



## wwPDB EM Validation Summary Report ⓘ

Jun 28, 2023 – 12:36 pm BST

PDB ID : 7ZQB  
EMDB ID : EMD-14869  
Title : Tail tip of siphophage T5 : full structure  
Authors : Linares, R.; Arnaud, C.A.; Effantin, G.; Darnault, C.; Epalle, N.; Boeri Erba, E.; Schoehn, G.; Breyton, C.  
Deposited on : 2022-04-29  
Resolution : 3.88 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.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.88 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

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	h	688	66% 76% 23%
1	i	688	65% 76% 23%
1	j	688	64% 76% 23%
2	J	140	12% 99% .
2	K	140	12% 99% .
2	L	140	13% 100%
2	M	140	13% 100%
2	N	140	13% 99% .
2	O	140	14% 99% .

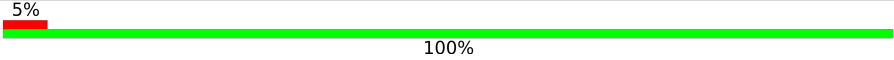
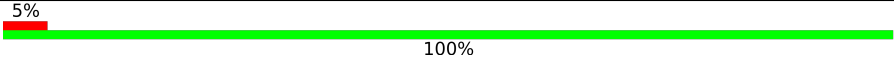
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Mol	Chain	Length	Quality of chain
2	P	140	12% 100%
2	Q	140	12% 100%
2	R	140	14% 99%
2	S	140	12% 99%
2	T	140	13% 100%
2	U	140	12% 100%
3	G	298	• 100%
3	H	298	• 100%
3	I	298	• 100%
4	V	204	• 100%
4	W	204	• 100%
4	X	204	• 100%
4	Y	204	• 100%
4	Z	204	• 100%
4	a	204	• 100%
5	A	464	44% 100%
5	B	464	44% 100%
5	C	464	45% 100%
5	D	464	13% 100%
5	E	464	13% 100%
5	F	464	13% 100%
6	e	1219	• 97%
6	f	1219	• 97%
6	g	1219	• 97%
7	b	949	5% 100%

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Mol	Chain	Length	Quality of chain
7	c	949	 5% 100%
7	d	949	 5% 100%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 86580 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 Probable central straight fiber.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	i	527	4078	2598	680	787	13	0	0
1	h	527	4078	2598	680	787	13	0	0
1	j	527	4078	2598	680	787	13	0	0

- Molecule 2 is a protein called L-shaped tail fiber protein p132.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	139	1048	653	175	217	3	0	0
2	Q	140	1056	658	176	218	4	0	0
2	S	139	1048	653	175	217	3	0	0
2	N	139	1048	653	175	217	3	0	0
2	M	140	1056	658	176	218	4	0	0
2	O	139	1048	653	175	217	3	0	0
2	J	139	1048	653	175	217	3	0	0
2	L	140	1056	658	176	218	4	0	0
2	U	140	1056	658	176	218	4	0	0
2	K	139	1048	653	175	217	3	0	0
2	P	140	1056	658	176	218	4	0	0
2	T	140	1056	658	176	218	4	0	0

- Molecule 3 is a protein called Minor tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	298	Total	C	N	O	S	0	0
			2423	1551	398	464	10		
3	H	298	Total	C	N	O	S	0	0
			2423	1551	398	464	10		
3	G	298	Total	C	N	O	S	0	0
			2423	1551	398	464	10		

- Molecule 4 is a protein called Distal tail protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
4	X	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
4	Y	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
4	W	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
4	V	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		
4	Z	204	Total	C	N	O	S	0	0
			1610	1030	264	313	3		

- Molecule 5 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
5	E	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
5	C	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
5	D	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
5	A	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		
5	B	464	Total	C	N	O	S	0	0
			3546	2217	597	722	10		

- Molecule 6 is a protein called Pore-forming tail tip protein pb2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	f	35	Total	C	N	O	0	0
			262	158	47	57		
6	g	35	Total	C	N	O	0	0
			262	158	47	57		
6	e	35	Total	C	N	O	0	0
			262	158	47	57		

- Molecule 7 is a protein called Probable baseplate hub protein.

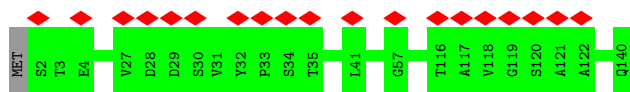
Mol	Chain	Residues	Atoms					AltConf	Trace
7	b	949	Total	C	N	O	S	0	0
			7577	4811	1274	1482	10		
7	d	949	Total	C	N	O	S	0	0
			7577	4811	1274	1482	10		
7	c	949	Total	C	N	O	S	0	0
			7577	4811	1274	1482	10		



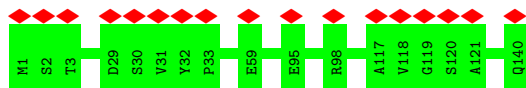








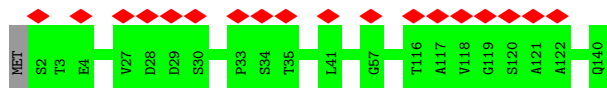
- Molecule 2: L-shaped tail fiber protein p132



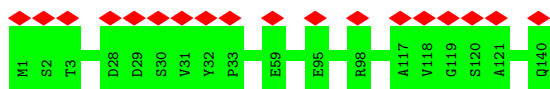
- Molecule 2: L-shaped tail fiber protein p132



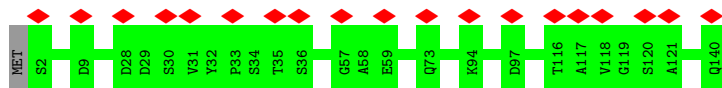
- Molecule 2: L-shaped tail fiber protein p132



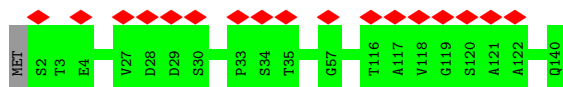
- Molecule 2: L-shaped tail fiber protein p132



- Molecule 2: L-shaped tail fiber protein p132



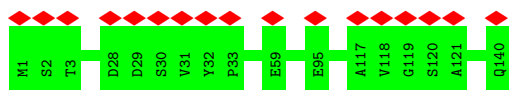
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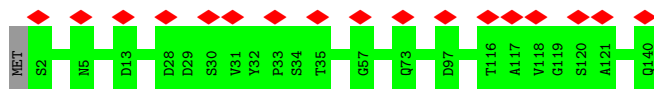
- Molecule 2: L-shaped tail fiber protein p132



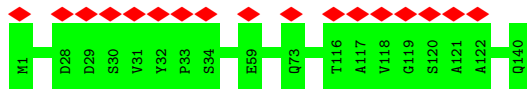
- Molecule 2: L-shaped tail fiber protein p132



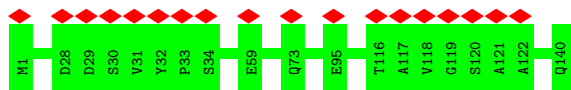
- Molecule 2: L-shaped tail fiber protein p132



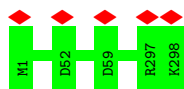
- Molecule 2: L-shaped tail fiber protein p132



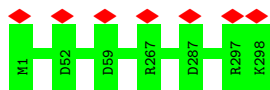
- Molecule 2: L-shaped tail fiber protein p132



- Molecule 3: Minor tail protein

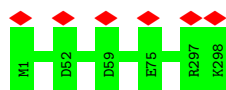


- Molecule 3: Minor tail protein



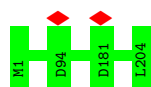
- Molecule 3: Minor tail protein

Chain G:  100%



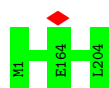
- Molecule 4: Distal tail protein

Chain a:  100%



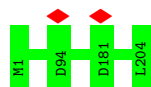
- Molecule 4: Distal tail protein

Chain X:  100%



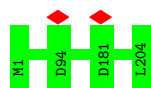
- Molecule 4: Distal tail protein

Chain Y:  100%



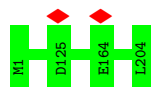
- Molecule 4: Distal tail protein

Chain W:  100%



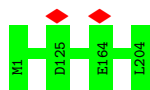
- Molecule 4: Distal tail protein

Chain V:  100%

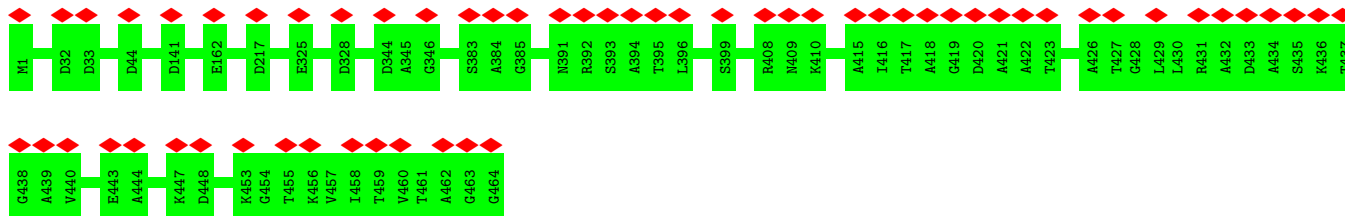


- Molecule 4: Distal tail protein

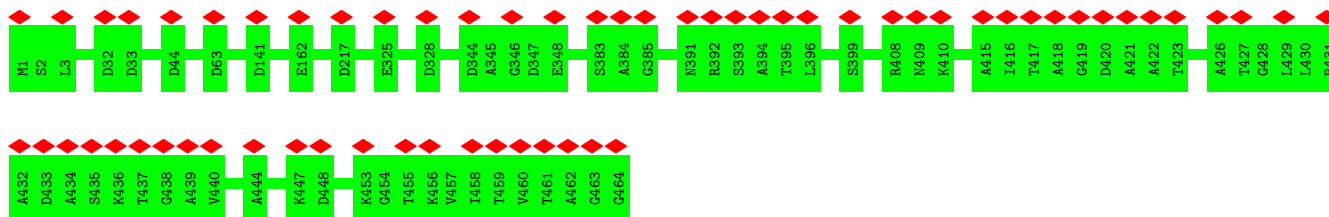
Chain Z:  100%



• Molecule 5: Tail tube protein



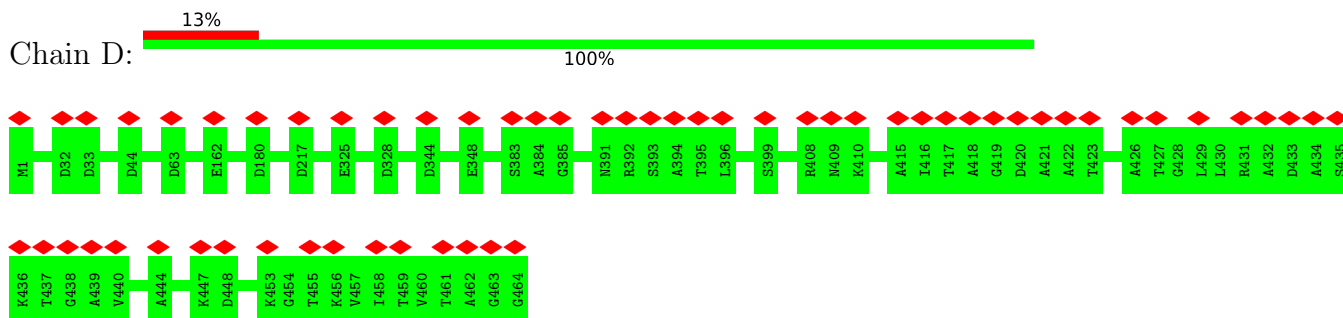
• Molecule 5: Tail tube protein



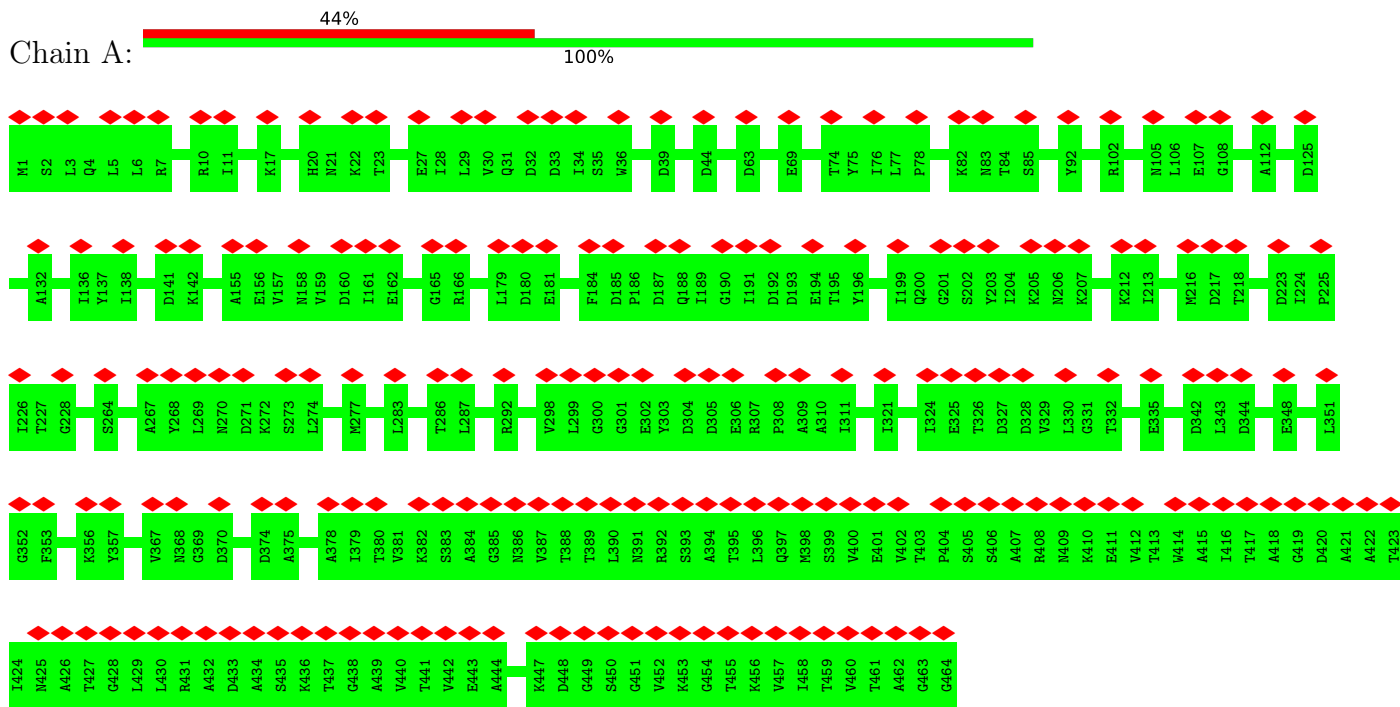
• Molecule 5: Tail tube protein



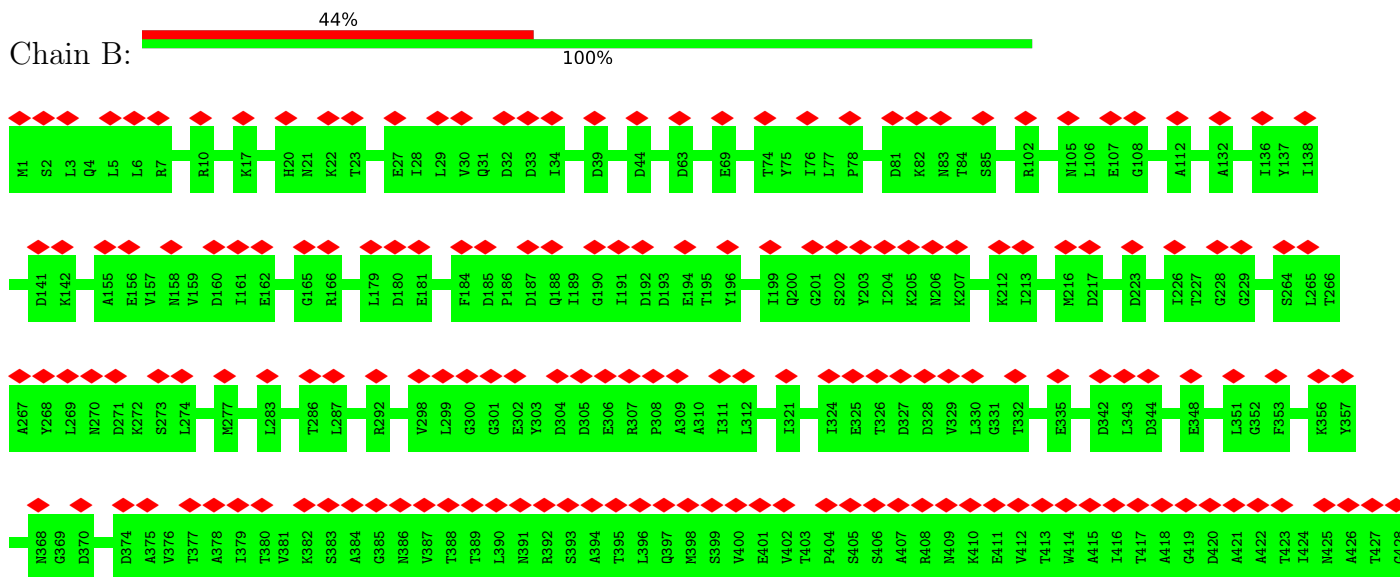
• Molecule 5: Tail tube protein



• Molecule 5: Tail tube protein



• Molecule 5: Tail tube protein



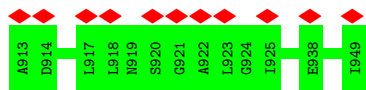












## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	9290	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	621.45996, 621.45996, 621.45996	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.351, 1.351, 1.351	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	h	0.26	0/4165	0.50	0/5665
1	i	0.26	0/4165	0.50	0/5665
1	j	0.26	0/4165	0.51	0/5665
2	J	0.26	0/1062	0.54	0/1443
2	K	0.26	0/1062	0.54	0/1443
2	L	0.30	0/1070	0.55	0/1453
2	M	0.26	0/1070	0.54	0/1453
2	N	0.26	0/1062	0.54	0/1443
2	O	0.26	0/1062	0.53	0/1443
2	P	0.30	0/1070	0.55	0/1453
2	Q	0.26	0/1070	0.53	0/1453
2	R	0.26	0/1062	0.54	0/1443
2	S	0.27	0/1062	0.54	0/1443
2	T	0.30	0/1070	0.55	0/1453
2	U	0.26	0/1070	0.53	0/1453
3	G	0.28	0/2483	0.50	0/3370
3	H	0.28	0/2483	0.50	0/3370
3	I	0.28	0/2483	0.50	0/3370
4	V	0.28	0/1649	0.48	0/2239
4	W	0.27	0/1649	0.47	0/2239
4	X	0.28	0/1649	0.48	0/2239
4	Y	0.27	0/1649	0.47	0/2239
4	Z	0.28	0/1649	0.48	0/2239
4	a	0.27	0/1649	0.47	0/2239
5	A	0.26	0/3604	0.50	0/4904
5	B	0.26	0/3604	0.50	0/4904
5	C	0.26	0/3604	0.50	0/4904
5	D	0.26	0/3604	0.50	0/4904
5	E	0.26	0/3604	0.50	0/4904
5	F	0.26	0/3604	0.50	0/4904
6	e	0.33	0/264	0.39	0/354
6	f	0.33	0/264	0.39	0/354
6	g	0.33	0/264	0.39	0/354
7	b	0.28	0/7741	0.48	0/10502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	c	0.28	0/7741	0.48	0/10502
7	d	0.28	0/7741	0.48	0/10502
All	All	0.27	0/88269	0.50	0/119907

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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	h	523/688 (76%)	467 (89%)	55 (10%)	1 (0%)	47	79
1	i	523/688 (76%)	467 (89%)	55 (10%)	1 (0%)	47	79
1	j	523/688 (76%)	467 (89%)	55 (10%)	1 (0%)	47	79
2	J	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
2	K	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
2	L	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	M	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
2	N	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
2	O	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
2	P	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	Q	138/140 (99%)	131 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
2	S	137/140 (98%)	133 (97%)	4 (3%)	0	100	100
2	T	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
2	U	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
3	G	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
3	H	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
3	I	296/298 (99%)	286 (97%)	10 (3%)	0	100	100
4	V	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
4	W	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
4	X	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
4	Y	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
4	Z	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
4	a	202/204 (99%)	197 (98%)	5 (2%)	0	100	100
5	A	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
5	B	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
5	C	462/464 (100%)	445 (96%)	17 (4%)	0	100	100
5	D	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
5	E	462/464 (100%)	446 (96%)	16 (4%)	0	100	100
5	F	462/464 (100%)	447 (97%)	15 (3%)	0	100	100
6	e	33/1219 (3%)	32 (97%)	1 (3%)	0	100	100
6	f	33/1219 (3%)	32 (97%)	1 (3%)	0	100	100
6	g	33/1219 (3%)	32 (97%)	1 (3%)	0	100	100
7	b	947/949 (100%)	907 (96%)	40 (4%)	0	100	100
7	c	947/949 (100%)	906 (96%)	41 (4%)	0	100	100
7	d	947/949 (100%)	907 (96%)	40 (4%)	0	100	100
All	All	11031/15150 (73%)	10524 (95%)	504 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	i	250	GLU
1	h	250	GLU
1	j	250	GLU



### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	441/572 (77%)	439 (100%)	2 (0%)	88	93
1	i	441/572 (77%)	439 (100%)	2 (0%)	88	93
1	j	441/572 (77%)	439 (100%)	2 (0%)	88	93
2	J	118/119 (99%)	118 (100%)	0	100	100
2	K	118/119 (99%)	118 (100%)	0	100	100
2	L	119/119 (100%)	119 (100%)	0	100	100
2	M	119/119 (100%)	119 (100%)	0	100	100
2	N	118/119 (99%)	118 (100%)	0	100	100
2	O	118/119 (99%)	118 (100%)	0	100	100
2	P	119/119 (100%)	119 (100%)	0	100	100
2	Q	119/119 (100%)	119 (100%)	0	100	100
2	R	118/119 (99%)	118 (100%)	0	100	100
2	S	118/119 (99%)	118 (100%)	0	100	100
2	T	119/119 (100%)	119 (100%)	0	100	100
2	U	119/119 (100%)	119 (100%)	0	100	100
3	G	273/273 (100%)	273 (100%)	0	100	100
3	H	273/273 (100%)	273 (100%)	0	100	100
3	I	273/273 (100%)	273 (100%)	0	100	100
4	V	181/181 (100%)	181 (100%)	0	100	100
4	W	181/181 (100%)	181 (100%)	0	100	100
4	X	181/181 (100%)	181 (100%)	0	100	100
4	Y	181/181 (100%)	181 (100%)	0	100	100
4	Z	181/181 (100%)	181 (100%)	0	100	100
4	a	181/181 (100%)	181 (100%)	0	100	100
5	A	394/394 (100%)	394 (100%)	0	100	100
5	B	394/394 (100%)	394 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	C	394/394 (100%)	394 (100%)	0	100	100
5	D	394/394 (100%)	394 (100%)	0	100	100
5	E	394/394 (100%)	394 (100%)	0	100	100
5	F	394/394 (100%)	394 (100%)	0	100	100
6	e	28/980 (3%)	28 (100%)	0	100	100
6	f	28/980 (3%)	28 (100%)	0	100	100
6	g	28/980 (3%)	28 (100%)	0	100	100
7	b	834/834 (100%)	832 (100%)	2 (0%)	93	96
7	c	834/834 (100%)	832 (100%)	2 (0%)	93	96
7	d	834/834 (100%)	832 (100%)	2 (0%)	93	96
All	All	9600/12855 (75%)	9588 (100%)	12 (0%)	93	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	b	863	VAL
7	d	700	ARG
7	c	863	VAL
7	d	863	VAL
1	h	458	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	A	151	GLN
5	B	151	GLN
7	c	721	GLN
6	e	1209	ASN
7	d	721	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

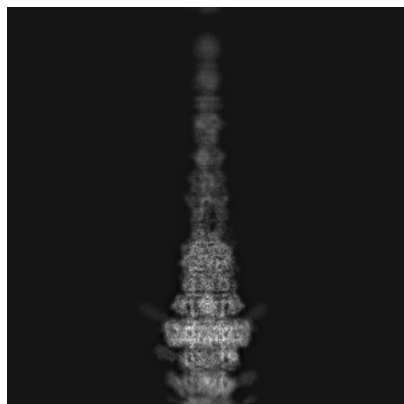
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14869. These allow visual inspection of the internal detail of the map and identification of artifacts.

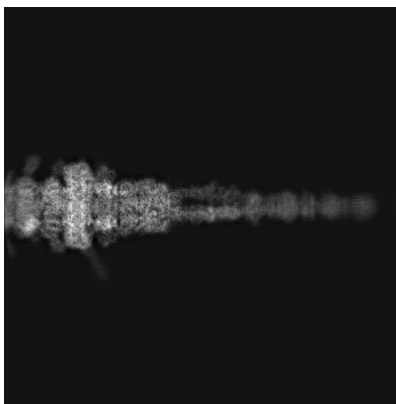
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

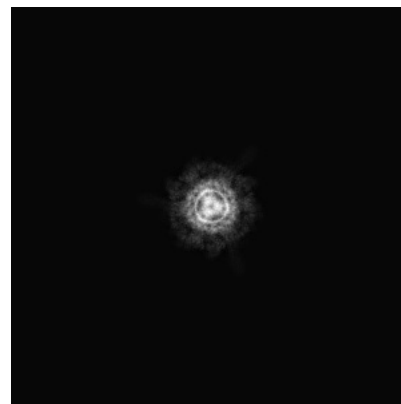
#### 6.1.1 Primary map



X

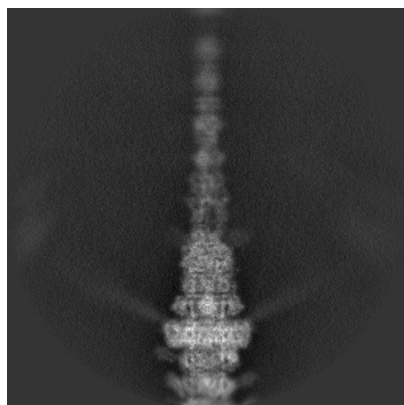


Y

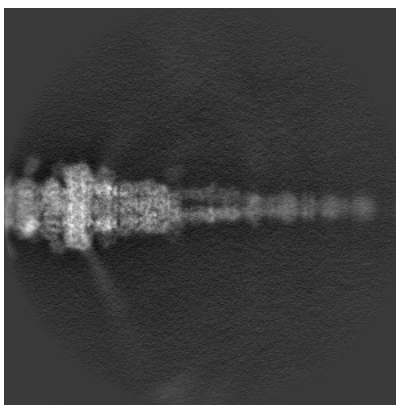


Z

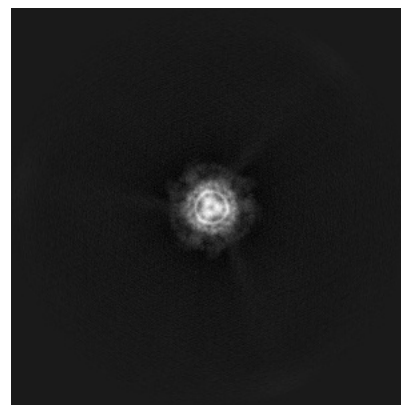
#### 6.1.2 Raw map



X



Y

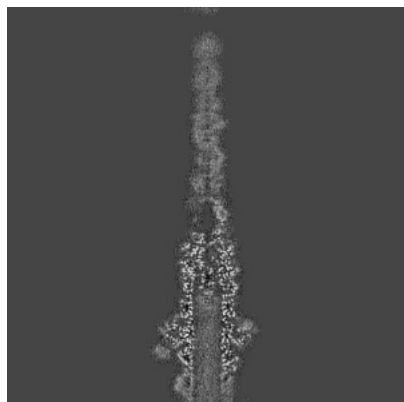


Z

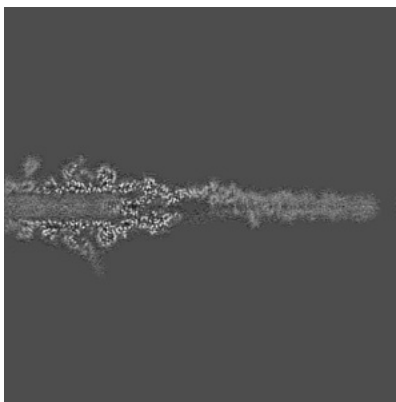
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

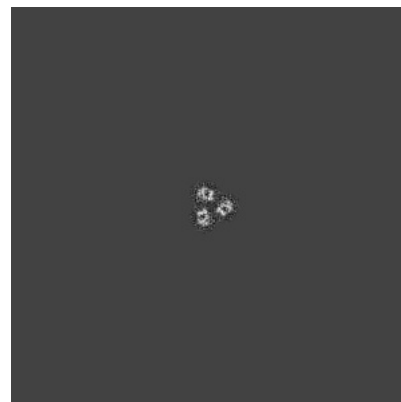
### 6.2.1 Primary map



X Index: 230

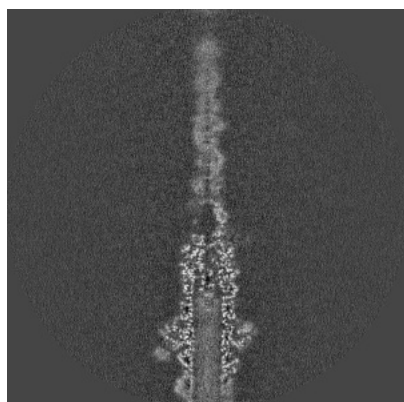


Y Index: 230

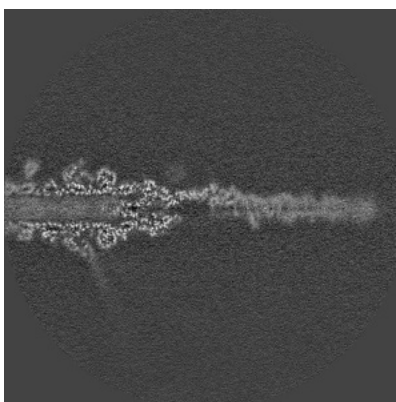


Z Index: 230

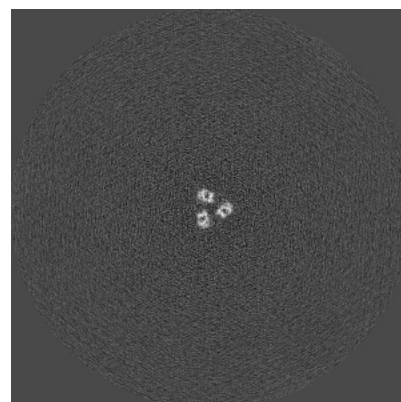
### 6.2.2 Raw map



X Index: 230



Y Index: 230

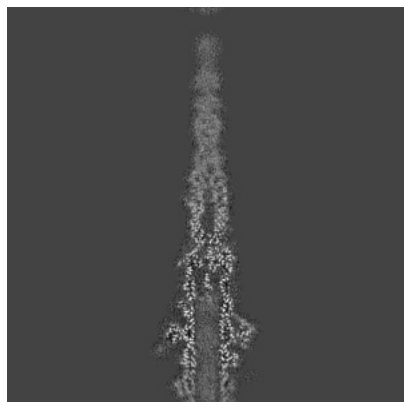


Z Index: 230

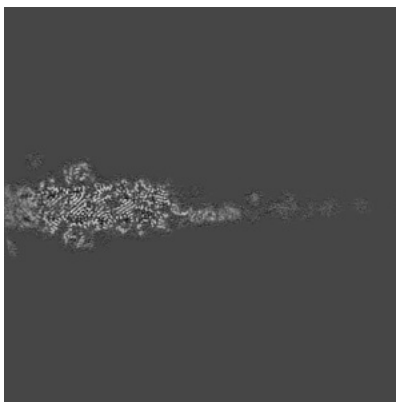
The images above show central slices of the map in three orthogonal directions.

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

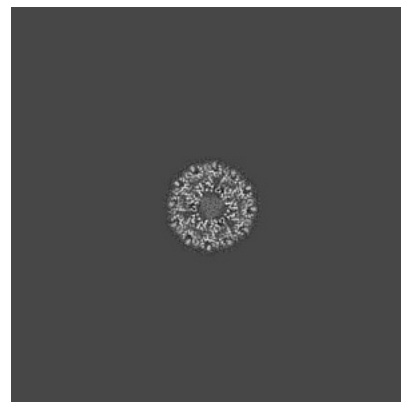
### 6.3.1 Primary map



X Index: 223

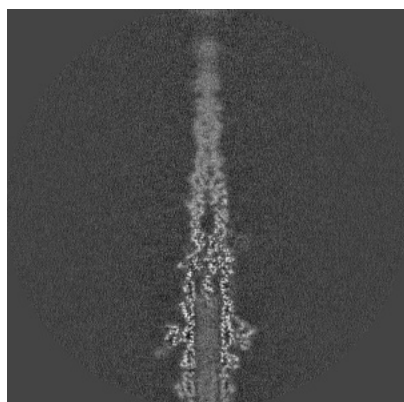


Y Index: 213

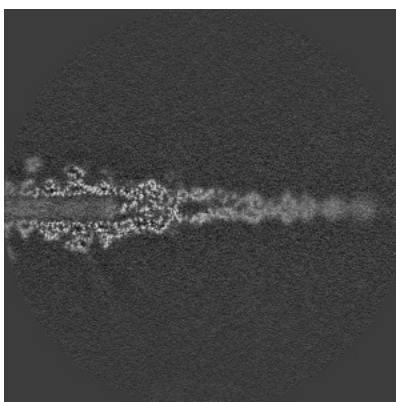


Z Index: 77

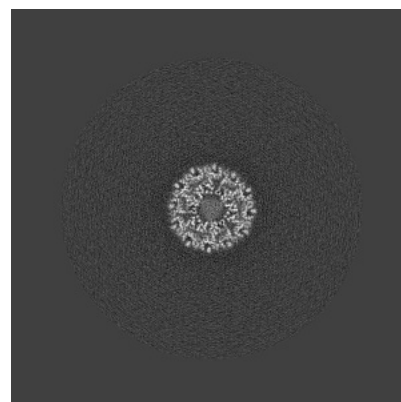
### 6.3.2 Raw map



X Index: 224



Y Index: 223

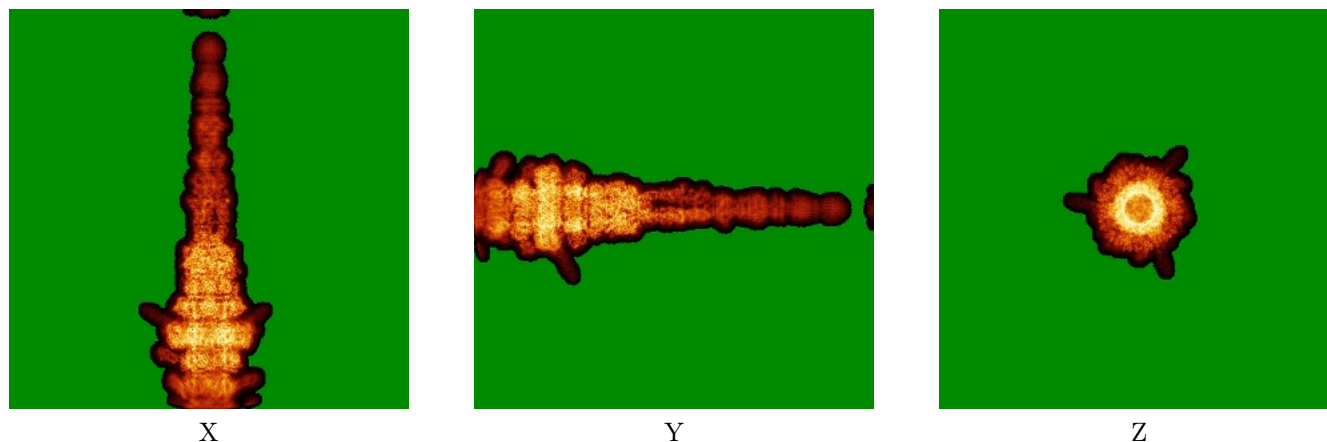


Z Index: 77

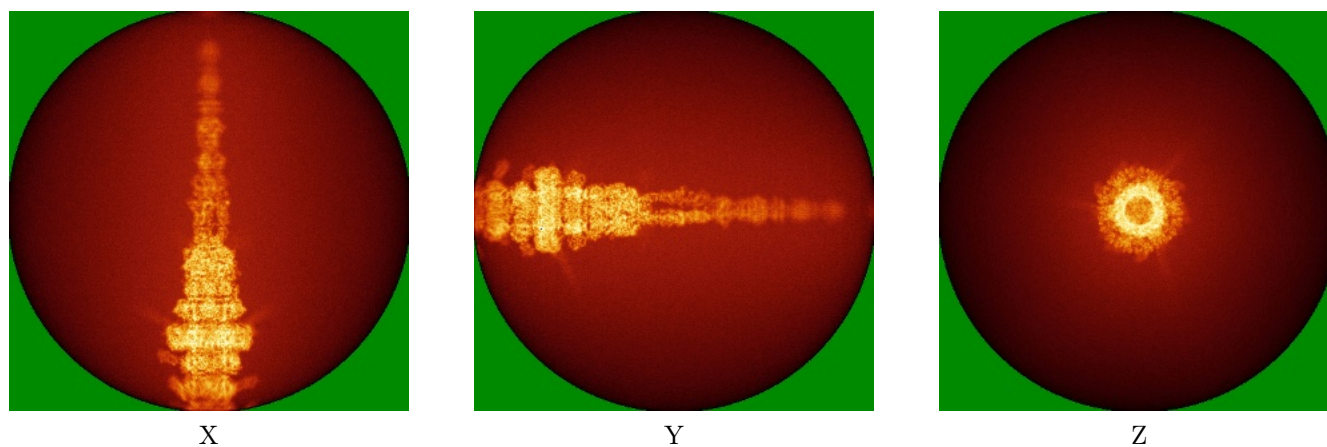
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



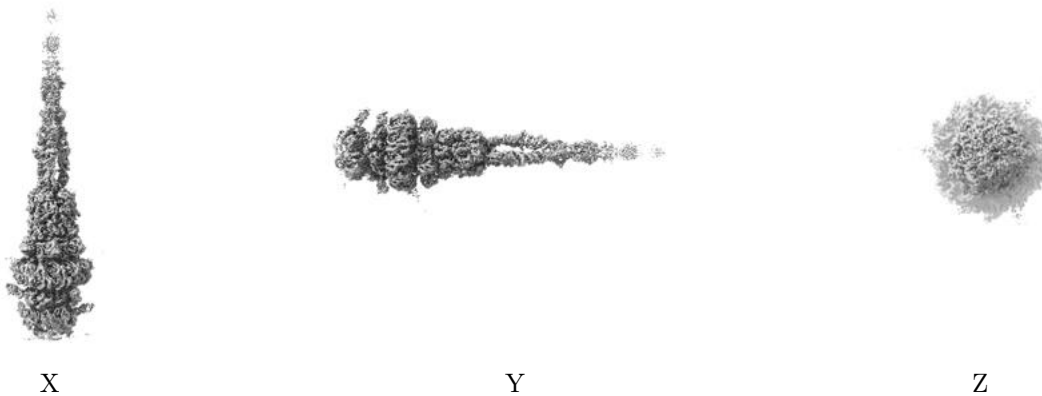
### 6.4.2 Raw map



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.

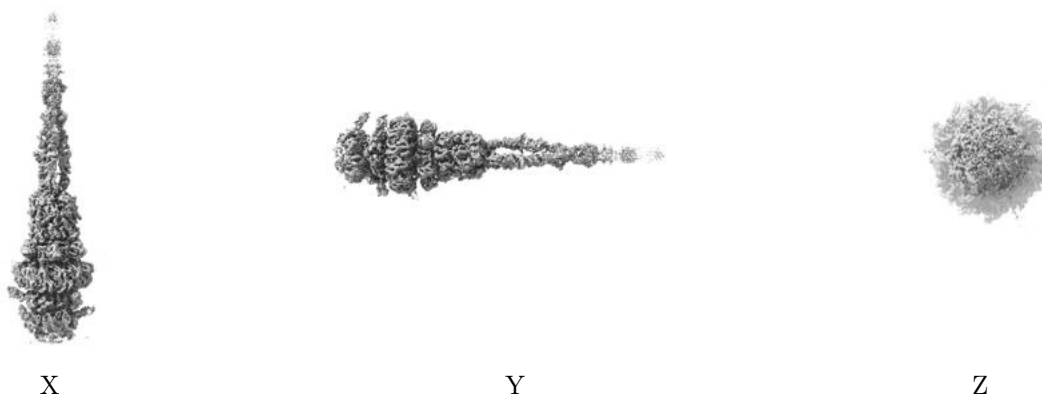
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. 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](#)

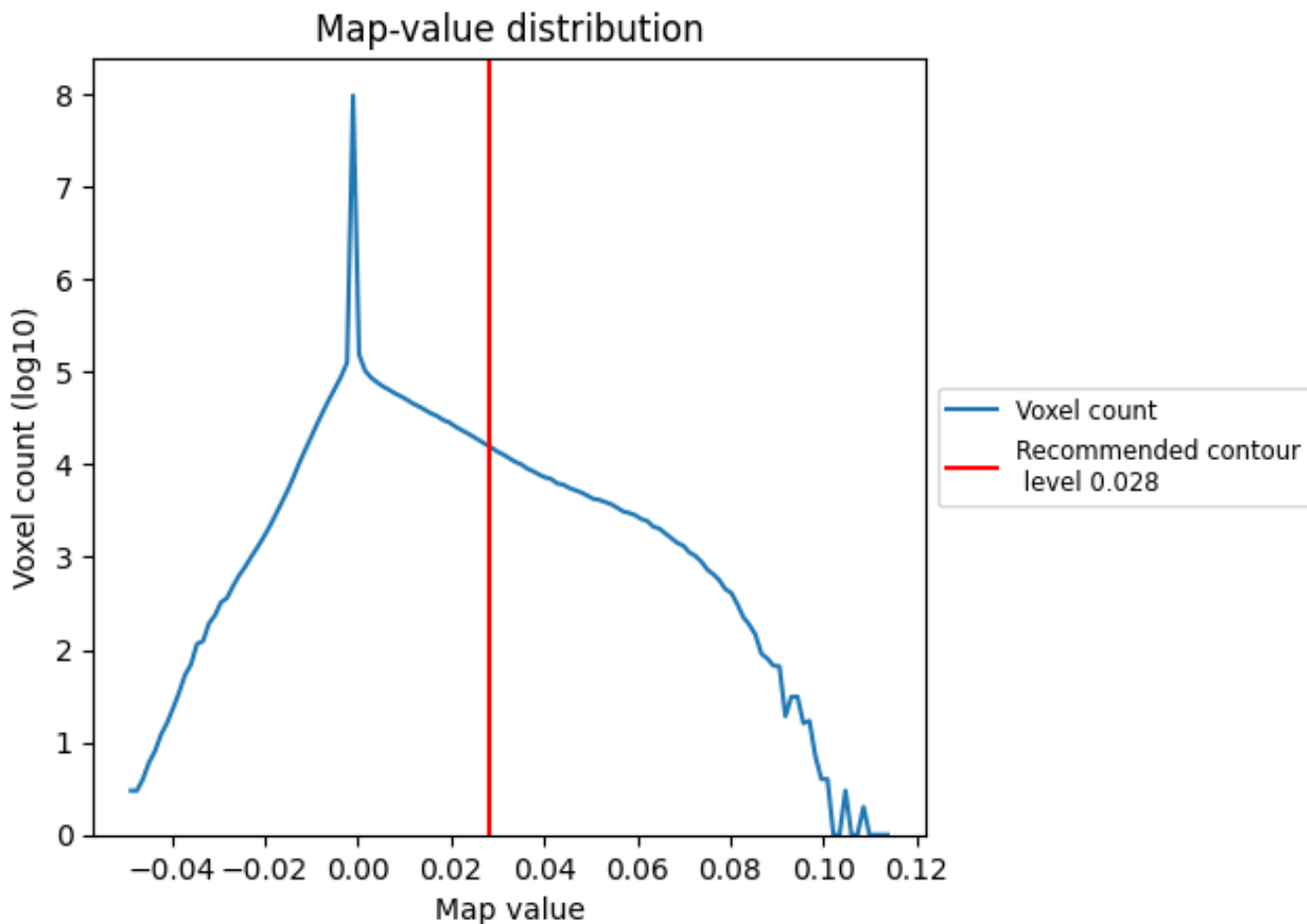
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

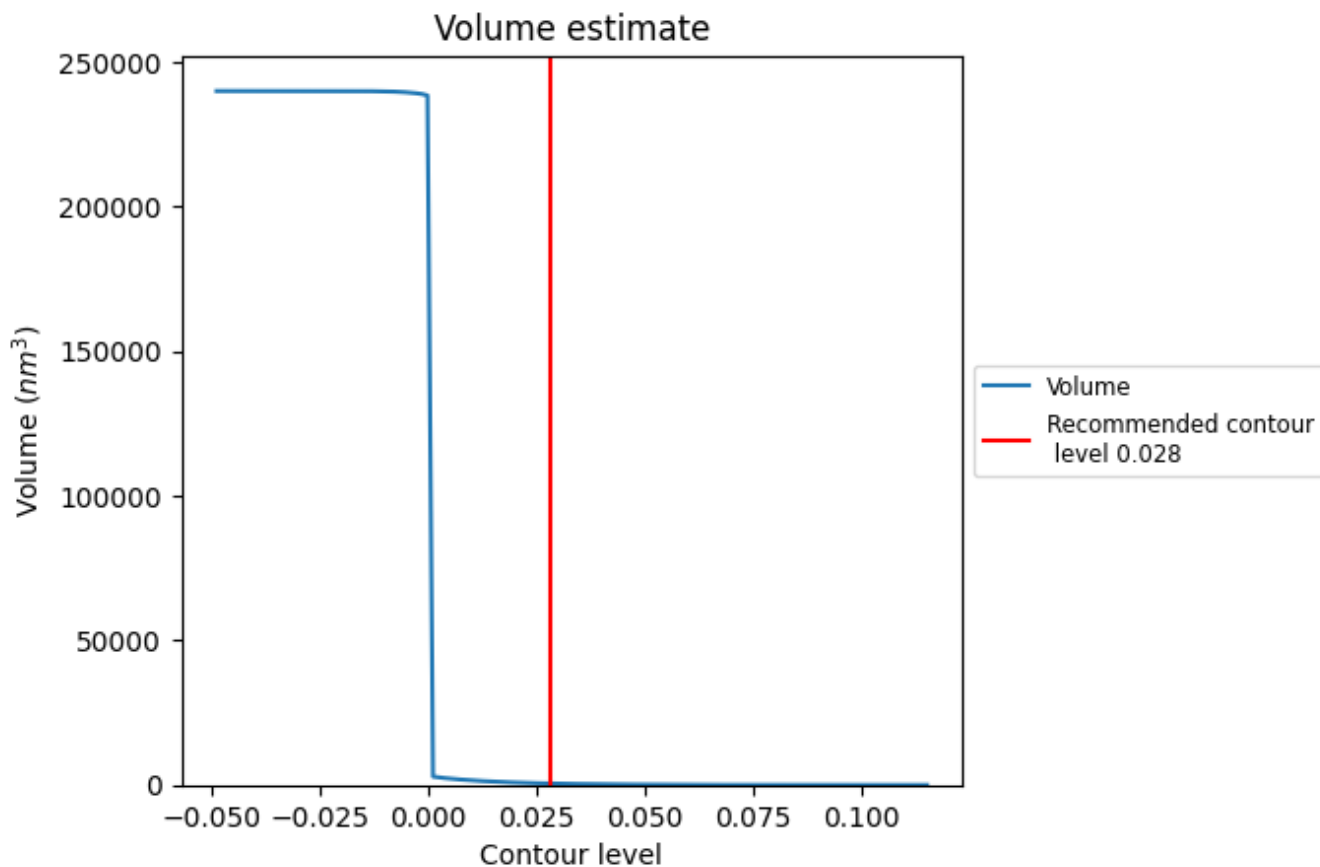
This section contains the results of statistical analysis of the map.

### 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.

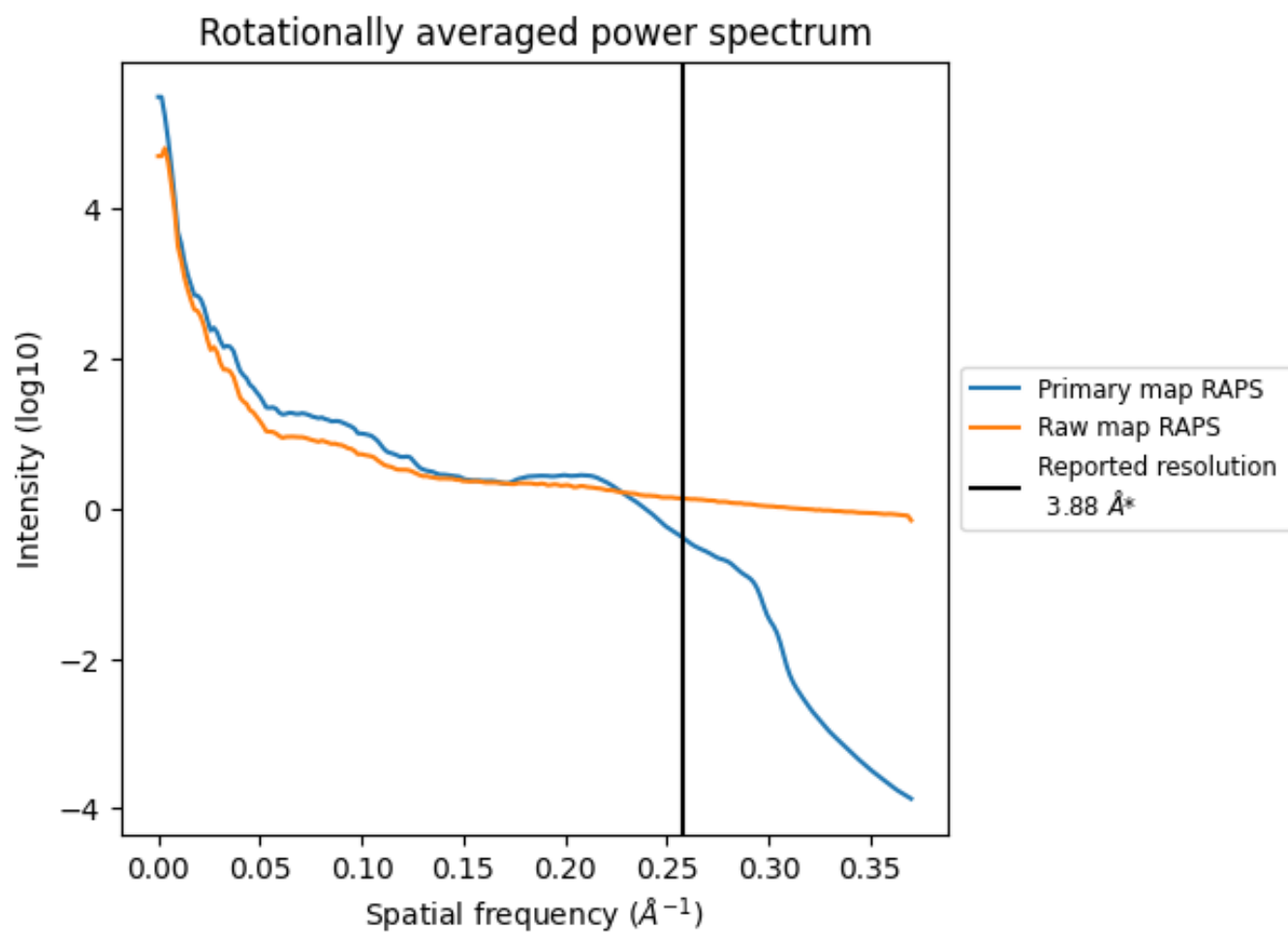
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 504 nm<sup>3</sup>; this corresponds to an approximate mass of 455 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

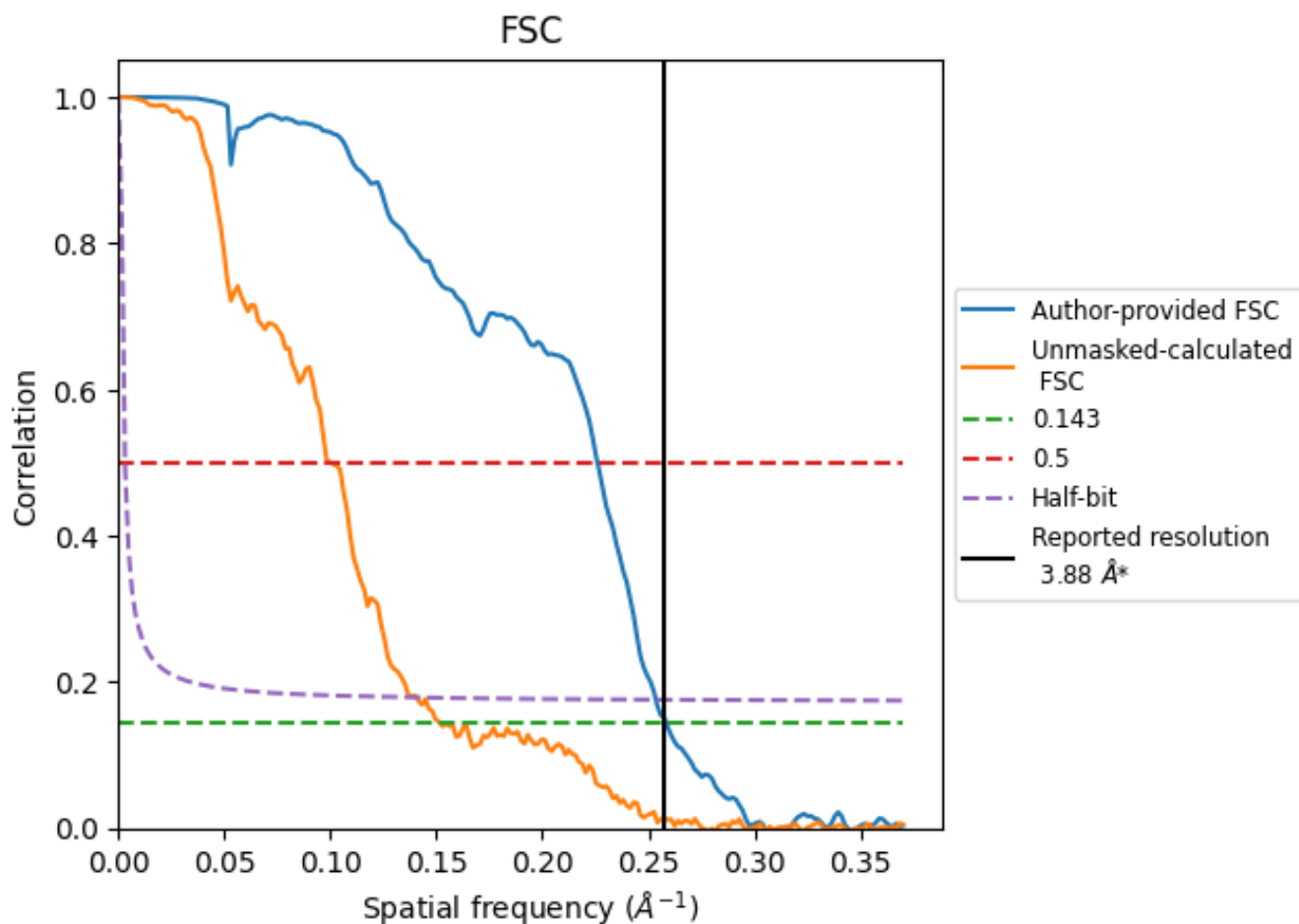


\*Reported resolution corresponds to spatial frequency of 0.258 Å<sup>-1</sup>

## 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 0.258 Å<sup>-1</sup>

## 8.2 Resolution estimates

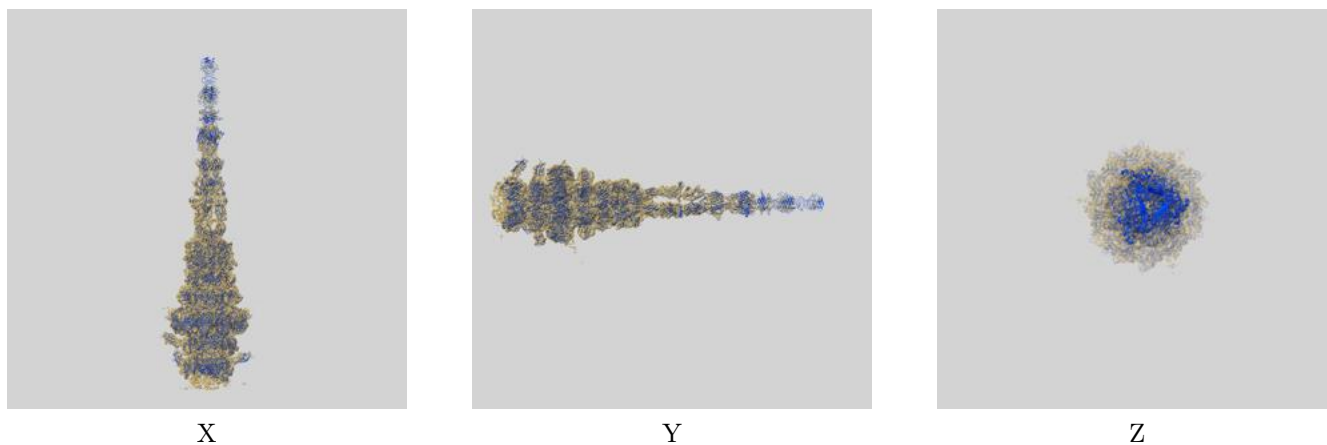
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.88	-	-
Author-provided FSC curve	3.87	4.43	3.94
Unmasked-calculated*	6.59	9.99	7.11

\*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 6.59 differs from the reported value 3.88 by more than 10 %

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

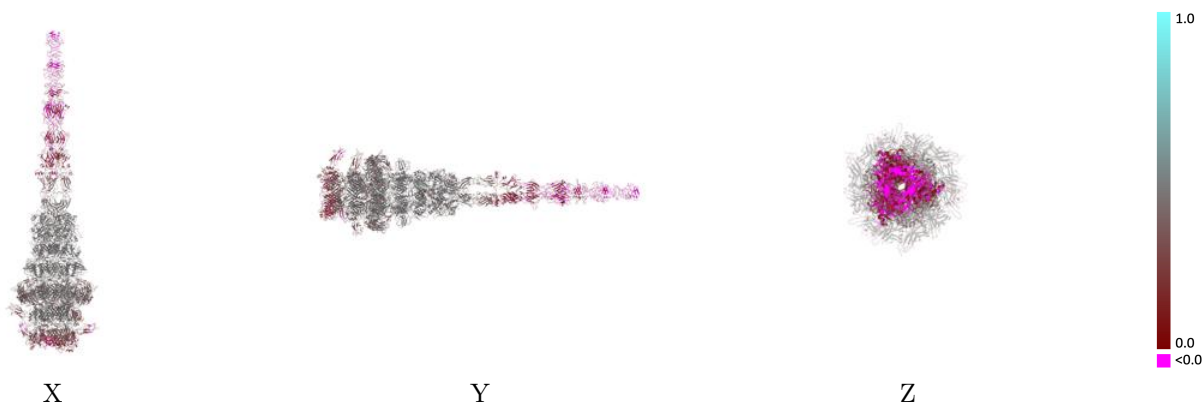
This section contains information regarding the fit between EMDB map EMD-14869 and PDB model 7ZQB. Per-residue inclusion information can be found in section 3 on page 8.

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



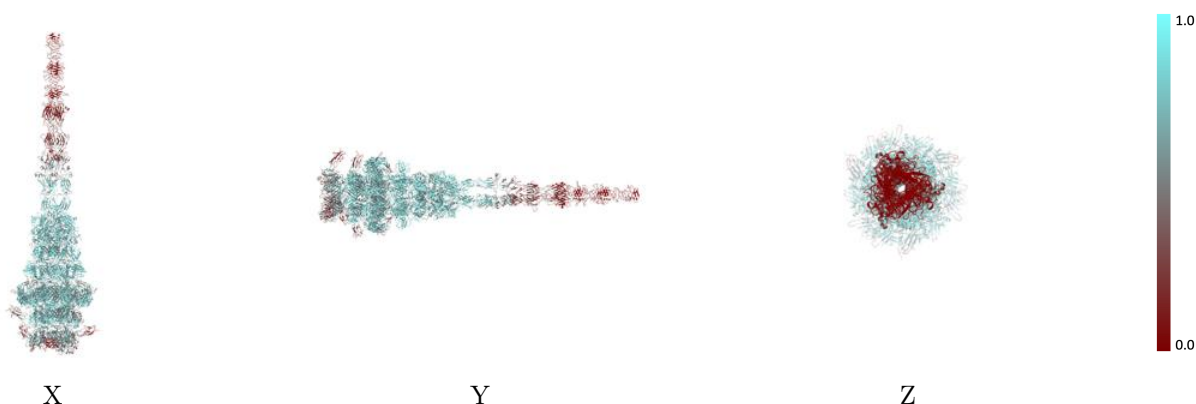
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



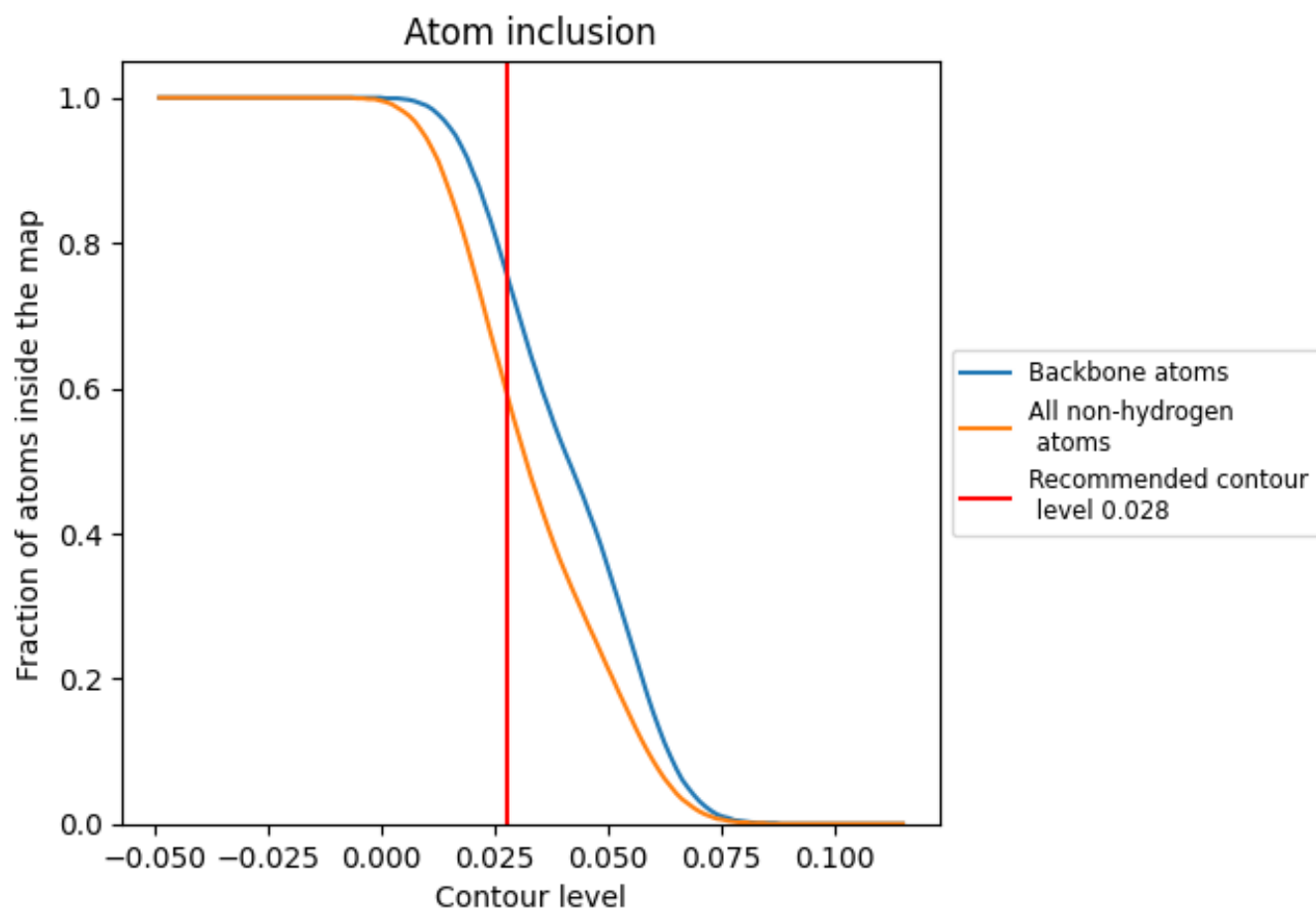
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 75% of all backbone atoms, 59% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.3570
A	 0.4270	 0.2420
B	 0.4270	 0.2430
C	 0.4230	 0.2420
D	 0.6590	 0.4180
E	 0.6590	 0.4170
F	 0.6590	 0.4180
G	 0.7360	 0.4710
H	 0.7430	 0.4700
I	 0.7460	 0.4700
J	 0.6180	 0.3810
K	 0.6290	 0.3810
L	 0.6200	 0.3980
M	 0.6460	 0.4180
N	 0.6140	 0.3710
O	 0.6350	 0.3770
P	 0.6190	 0.3930
Q	 0.6530	 0.4160
R	 0.6110	 0.3720
S	 0.6320	 0.3810
T	 0.6180	 0.3970
U	 0.6530	 0.4180
V	 0.7510	 0.4550
W	 0.7550	 0.4600
X	 0.7460	 0.4510
Y	 0.7430	 0.4560
Z	 0.7500	 0.4530
a	 0.7510	 0.4590
b	 0.7160	 0.4300
c	 0.7170	 0.4320
d	 0.7110	 0.4250
e	 0.6700	 0.4200
f	 0.6860	 0.4260
g	 0.6630	 0.4260
h	 0.1630	 0.0900



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Chain	Atom inclusion	Q-score
i	 0.1640	 0.0780
j	 0.1630	 0.0790