residues	Atoms				AltConf	Trace
20	p	444	Total	C	N	O	5	0
			2239	1351	444	444		

- Molecule 21 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	143	Total	C	N	O	P	0	0
			3021	1351	511	1017	142		



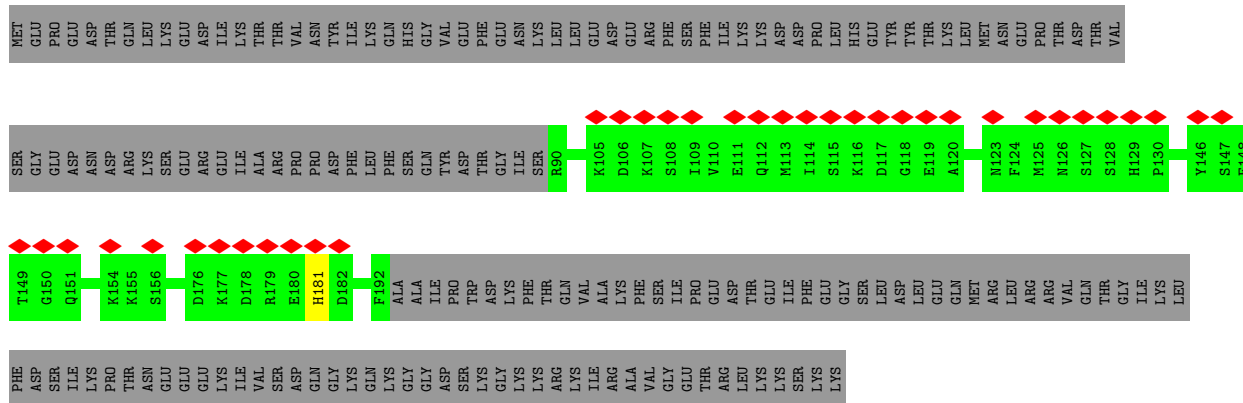




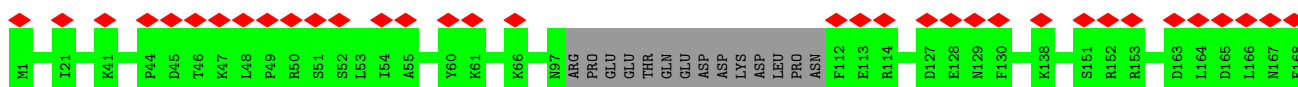
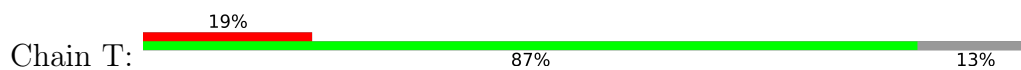
• Molecule 3: Pre-mRNA-splicing factor PRP11



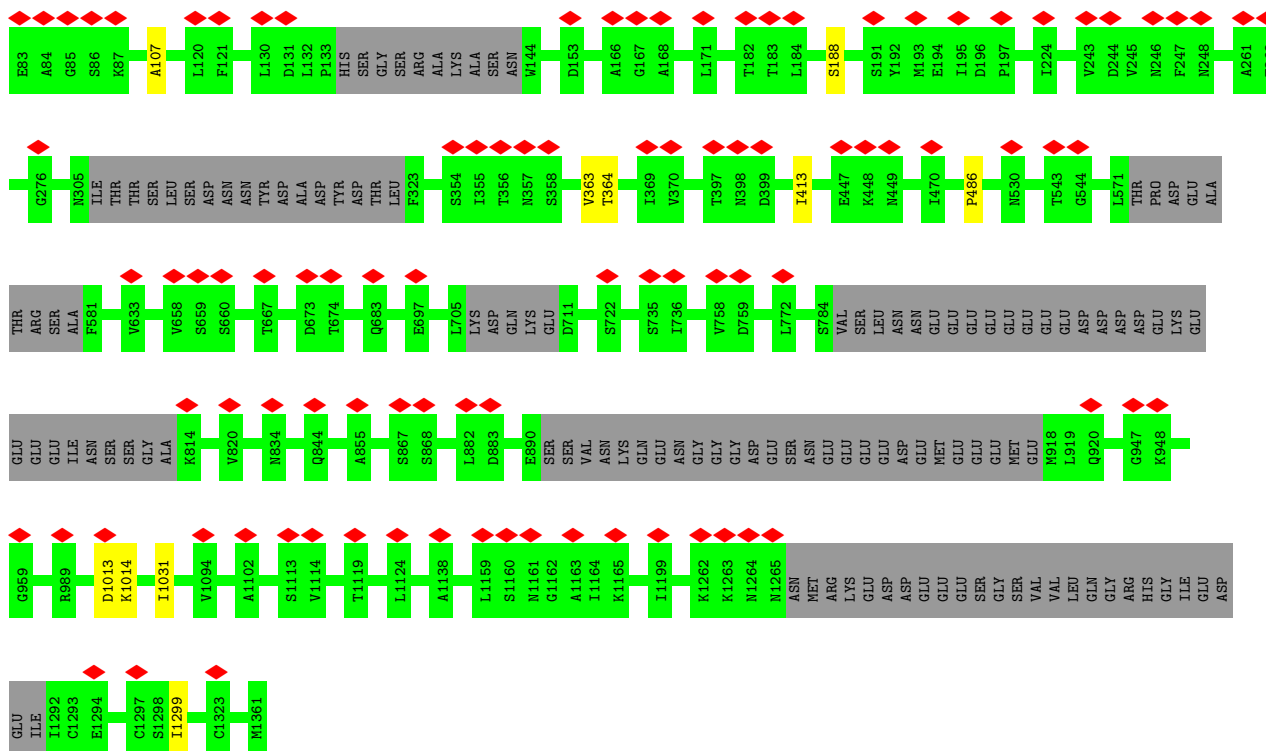
• Molecule 4: Pre-mRNA-splicing factor PRP21



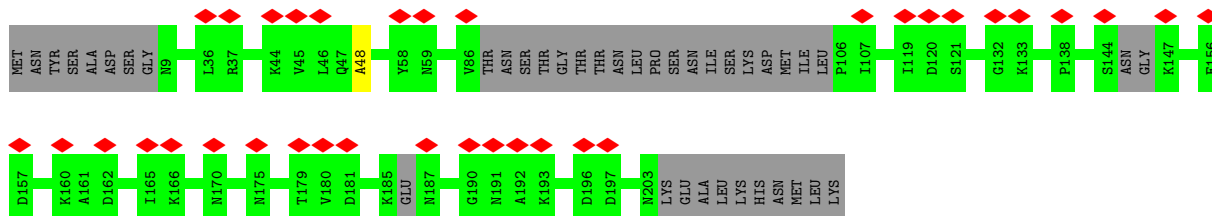
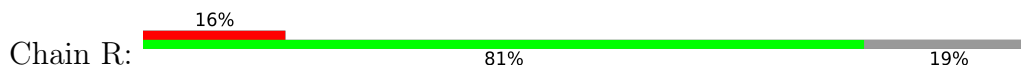
• Molecule 5: Pre-mRNA-splicing factor PRP9



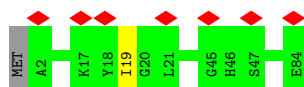




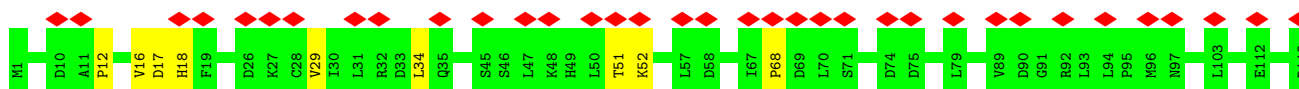
• Molecule 9: Protein HSH49



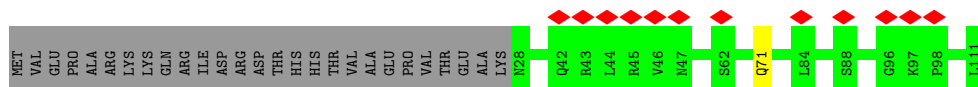
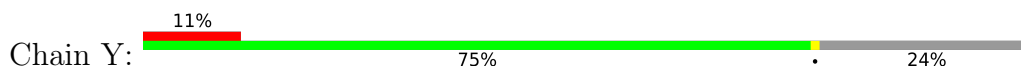
• Molecule 10: RDS3 complex subunit 10



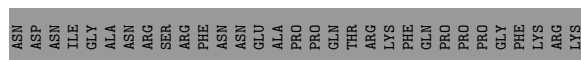
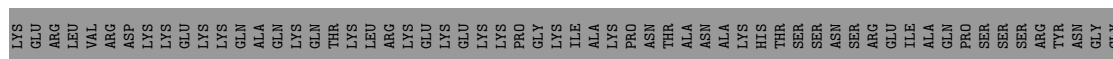
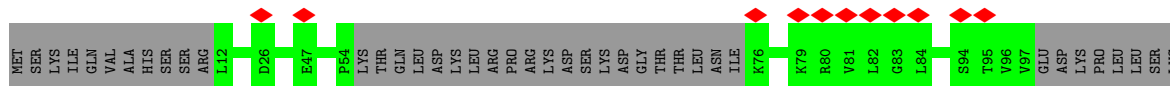
• Molecule 11: U2 small nuclear ribonucleoprotein A'



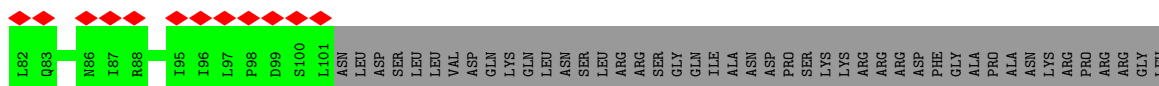
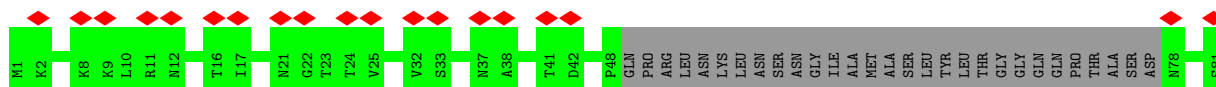
- Molecule 12: U2 small nuclear ribonucleoprotein B''



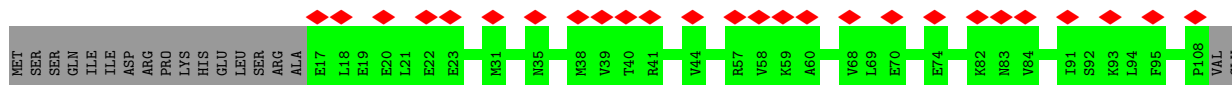
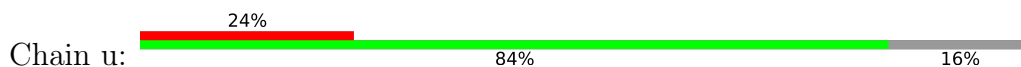
- Molecule 13: Small nuclear ribonucleoprotein-associated protein B



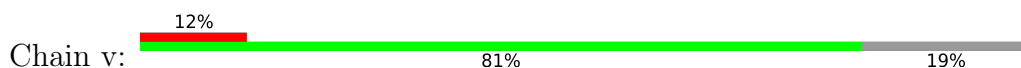
- Molecule 14: Small nuclear ribonucleoprotein Sm D1



- Molecule 15: Small nuclear ribonucleoprotein Sm D2



- Molecule 16: Small nuclear ribonucleoprotein Sm D3









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160894	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 ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.038	Depositor
Map size ( $\text{\AA}$ )	510.4, 510.4, 510.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	2.32, 2.32, 2.32	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	O	0.42	0/4149	0.77	30/5819 (0.5%)
2	I	0.69	6/534 (1.1%)	0.86	0/827
3	U	0.22	0/867	0.43	0/1208
4	V	0.38	0/515	0.43	0/719
5	T	0.27	0/2324	0.44	0/3248
6	S	0.27	0/463	0.49	0/645
7	Q	0.27	0/1137	0.47	0/1593
8	P	0.28	1/6009 (0.0%)	0.54	0/8407
9	R	0.28	0/869	0.46	0/1209
10	Z	0.26	0/412	0.41	0/573
11	W	0.32	0/869	0.60	0/1219
12	Y	0.27	0/418	0.49	0/582
13	s	0.30	0/322	0.57	0/446
14	t	0.33	0/364	0.56	0/507
15	u	0.32	0/465	0.53	0/650
16	v	0.29	0/415	0.54	0/579
17	w	0.29	0/392	0.54	0/546
18	x	0.31	0/367	0.58	0/510
19	y	0.26	0/374	0.50	0/520
20	p	0.55	1/2269 (0.0%)	0.66	3/3172 (0.1%)
21	2	4.64	44/3363 (1.3%)	2.45	107/5218 (2.1%)
All	All	1.68	52/26897 (0.2%)	1.06	140/38197 (0.4%)

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
5	T	0	1
8	P	0	2
11	W	0	1
21	2	0	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	6

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	35	U	C1'-N1	151.34	3.75	1.48
21	2	42	U	C1'-N1	150.88	3.75	1.48
21	2	44	U	C1'-N1	149.94	3.73	1.48
20	p	271	THR	C-N	20.19	1.80	1.34
21	2	1161	U	O3'-P	-15.60	1.42	1.61

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	44	U	C6-N1-C1'	-74.41	17.03	121.20
21	2	42	U	C6-N1-C1'	-73.72	17.98	121.20
21	2	35	U	C6-N1-C1'	-73.61	18.15	121.20
21	2	44	U	O4'-C1'-N1	-27.52	86.18	108.20
21	2	42	U	O4'-C1'-N1	-21.00	91.40	108.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	2	141	A	Sidechain
8	P	1013	ASP	Peptide
8	P	1014	LYS	Peptide
5	T	458	SER	Peptide
11	W	16	VAL	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	O	810/971 (83%)	770 (95%)	37 (5%)	3 (0%)	34	72
3	U	166/282 (59%)	141 (85%)	24 (14%)	1 (1%)	25	66
4	V	101/280 (36%)	90 (89%)	10 (10%)	1 (1%)	15	55
5	T	454/530 (86%)	414 (91%)	40 (9%)	0	100	100
6	S	90/107 (84%)	79 (88%)	11 (12%)	0	100	100
7	Q	214/436 (49%)	202 (94%)	11 (5%)	1 (0%)	29	69
8	P	1170/1361 (86%)	1059 (90%)	104 (9%)	7 (1%)	25	66
9	R	165/213 (78%)	161 (98%)	3 (2%)	1 (1%)	25	66
10	Z	81/84 (96%)	76 (94%)	4 (5%)	1 (1%)	13	50
11	W	168/238 (71%)	129 (77%)	28 (17%)	11 (6%)	1	16
12	Y	82/111 (74%)	76 (93%)	5 (6%)	1 (1%)	13	50
13	s	61/196 (31%)	58 (95%)	3 (5%)	0	100	100
14	t	68/146 (47%)	67 (98%)	1 (2%)	0	100	100
15	u	90/110 (82%)	89 (99%)	1 (1%)	0	100	100
16	v	80/101 (79%)	77 (96%)	3 (4%)	0	100	100
17	w	73/93 (78%)	72 (99%)	1 (1%)	0	100	100
18	x	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
19	y	73/77 (95%)	64 (88%)	6 (8%)	3 (4%)	3	23
20	p	445/849 (52%)	431 (97%)	13 (3%)	1 (0%)	47	81
All	All	4462/6271 (71%)	4124 (92%)	307 (7%)	31 (1%)	26	63

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Q	368	ILE
8	P	1299	ILE
11	W	34	LEU
11	W	52	LYS
19	y	50	ASP

### 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	O	42/867 (5%)	42 (100%)	0	100	100
3	U	7/236 (3%)	7 (100%)	0	100	100
4	V	1/259 (0%)	1 (100%)	0	100	100
5	T	10/492 (2%)	10 (100%)	0	100	100
6	S	4/97 (4%)	4 (100%)	0	100	100
7	Q	18/392 (5%)	18 (100%)	0	100	100
8	P	45/1244 (4%)	45 (100%)	0	100	100
9	R	5/189 (3%)	5 (100%)	0	100	100
10	Z	1/76 (1%)	1 (100%)	0	100	100
11	W	8/219 (4%)	8 (100%)	0	100	100
12	Y	1/100 (1%)	1 (100%)	0	100	100
13	s	1/176 (1%)	1 (100%)	0	100	100
14	t	3/129 (2%)	3 (100%)	0	100	100
15	u	3/103 (3%)	3 (100%)	0	100	100
16	v	4/89 (4%)	4 (100%)	0	100	100
17	w	5/82 (6%)	5 (100%)	0	100	100
18	x	3/77 (4%)	3 (100%)	0	100	100
19	y	2/66 (3%)	2 (100%)	0	100	100
20	p	17/768 (2%)	17 (100%)	0	100	100
All	All	180/5661 (3%)	180 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	22/318 (6%)	11 (50%)	0
21	2	138/1175 (11%)	53 (38%)	27 (19%)
All	All	160/1493 (10%)	64 (40%)	27 (16%)

5 of 64 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	247	U
2	I	248	A
2	I	249	C
2	I	250	U
2	I	251	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	2	1119	C
21	2	1122	U
21	2	1144	U
21	2	1121	U
21	2	1123	C

## 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 ⓘ

There are no chain breaks in this entry.

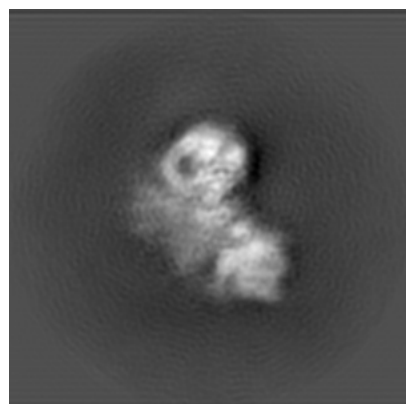
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13028. These allow visual inspection of the internal detail of the map and identification of artifacts.

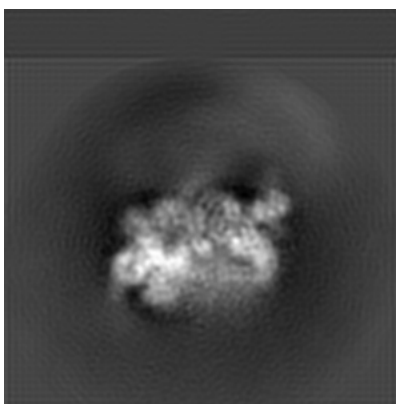
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

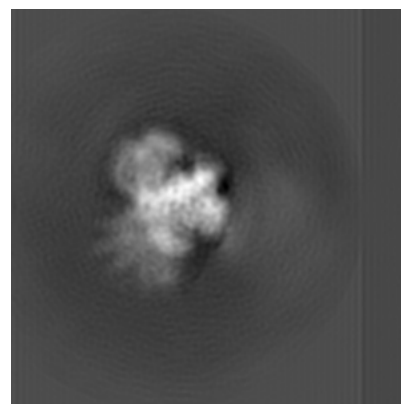
#### 6.1.1 Primary map



X

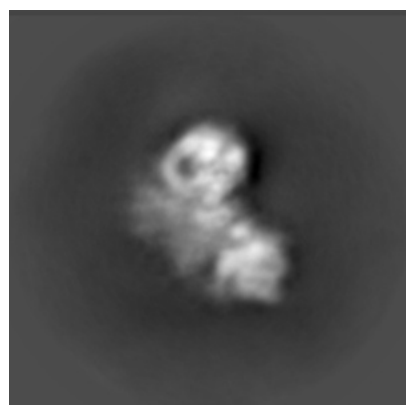


Y

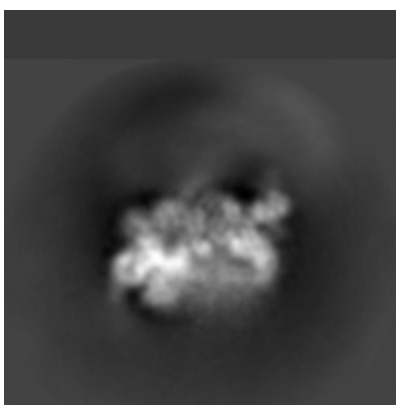


Z

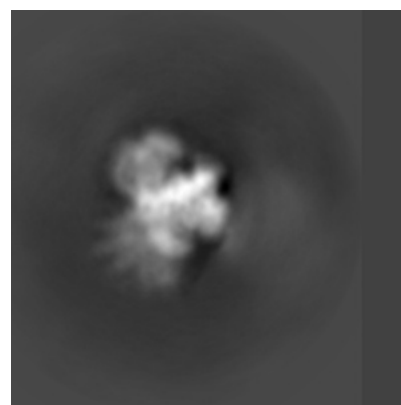
#### 6.1.2 Raw map



X



Y

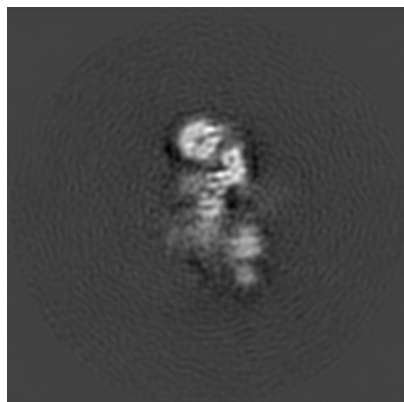


Z

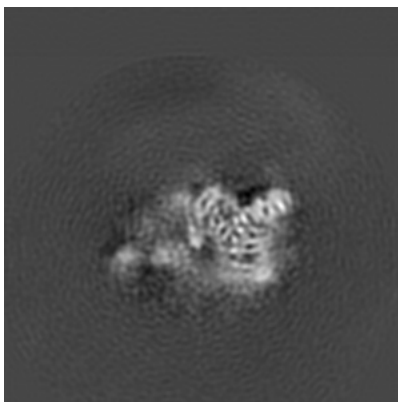
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

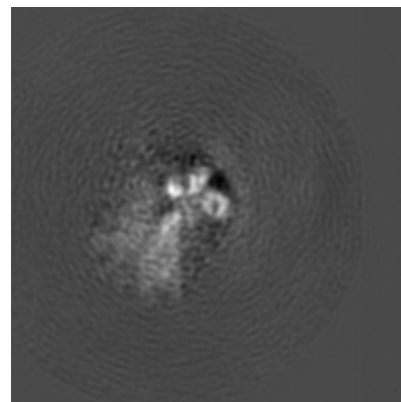
### 6.2.1 Primary map



X Index: 110

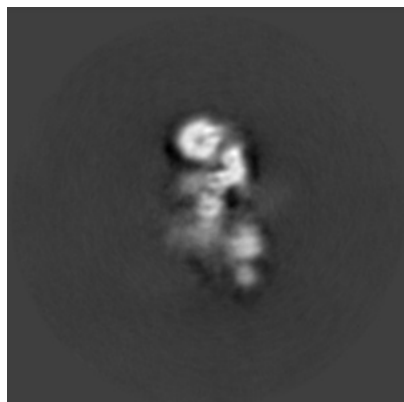


Y Index: 110

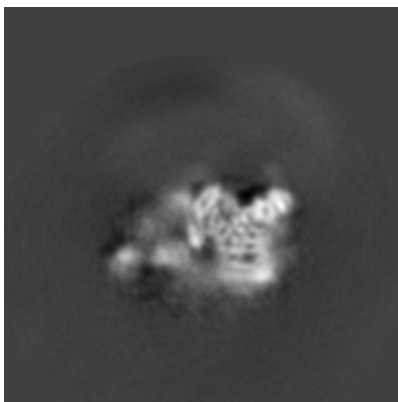


Z Index: 110

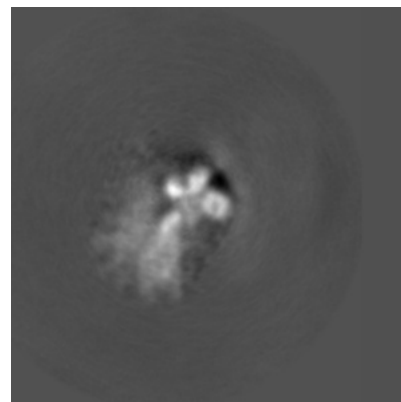
### 6.2.2 Raw map



X Index: 110



Y Index: 110



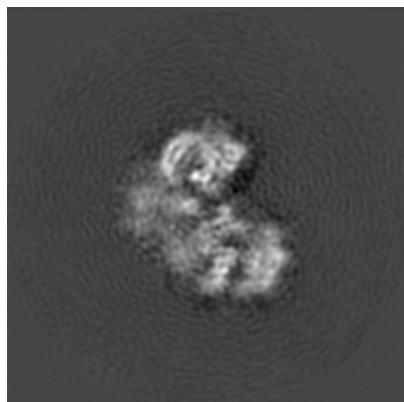
Z Index: 110

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

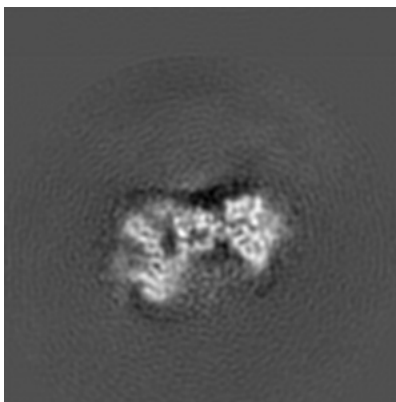


## 6.3 Largest variance slices [i](#)

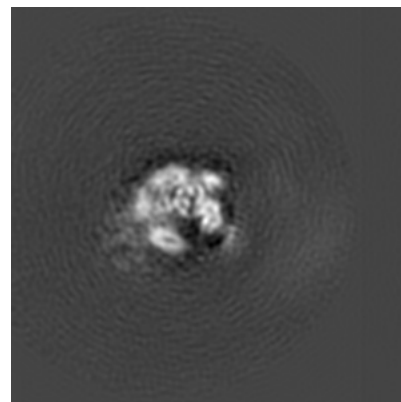
### 6.3.1 Primary map



X Index: 85

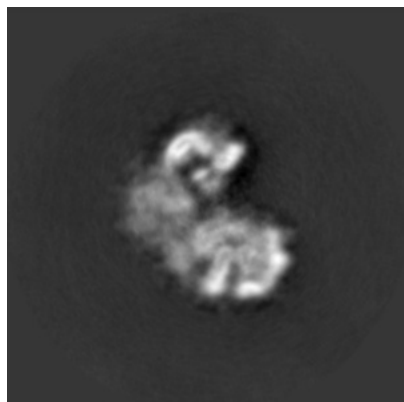


Y Index: 123

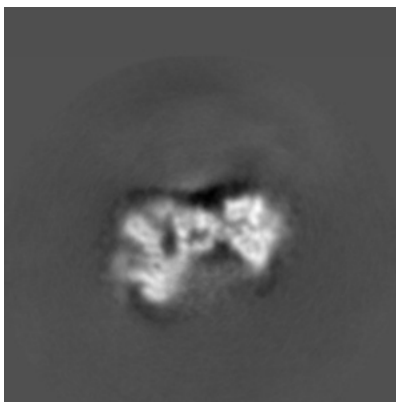


Z Index: 140

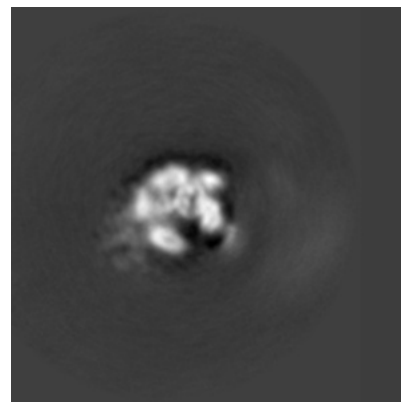
### 6.3.2 Raw map



X Index: 82



Y Index: 123

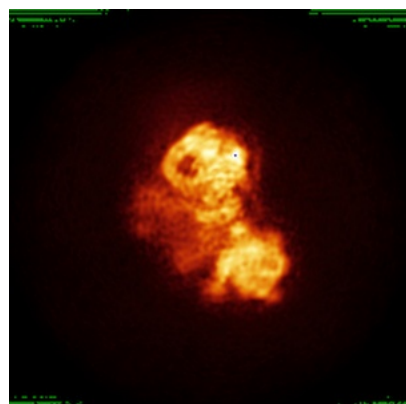


Z Index: 140

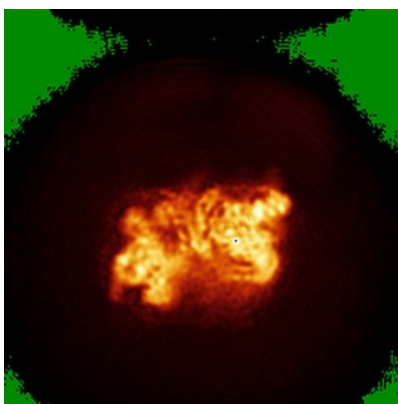
The images above show the largest variance slices of the map in three orthogonal directions.

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

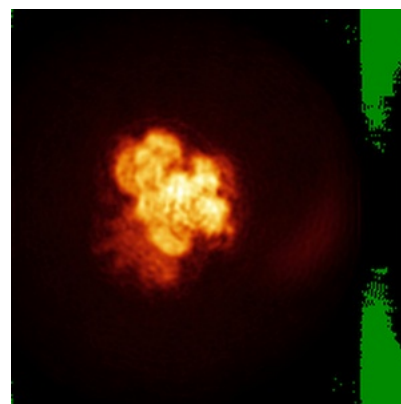
### 6.4.1 Primary map



X



Y

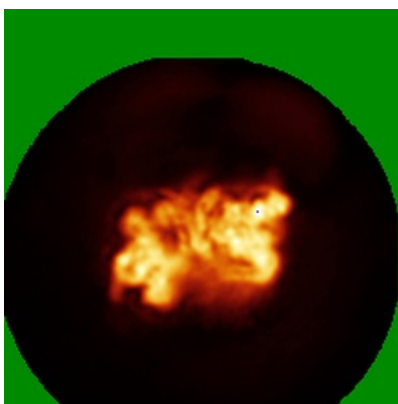


Z

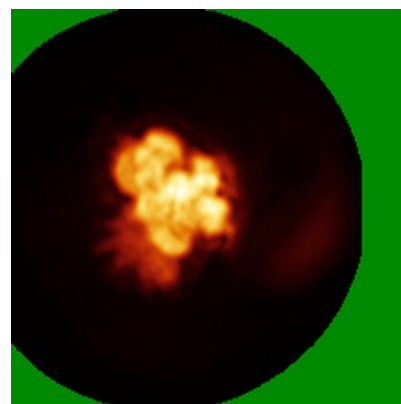
### 6.4.2 Raw map



X



Y

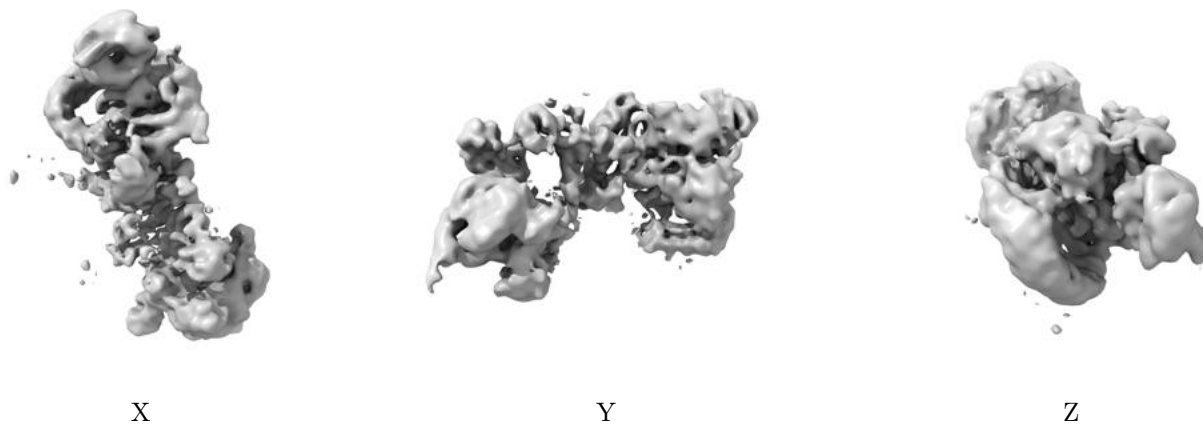


Z

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.

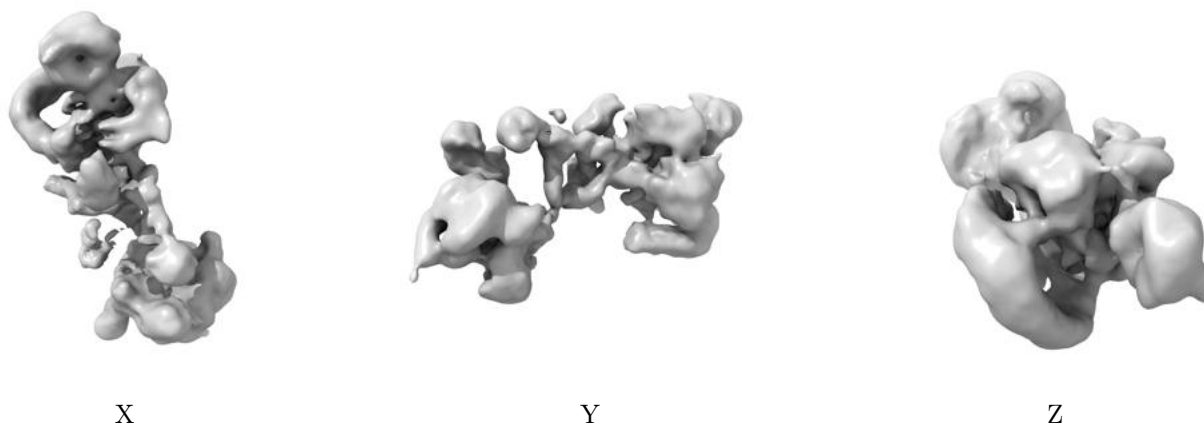
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.038. 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.

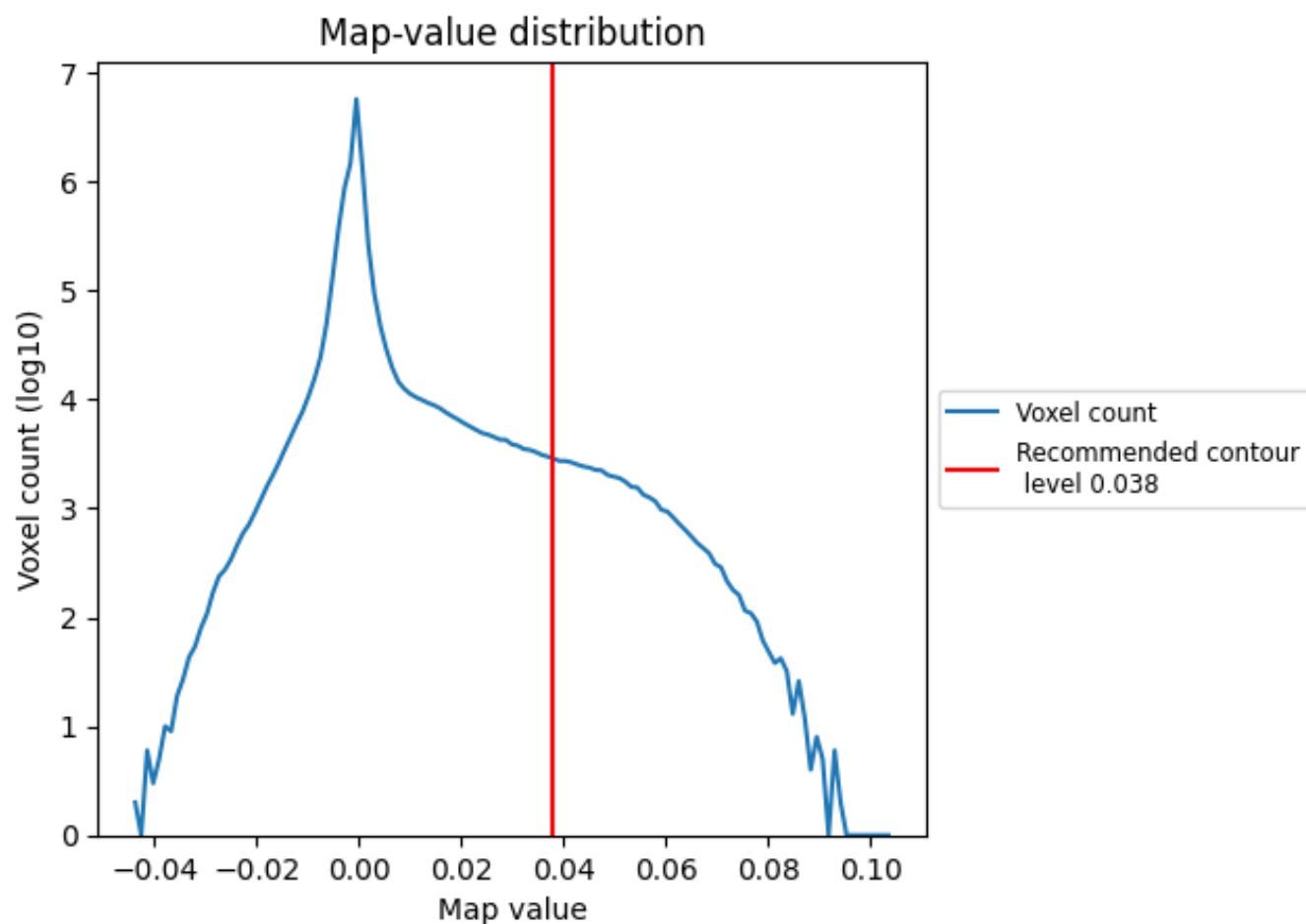
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

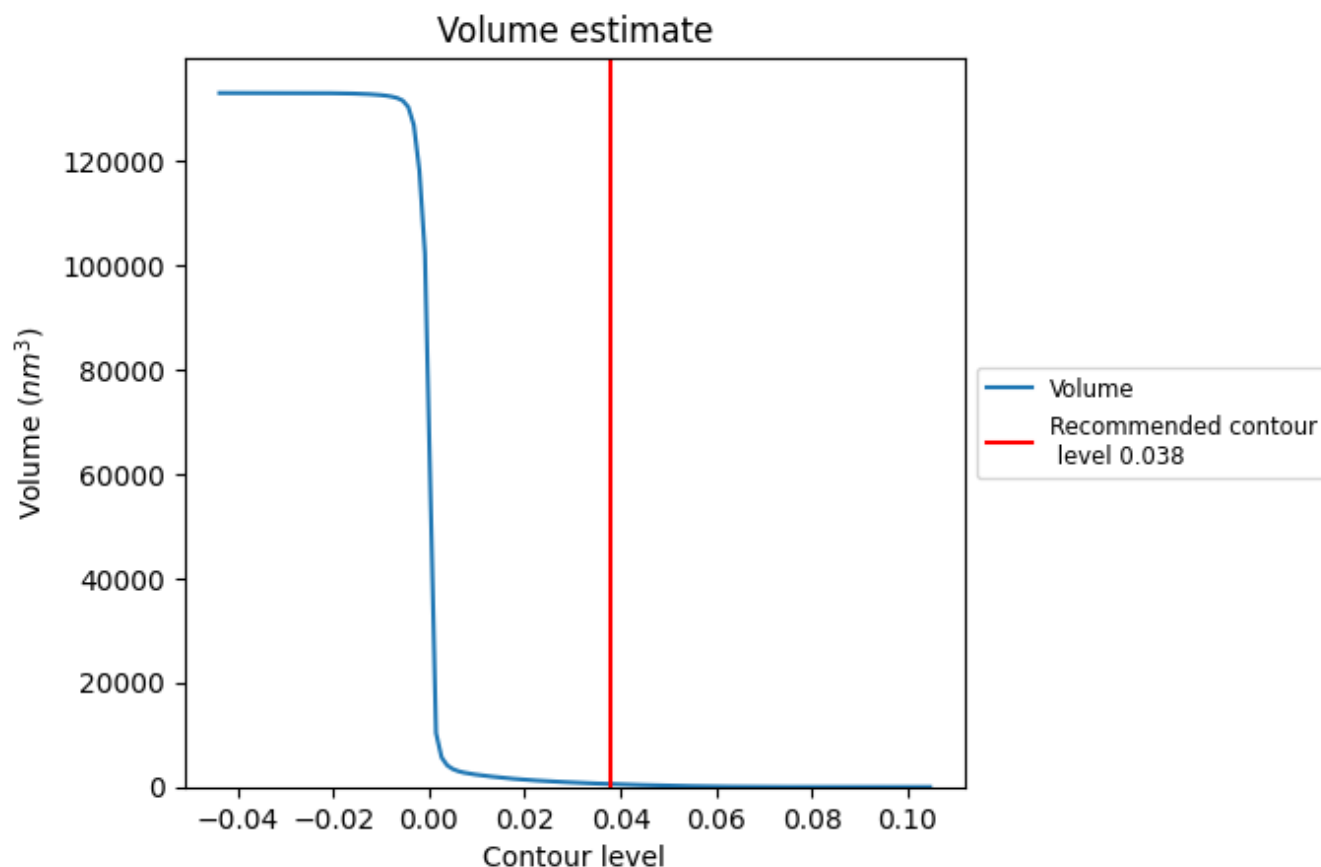
This section contains the results of statistical analysis of the map.

### 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.

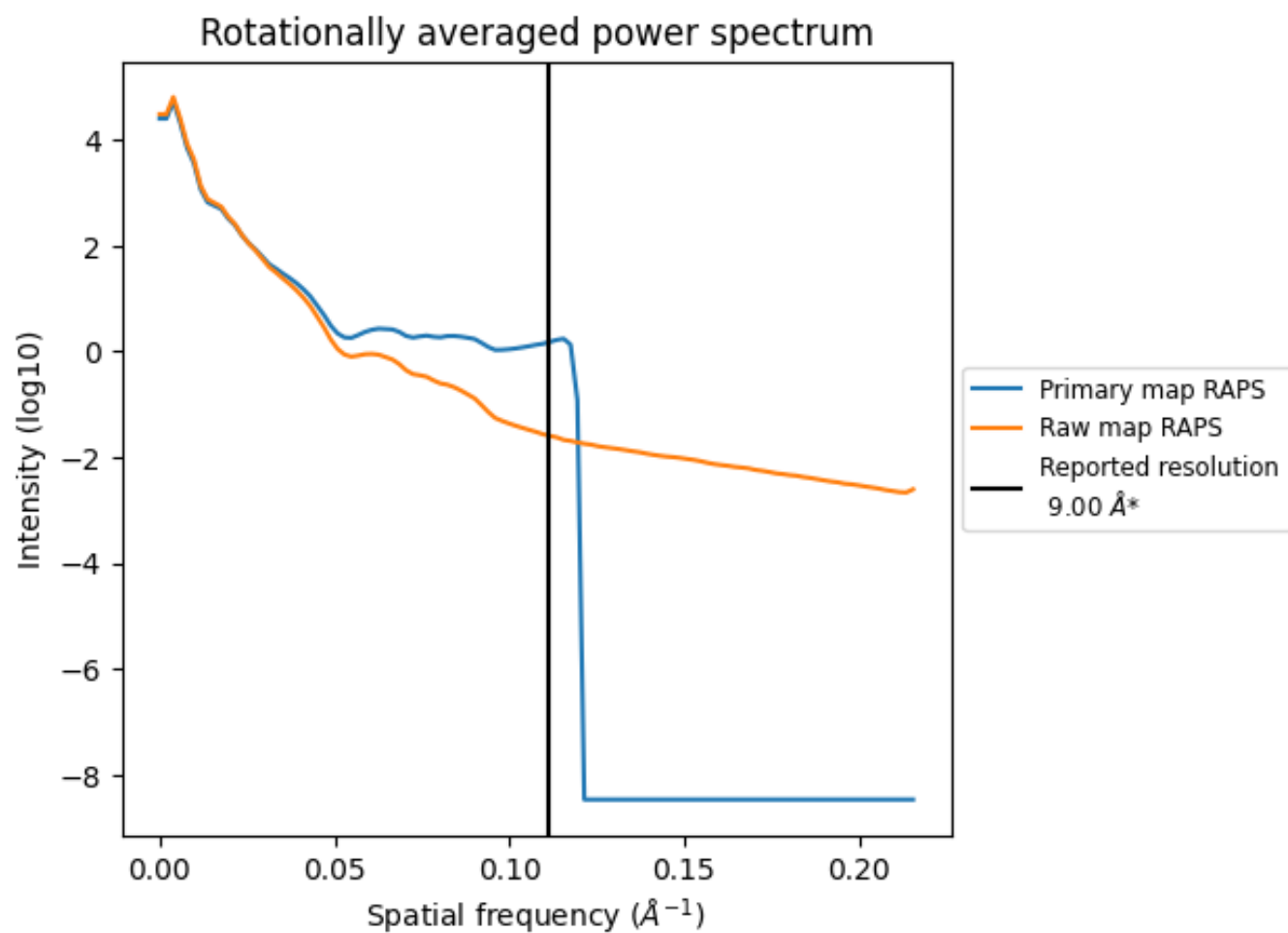
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 563  $\text{nm}^3$ ; this corresponds to an approximate mass of 509 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 ⓘ

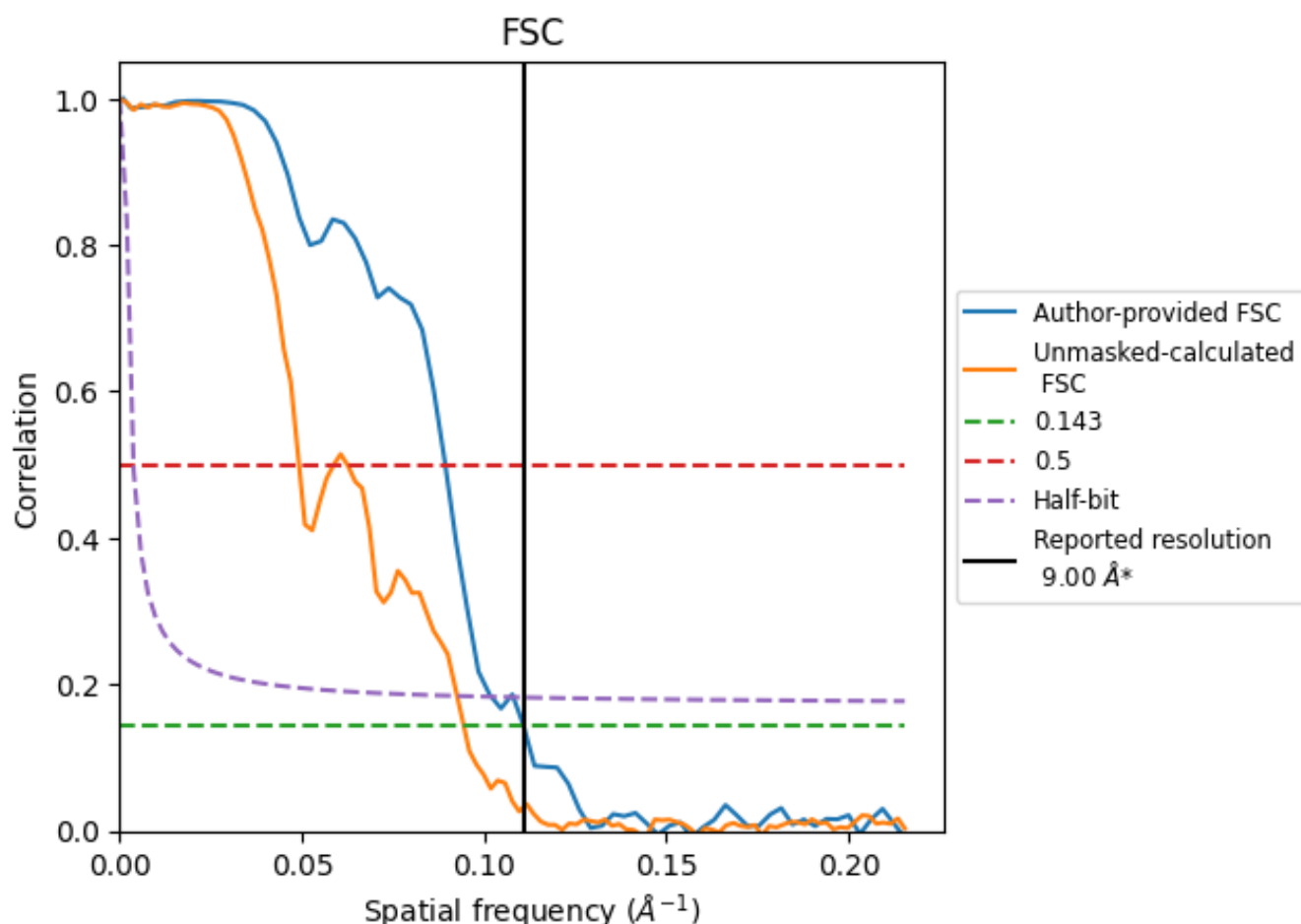


\*Reported resolution corresponds to spatial frequency of 0.111  $\text{\AA}^{-1}$

## 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 0.111 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	9.00	-	-
Author-provided FSC curve	9.02	11.19	9.87
Unmasked-calculated*	10.58	20.28	10.79

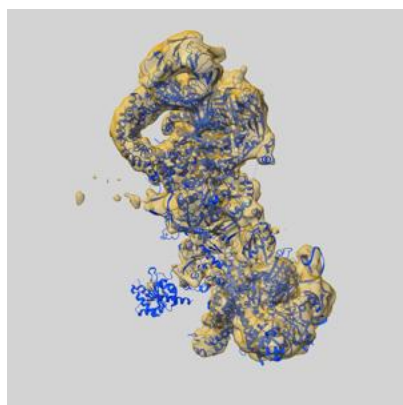
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.58 differs from the reported value 9.0 by more than 10 %



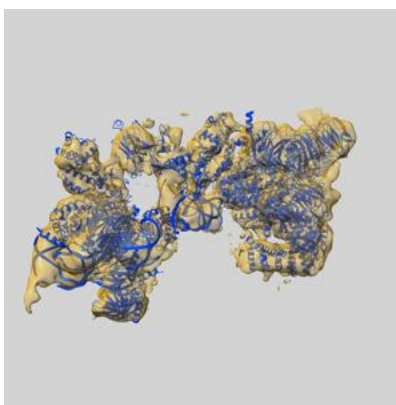
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13028 and PDB model 7OQB. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

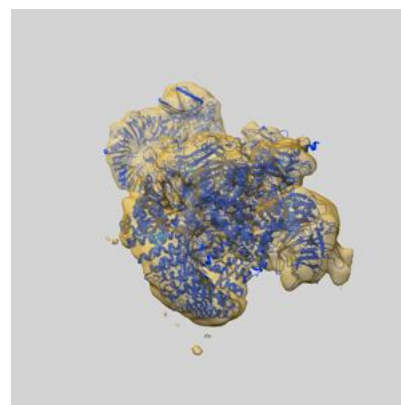
### 9.1 Map-model overlay [i](#)



X



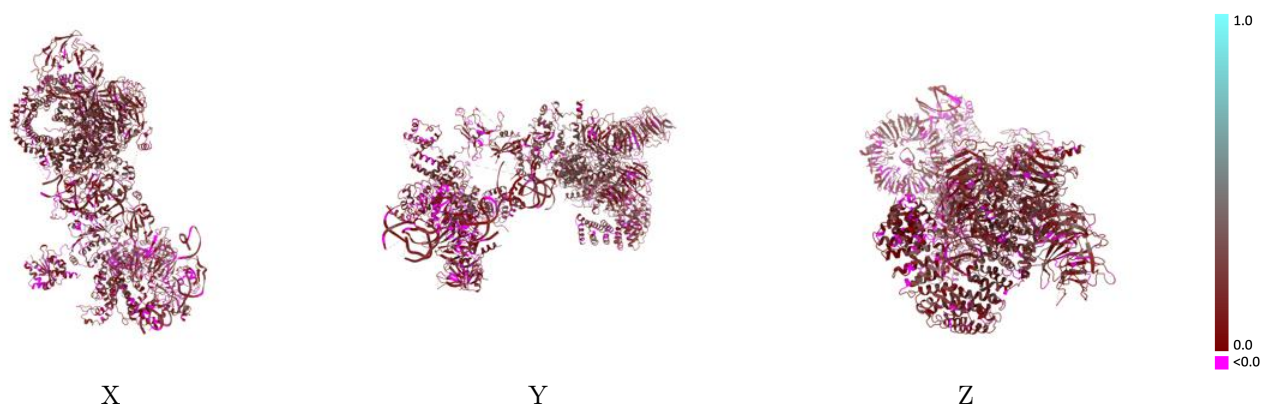
Y



Z

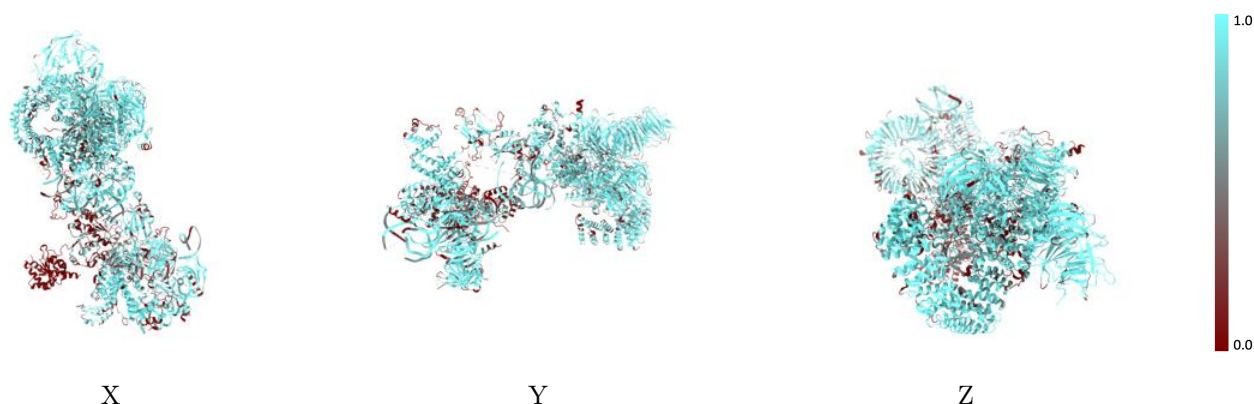
The images above show the 3D surface view of the map at the recommended contour level 0.038 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



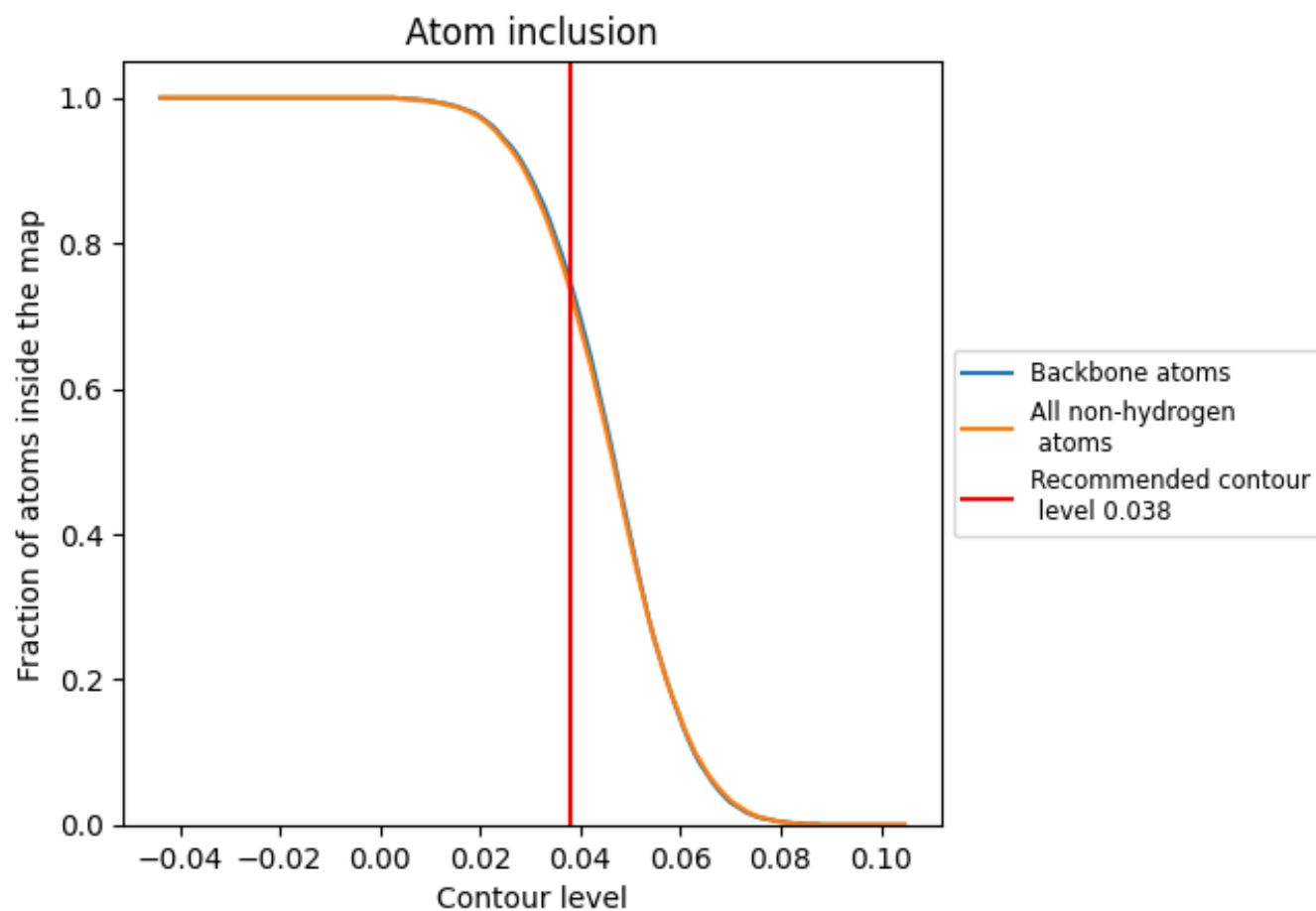
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.038).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.1330
2	 0.7650	 0.1140
I	 0.6650	 0.0960
O	 0.8420	 0.1490
P	 0.8830	 0.1630
Q	 0.5990	 0.1600
R	 0.7780	 0.1640
S	 0.7440	 0.1490
T	 0.7690	 0.1470
U	 0.4450	 0.0880
V	 0.6640	 0.1350
W	 0.6530	 0.1130
Y	 0.8330	 0.0250
Z	 0.9130	 0.2190
p	 0.2070	 0.0970
s	 0.7620	 0.1060
t	 0.5870	 0.0820
u	 0.7150	 0.0570
v	 0.8160	 0.1220
w	 0.8560	 0.0890
x	 0.7970	 0.0520
y	 0.8740	 0.1180

