



## wwPDB EM Validation Summary Report ⓘ

Dec 21, 2022 – 12:40 pm GMT

PDB ID : 7ZPM  
EMDB ID : EMD-14858  
Title : Influenza A/H7N9 polymerase apo-protein dimer complex  
Authors : Cusack, S.; Kouba, T.  
Deposited on : 2022-04-27  
Resolution : 2.81 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.dev43  
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) : 2.31.3

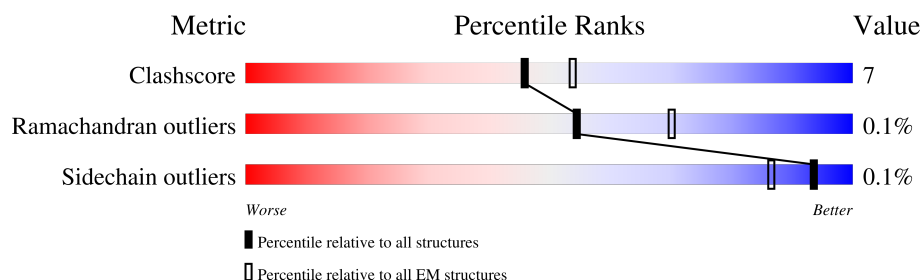
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.81 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	717	
1	D	717	
2	B	757	
2	E	757	
3	C	759	
3	F	759	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19330 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	515	Total	C	N	O	S	0	0
			4142	2622	703	787	30		
1	D	514	Total	C	N	O	S	0	0
			4133	2617	702	784	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP M9TI86
D	0	GLY	-	expression tag	UNP M9TI86

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	610	Total	C	N	O	S	0	0
			4853	3065	833	918	37		
2	E	613	Total	C	N	O	S	0	0
			4884	3087	841	919	37		

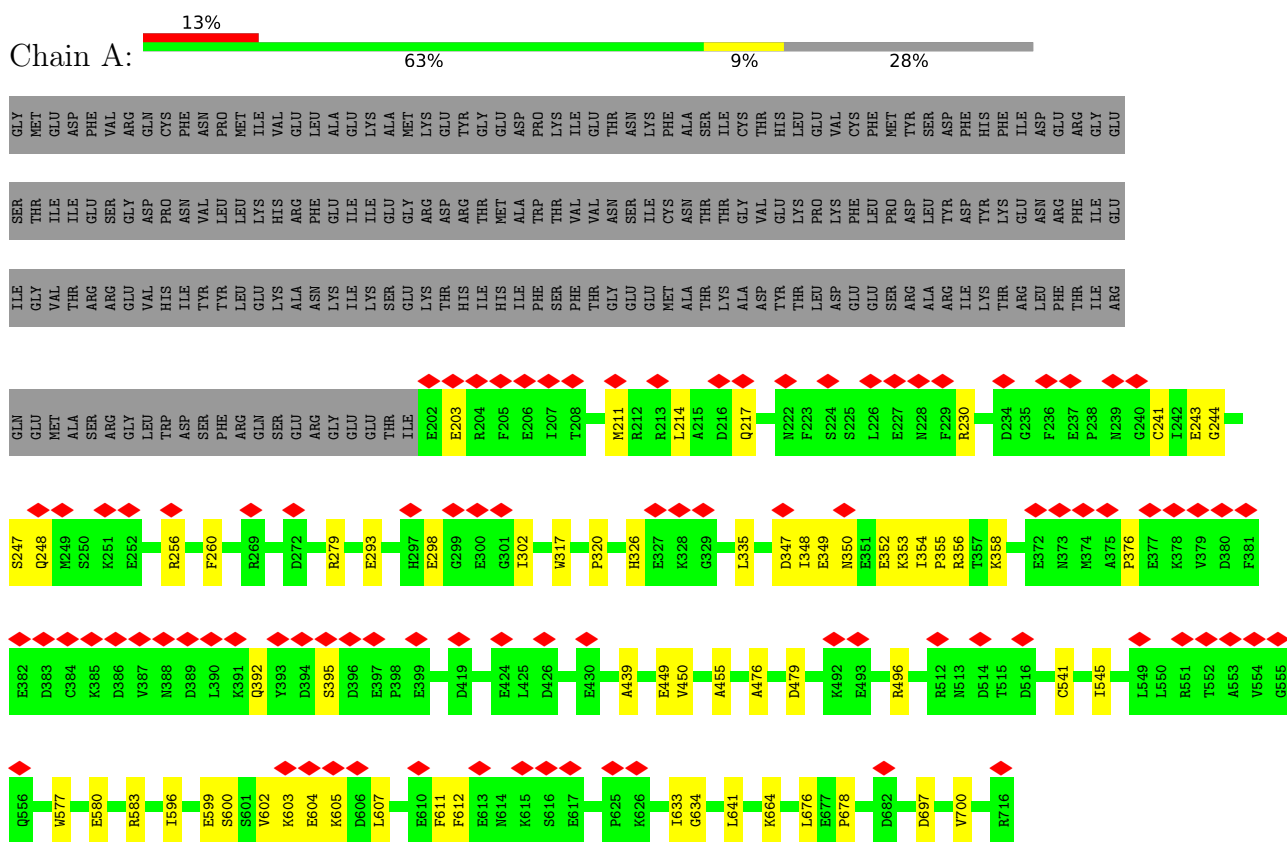
- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			659	420	115	117	7		
3	F	80	Total	C	N	O	S	0	0
			659	420	115	117	7		

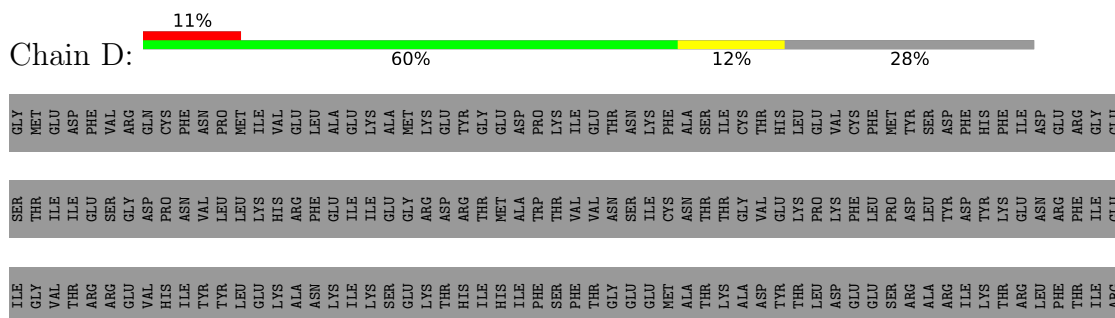
### 3 Residue-property plots

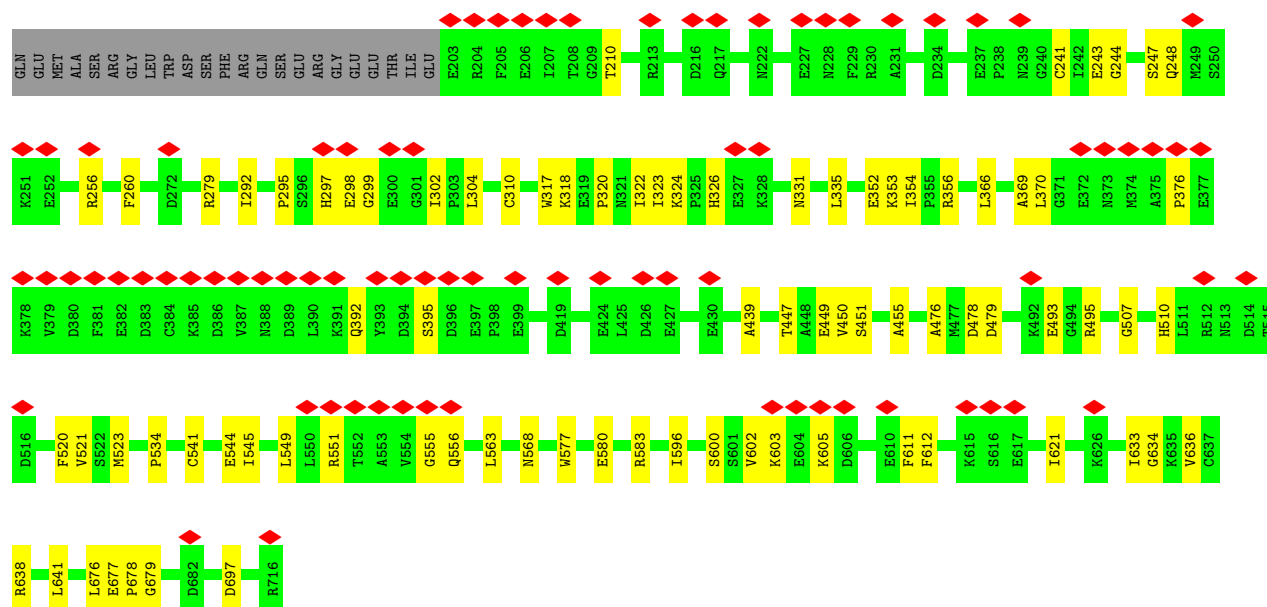
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Polymerase acidic protein

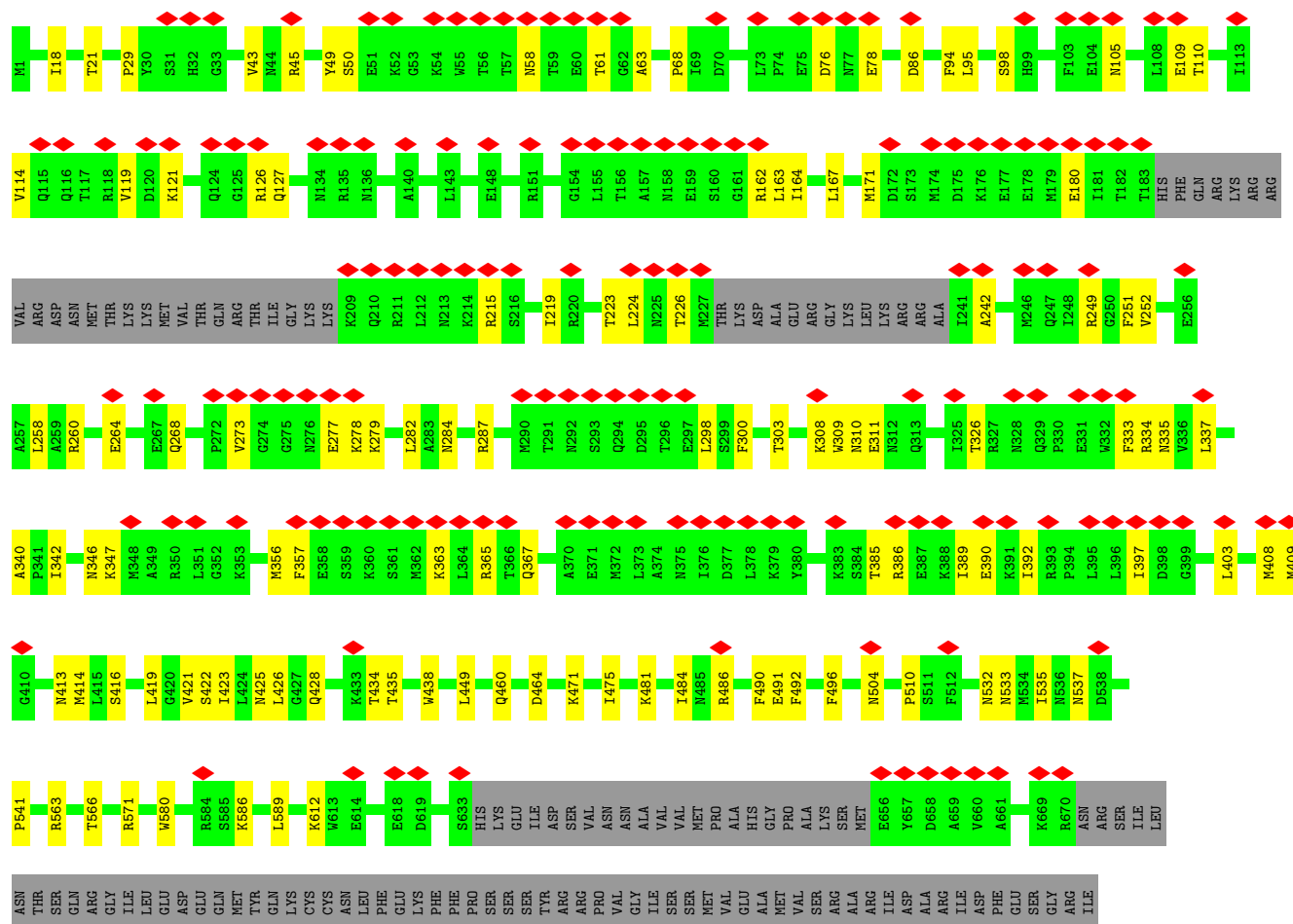


#### • Molecule 1: Polymerase acidic protein

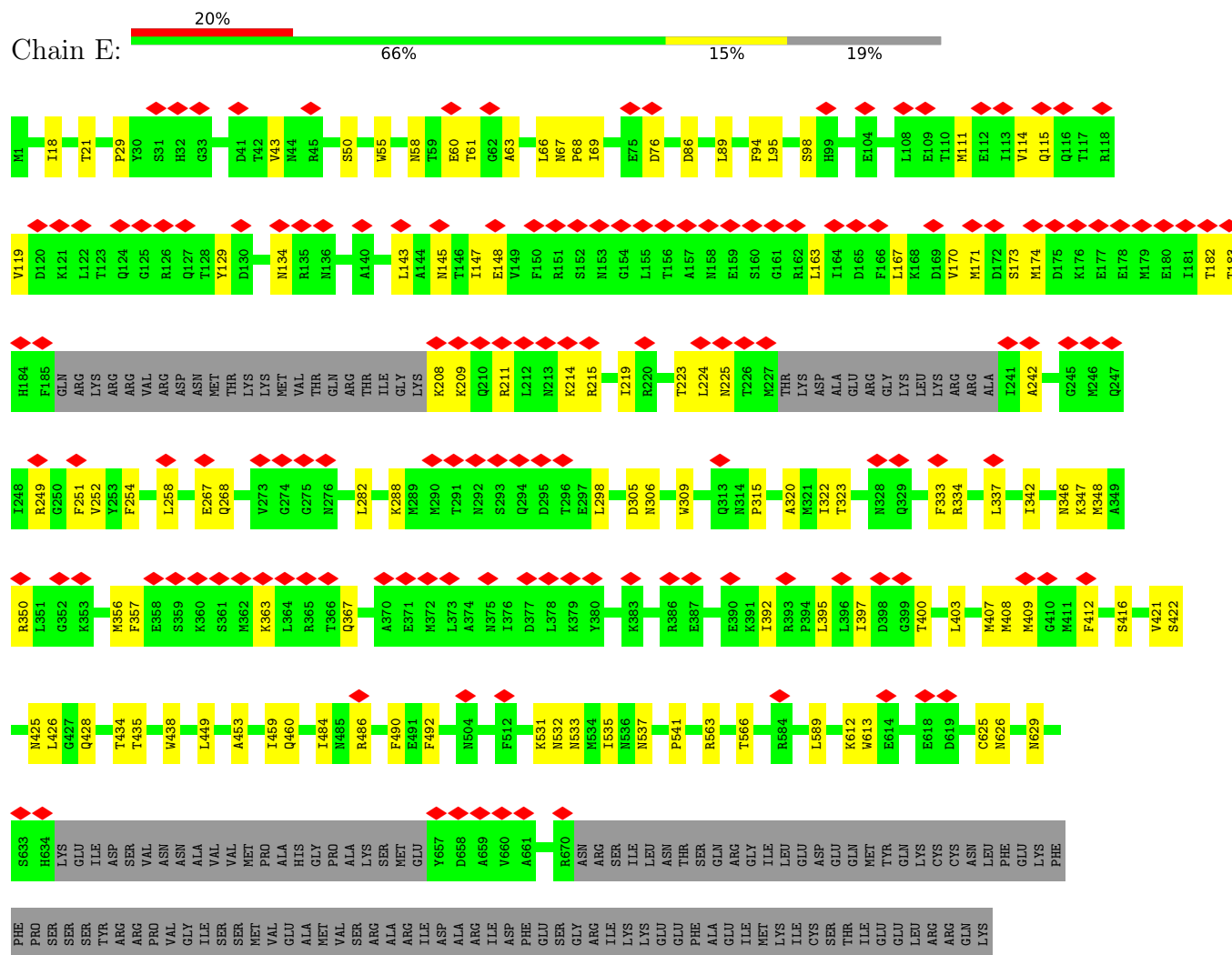




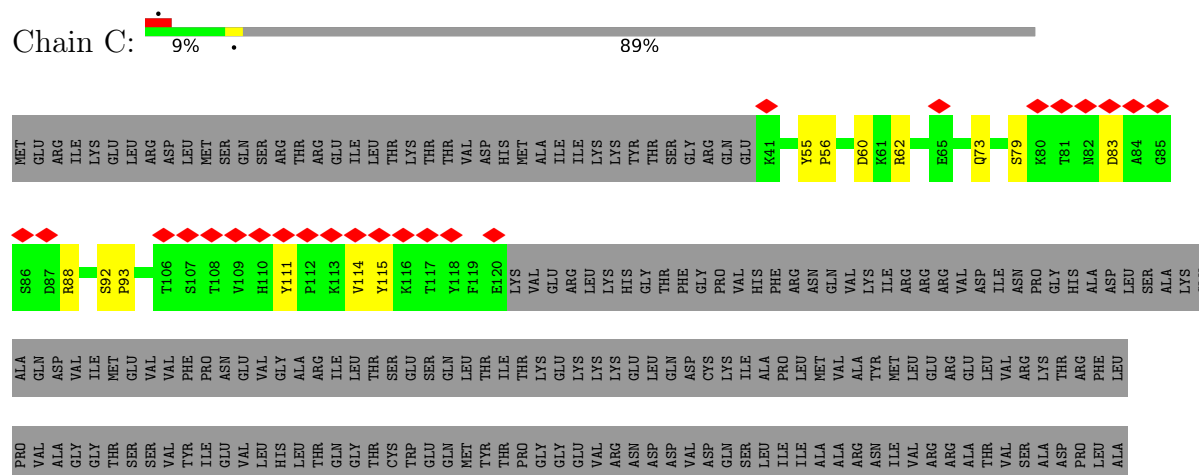
• Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 2: RNA-directed RNA polymerase catalytic subunit



- Molecule 3: Polymerase basic protein 2





ARG	LEU	SER	MET
MET	ILE	LEU	GLU
ALA	GLY	THR	PHE
ILE	LYS	VAL	PRO
ASN	GLU	VAL	PHE
	ASN	ARG	GLN
	LYS	GLY	SER
	ARG	SER	LEU
	TYR	GLY	VAL
	GLY	MET	PRO
	PRO	ARG	LYS
	ALA	ILE	ALA
	LEU	VAL	ALA
	SER	VAL	ARG
	ILE	ARG	GLY
	ASN	GLY	GLN
	GLU	ASN	TYR
	LEU	SER	SER
	SER	PRO	GLY
	ASN	VAL	PHE
	LEU	PHE	VAL
	ALA	ASN	ARG
	LYS	TYR	VAL
	GLY	ASN	LEU
	GLU	LYS	PHE
	LYS	ALA	GLN
	ALA	THR	GLN
	ASN	LYS	MET
	VAL	ARG	ARG
	LEU	LEU	ASP
	ILE	THR	VAL
	GLY	VAL	LEU
	GLN	LEU	GLY
	GLY	GLY	THR
	ASP	LYS	PHE
	VAL	ASP	LYS
	VAL	ALA	THR
	LEU	GLY	VAL
	VAL	ALA	GLN
	MET	LEU	ILE
	LYS	MET	ILE
	ARG	GLU	LYS
	LYS	ASP	LEU
	ARG	PRO	LEU
	ASP	ASP	PRO
	SER	GLY	PHE
	SER	GLY	ALA
	ILE	THR	ALA
	LEU	GLY	ALA
	THR	GLY	PRO
	ASP	VAL	PRO
	SER	GLU	GLU
	GLN	SER	GLN
	THR	ALA	SER
	ALA	VAL	ARG
	THR	LEU	MET
	LYS	ARG	GLN
	ARG	GLY	PHE
	ILE	THR	SER



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	101870	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.637	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	365.684, 365.684, 365.684	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8311, 0.8311, 0.8311	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/4231	0.47	0/5712
1	D	0.25	0/4222	0.47	0/5700
2	B	0.25	0/4952	0.48	0/6693
2	E	0.25	0/4986	0.48	0/6738
3	C	0.24	0/678	0.50	0/919
3	F	0.24	0/678	0.50	0/919
All	All	0.25	0/19747	0.48	0/26681

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4142	0	4109	48	0
1	D	4133	0	4103	54	0
2	B	4853	0	4815	86	0
2	E	4884	0	4845	81	0
3	C	659	0	655	9	0
3	F	659	0	655	6	0
All	All	19330	0	19182	254	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 7.

The worst 5 of 254 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)
1:A:217:GLN:NE2	2:B:58:ASN:OD1	1.82	1.12
2:E:183:THR:HG1	2:E:208:LYS:N	1.58	1.02
1:D:376:PRO:HB3	2:E:363:LYS:HG3	1.56	0.86
1:A:376:PRO:HB3	2:B:363:LYS:HG3	1.56	0.85
2:E:60:GLU:OE1	2:E:214:LYS:HE2	1.83	0.79

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	A	513/717 (72%)	497 (97%)	16 (3%)	0	100	100
1	D	512/717 (71%)	494 (96%)	16 (3%)	2 (0%)	34	64
2	B	602/757 (80%)	581 (96%)	21 (4%)	0	100	100
2	E	605/757 (80%)	580 (96%)	25 (4%)	0	100	100
3	C	78/759 (10%)	75 (96%)	3 (4%)	0	100	100
3	F	78/759 (10%)	75 (96%)	3 (4%)	0	100	100
All	All	2388/4466 (54%)	2302 (96%)	84 (4%)	2 (0%)	54	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	PRO
1	D	299	GLY

### 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	A	462/645 (72%)	461 (100%)	1 (0%)	93	98
1	D	461/645 (72%)	459 (100%)	2 (0%)	91	97
2	B	536/668 (80%)	536 (100%)	0	100	100
2	E	539/668 (81%)	539 (100%)	0	100	100
3	C	72/666 (11%)	72 (100%)	0	100	100
3	F	72/666 (11%)	72 (100%)	0	100	100
All	All	2142/3958 (54%)	2139 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	SER
1	D	298	GLU
1	D	395	SER

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

Mol	Chain	Res	Type
2	E	425	ASN
2	E	428	GLN
2	E	460	GLN
2	B	425	ASN
2	B	428	GLN

### 5.3.3 RNA ⓘ

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.

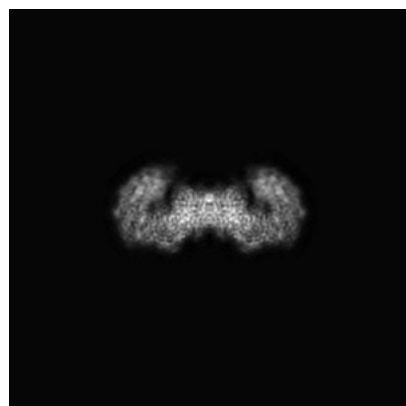
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14858. These allow visual inspection of the internal detail of the map and identification of artifacts.

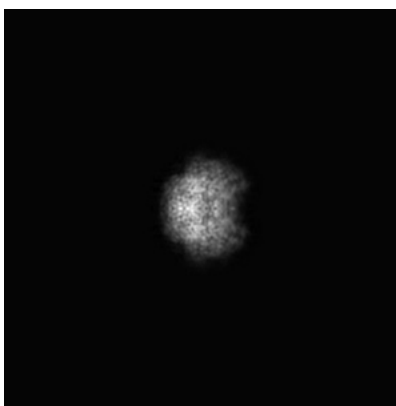
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

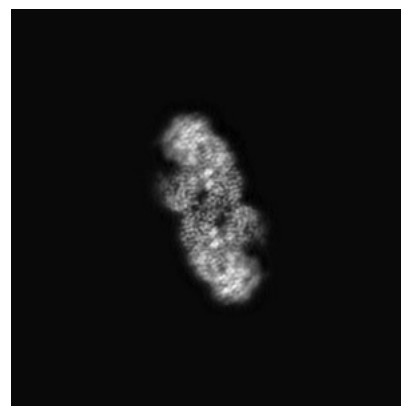
#### 6.1.1 Primary map



X

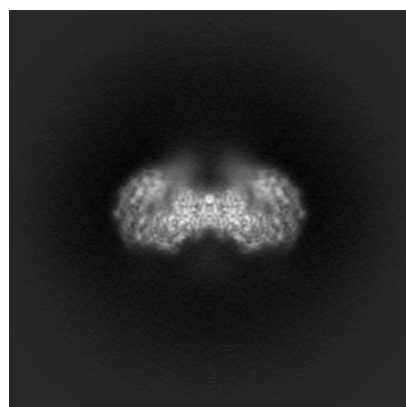


Y

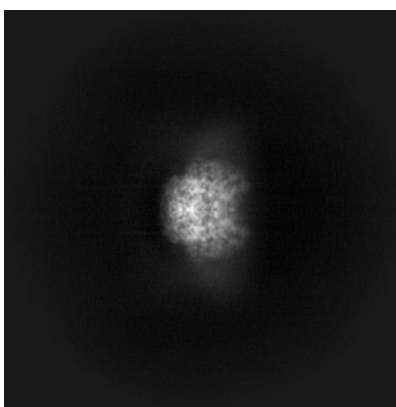


Z

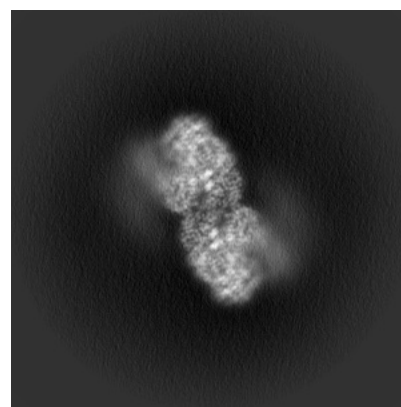
#### 6.1.2 Raw map



X



Y

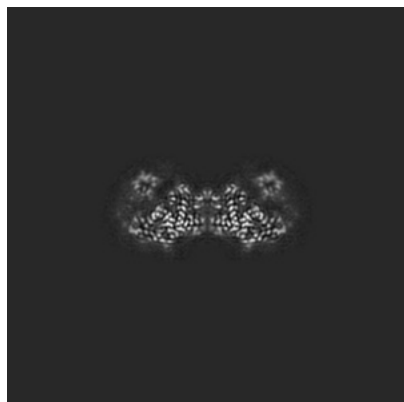


Z

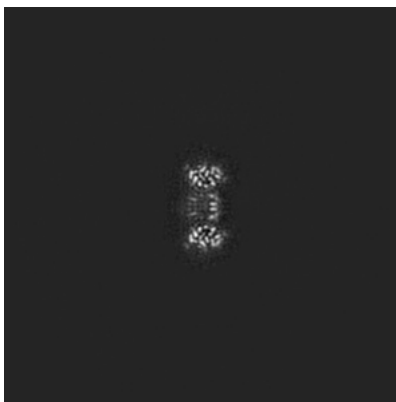
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

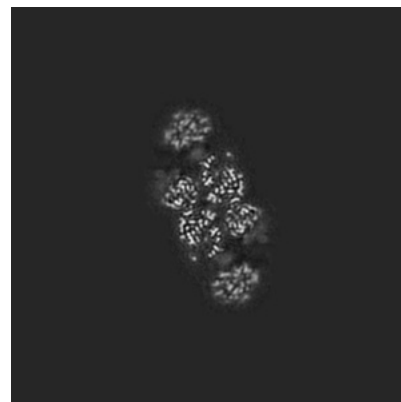
### 6.2.1 Primary map



X Index: 220

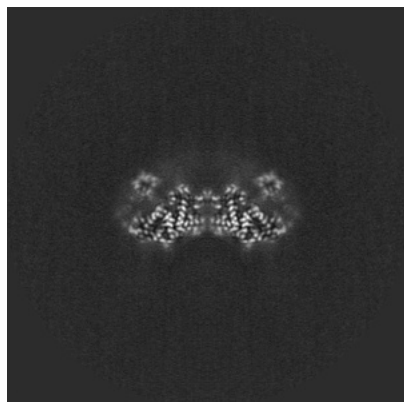


Y Index: 220

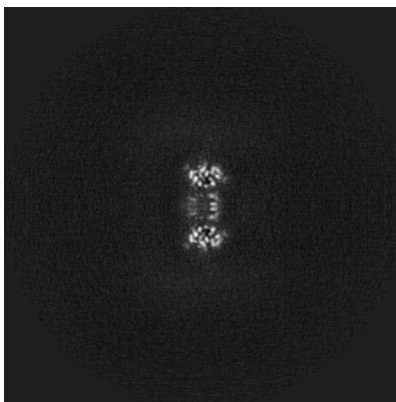


Z Index: 220

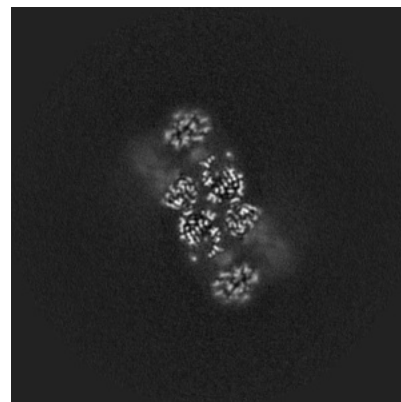
### 6.2.2 Raw map



X Index: 220



Y Index: 220

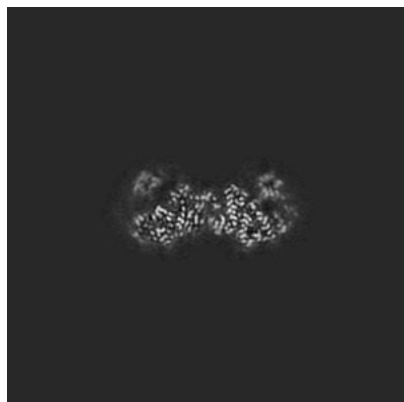


Z Index: 220

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

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

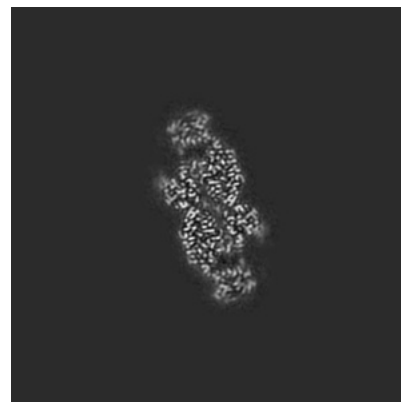
### 6.3.1 Primary map



X Index: 218

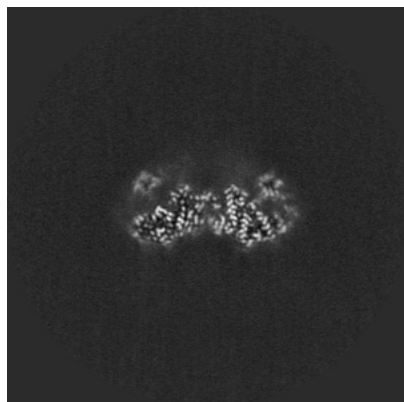


Y Index: 197

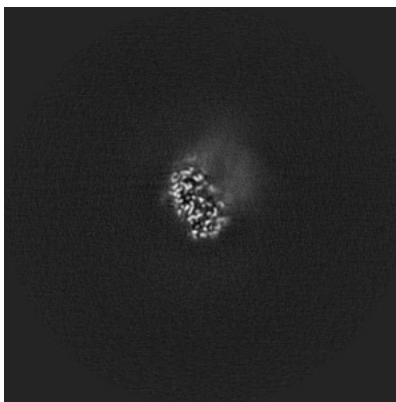


Z Index: 210

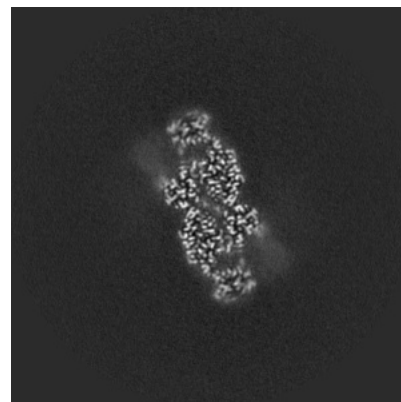
### 6.3.2 Raw map



X Index: 218



Y Index: 188



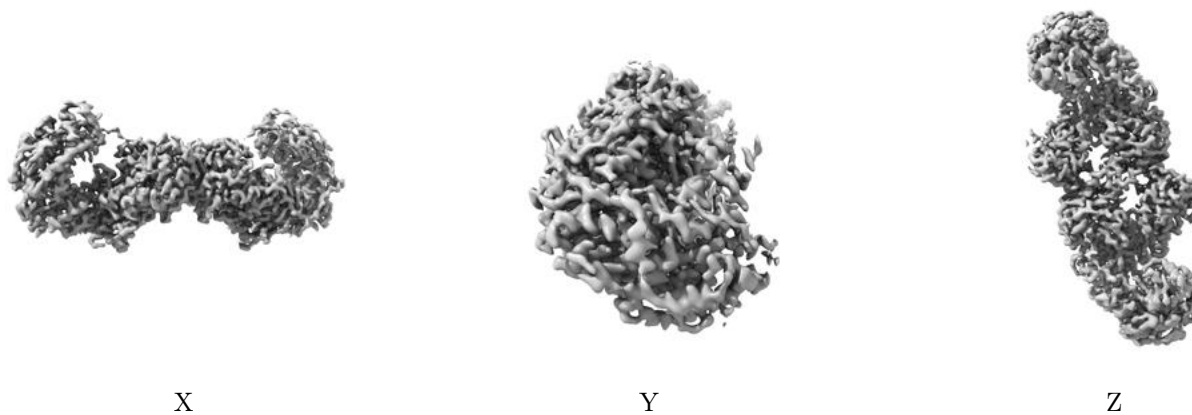
Z Index: 210

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



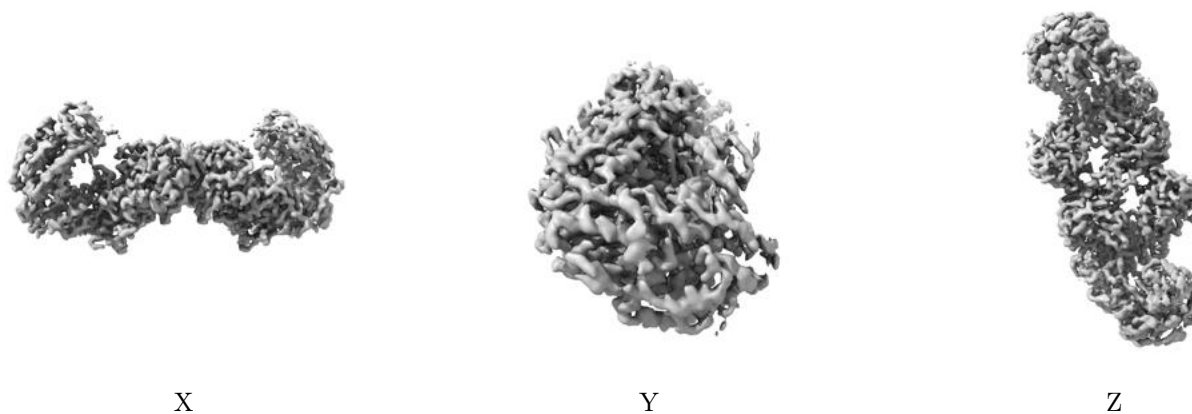
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

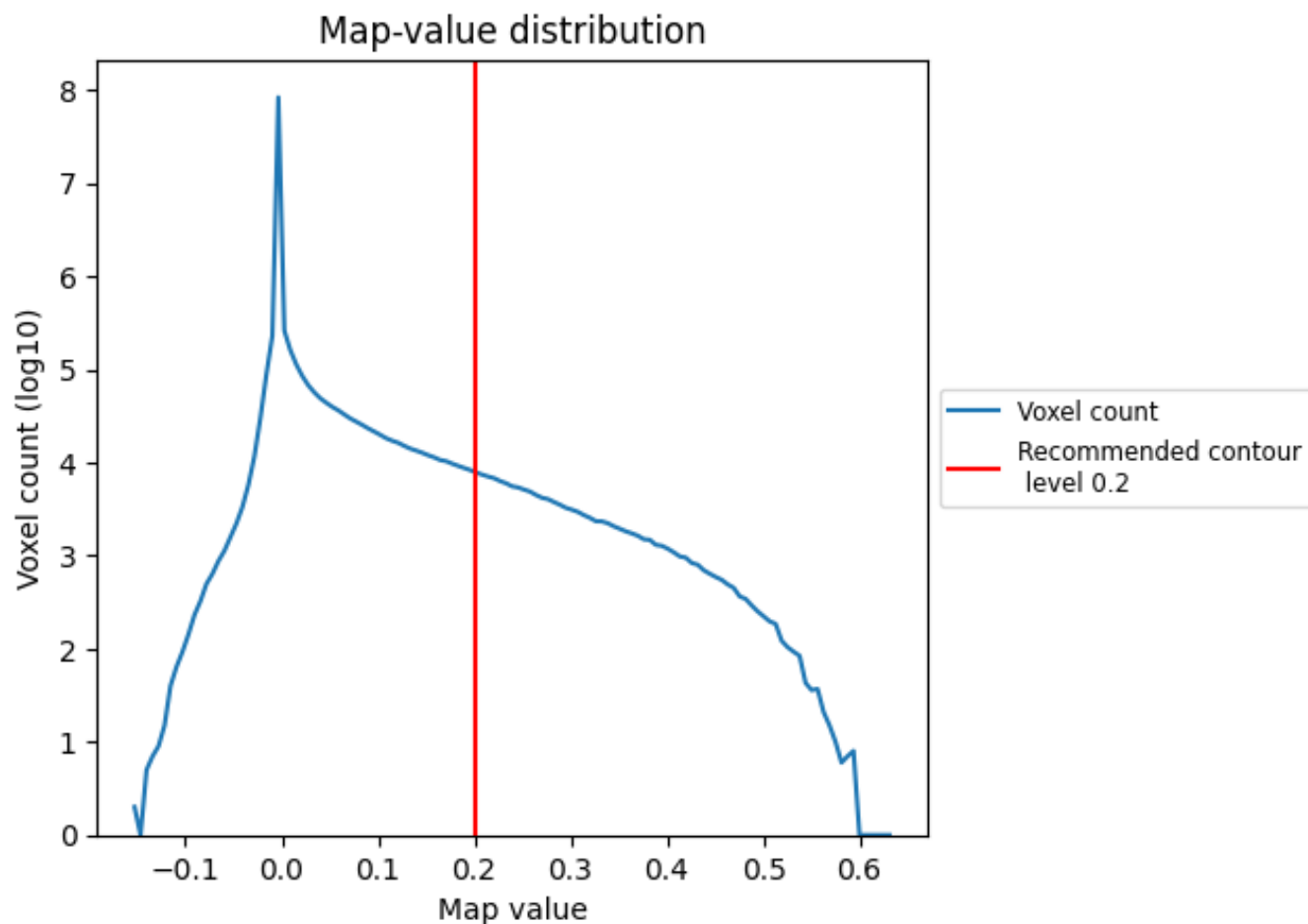
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

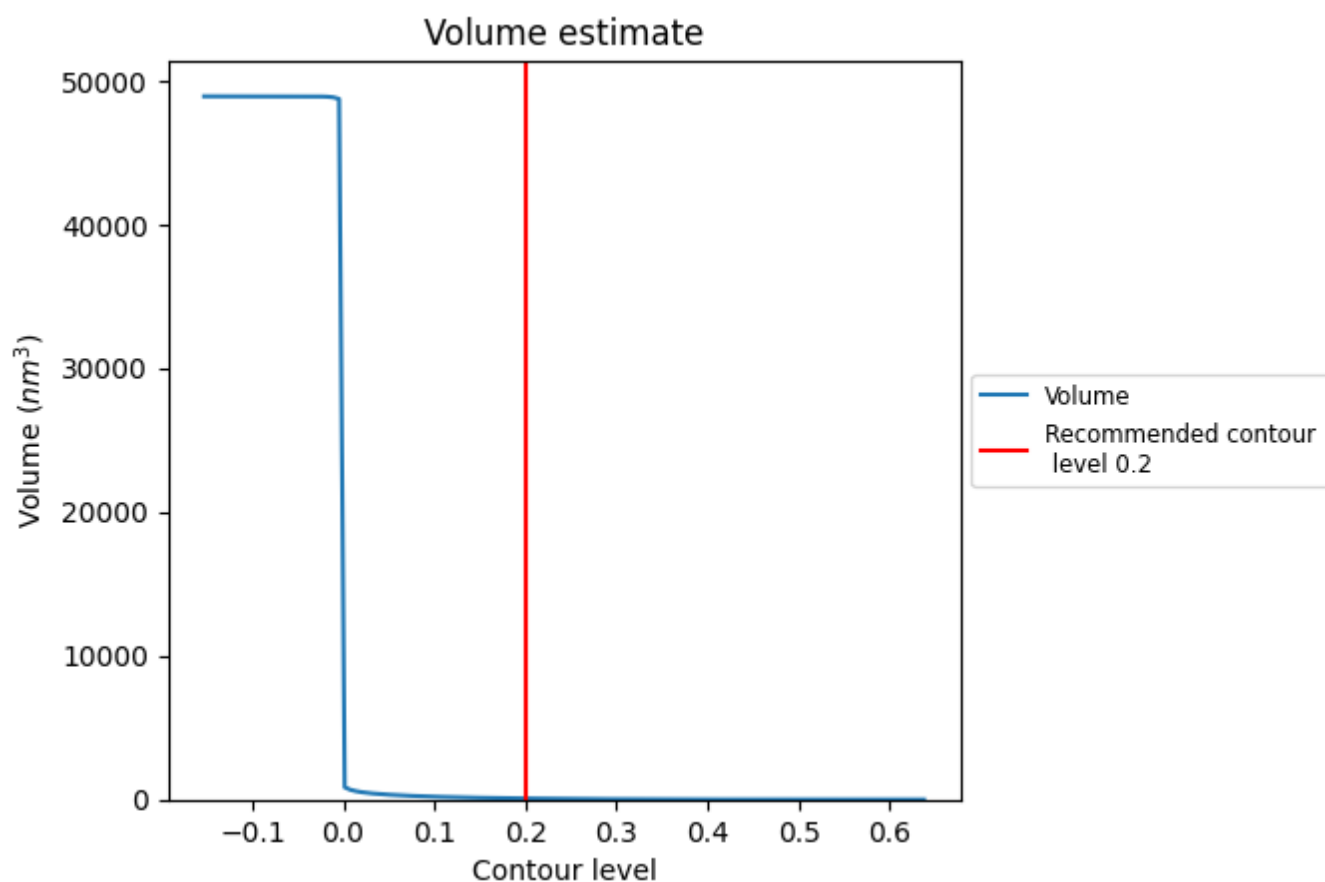
This section contains the results of statistical analysis of the map.

### 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.

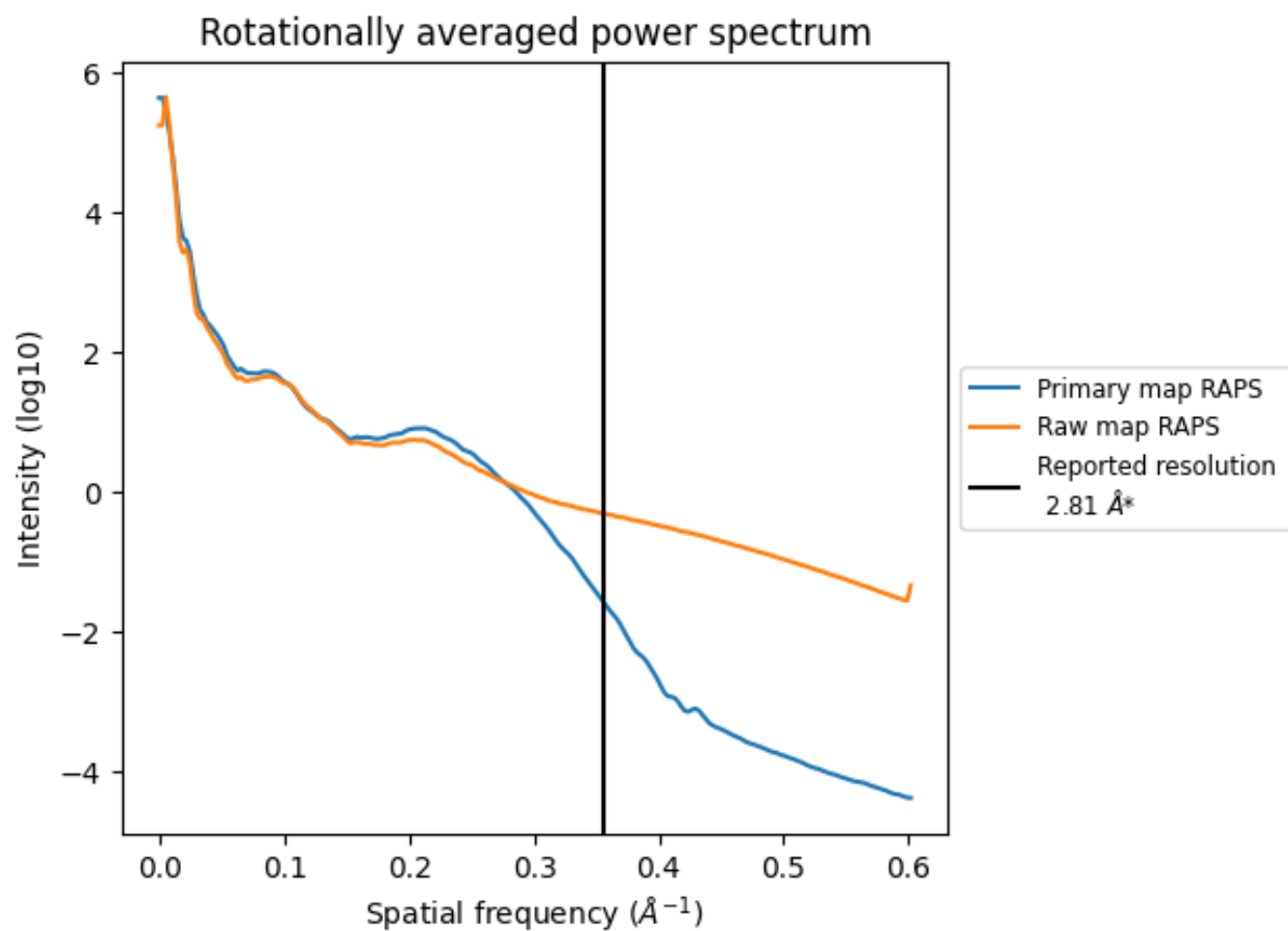
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 76 nm<sup>3</sup>; this corresponds to an approximate mass of 69 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 ⓘ

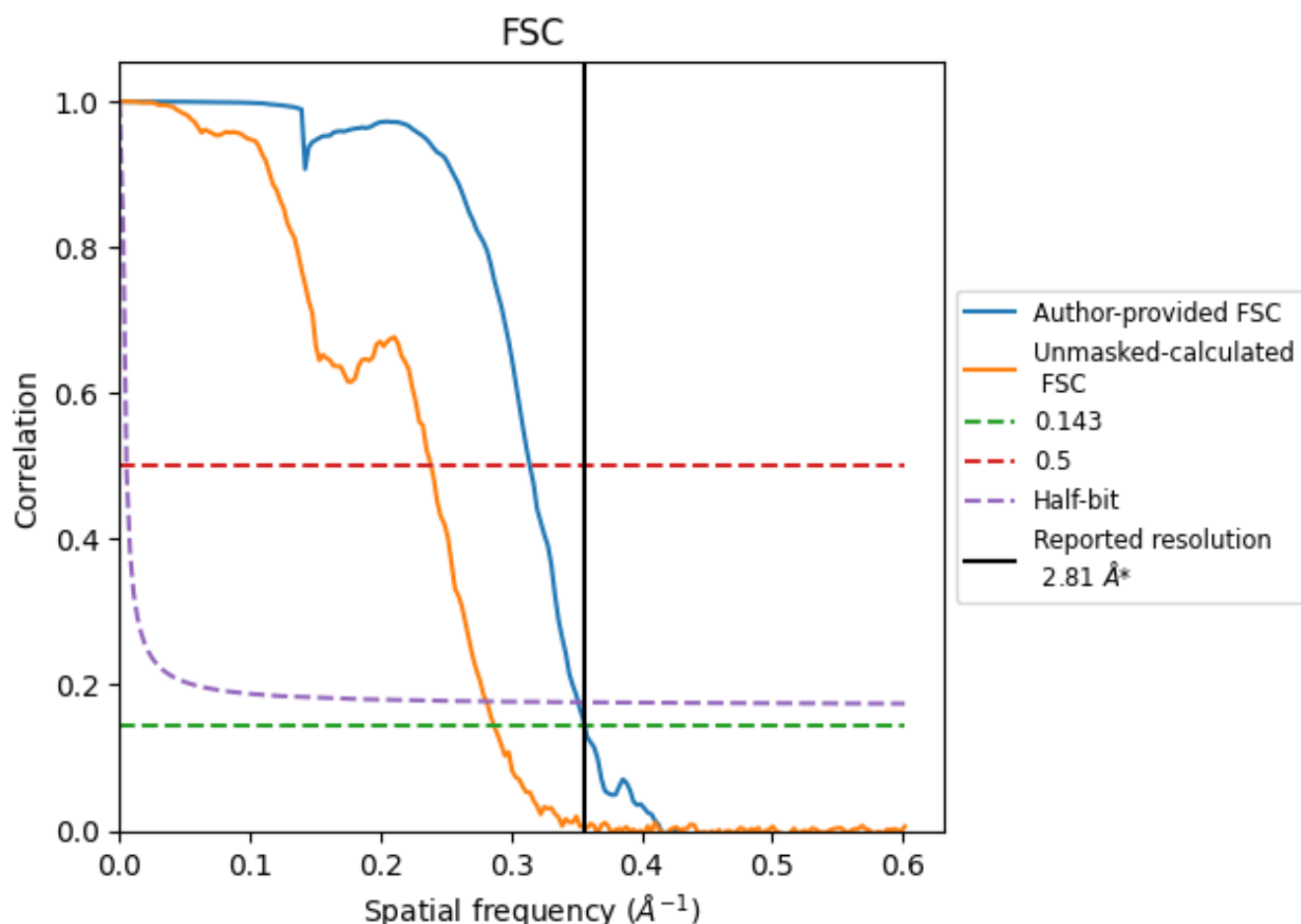


\*Reported resolution corresponds to spatial frequency of  $0.356 \text{ \AA}^{-1}$

## 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 0.356 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

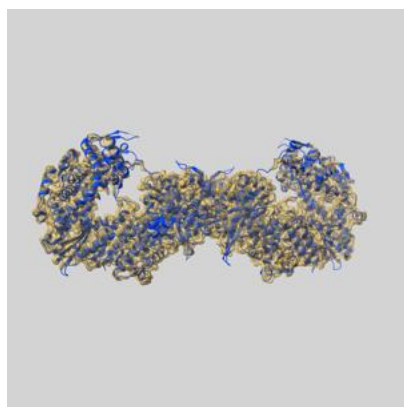
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.18	2.85
Unmasked-calculated*	3.48	4.19	3.56

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.81 by more than 10 %

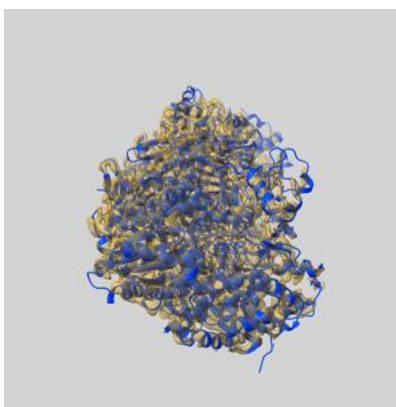
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14858 and PDB model 7ZPM. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

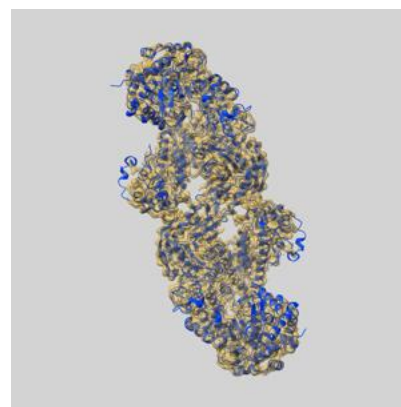
### 9.1 Map-model overlay [i](#)



X



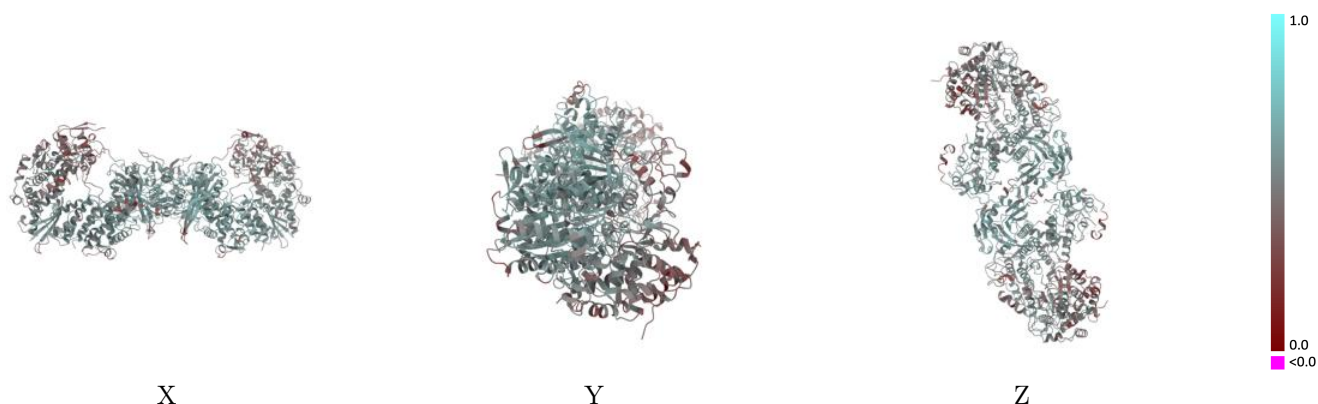
Y



Z

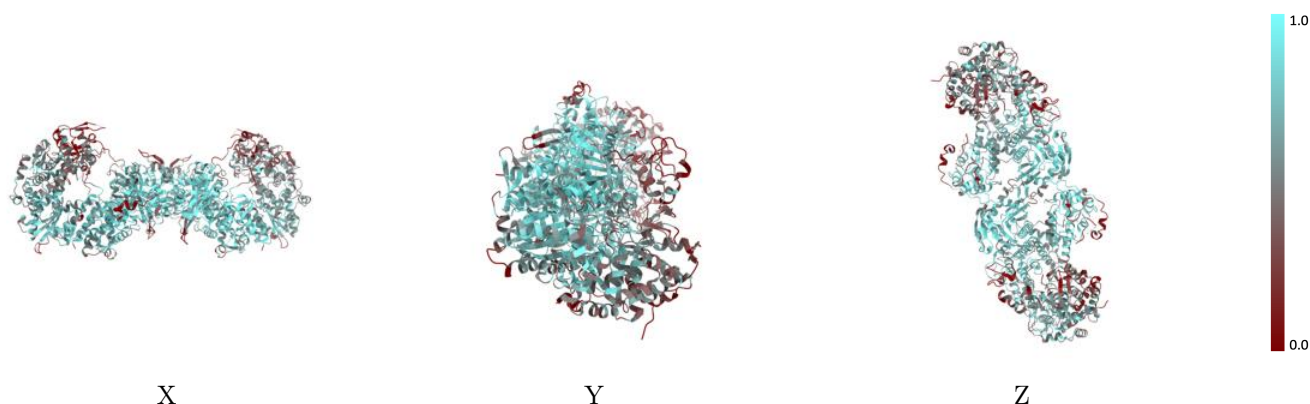
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

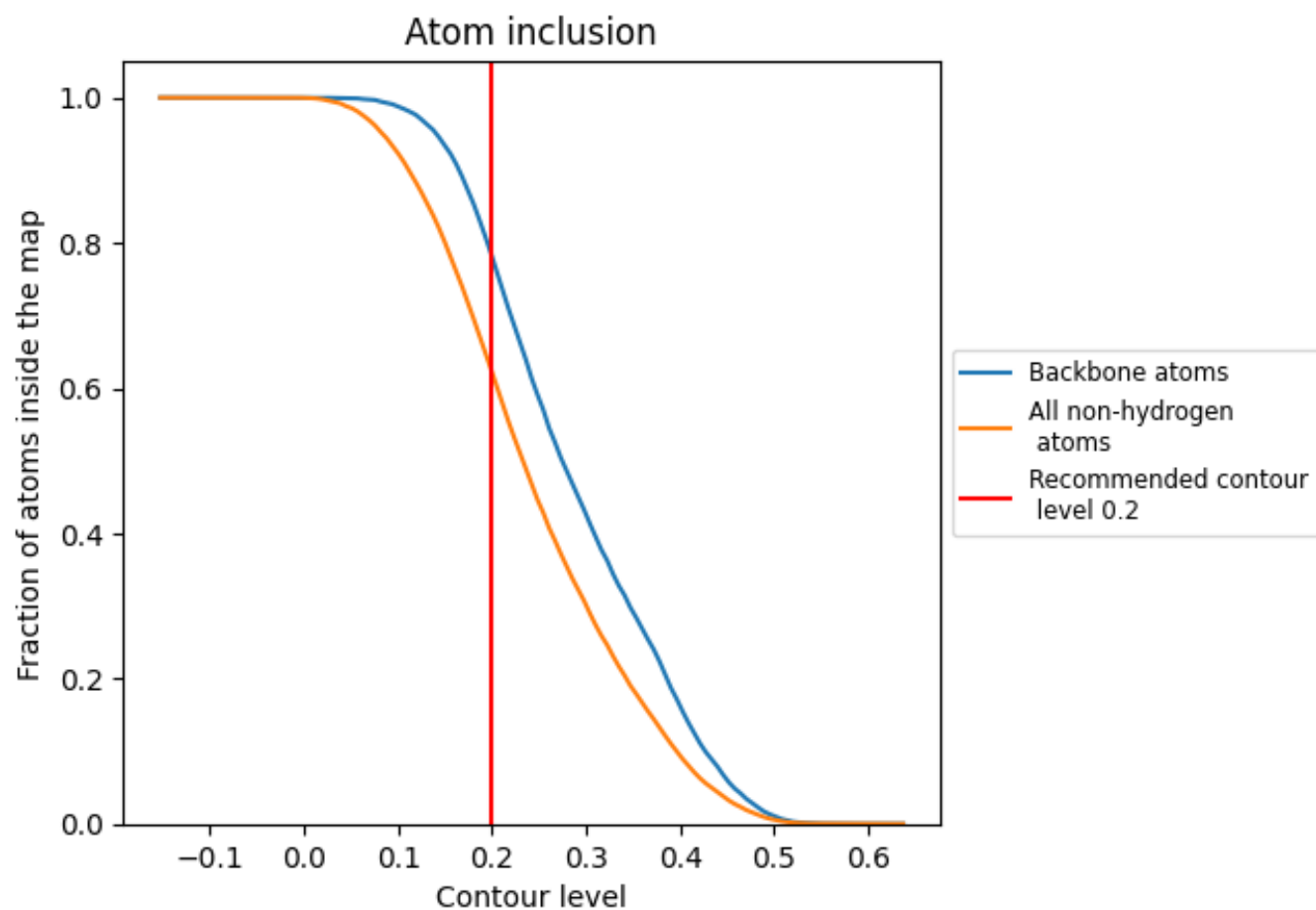
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.2).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.6222	<div><div></div></div> 0.5170
A	<div><div></div></div> 0.6770	<div><div></div></div> 0.5420
B	<div><div></div></div> 0.5697	<div><div></div></div> 0.4970
C	<div><div></div></div> 0.5491	<div><div></div></div> 0.4910
D	<div><div></div></div> 0.6908	<div><div></div></div> 0.5430
E	<div><div></div></div> 0.5900	<div><div></div></div> 0.4980
F	<div><div></div></div> 0.5429	<div><div></div></div> 0.4970

1.0

0.0

<0.0