

# Full wwPDB EM Validation Report (i)

Apr 18, 2024 – 04:04 pm BST

PDB ID : 8PTN

EMDB ID : EMD-17875

Title : Structure of the transcription termination factor Rho in complex with Rof

Authors: Said, N.; Hilal, T.; Wahl, M.C.

Deposited on : 2023-07-14

Resolution : 3.30 Å(reported)

Based on initial model : .

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

We welcome your comments at *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 (i) 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 (1)) 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)

 $MapQ \quad : \quad 1.9.13$ 

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

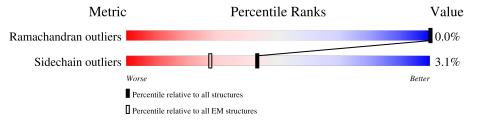
Validation Pipeline (wwPDB-VP) : 2.36

## 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 3.30 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 $(\# \mathrm{Entries})$	${ m EM~structures} \ (\#{ m Entries})$	
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 >=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 <=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	419	97%	·
1	В	419	97%	•
1	С	419	98%	•
1	D	419	96%	•
1	Е	419	97%	
1	F	419	96%	
2	a	86	92%	• 5%
2	b	86	91%	• • 5%
2	С	86	93%	• 5%



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Mol	Chain	Length	Quality of chain				
2	d	86	95%	5%			
2	e	86	7% 93%	•• 5%			



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22976 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	418	Total	С	N	О	S	0	0
1	Λ	410	3291	2071	585	618	17	0	
1	В	418	Total	С	N	О	S	0	0
1	Б	410	3291	2071	585	618	17	0	0
1	С	418	Total	С	N	О	S	0	0
1		410	3291	2071	585	618	17	U	0
1	D	418	Total	С	N	О	S	0	0
1	ט	410	3291	2071	585	618	17	0	0
1	Е	418	Total	С	N	О	S	0	0
1	E	410	3291	2071	585	618	17	U	0
1	F	418	Total	С	N	О	S	0	0
1	Г	410	3291	2071	585	618	17	U	U

• Molecule 2 is a protein called Protein rof.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	0	82	Total	С	N	О	S	0	0
	a	02	646	401	108	134	3	0	0
2	b	82	Total	С	N	О	S	0	0
	D	02	646	401	108	134	3	0	U
2		82	Total	С	N	О	S	0	0
	c	02	646	401	108	134	3	0	U
2	d	82	Total	С	N	О	S	0	0
	u	02	646	401	108	134	3	0	0
2		82	Total	С	N	О	S	0	0
	е	02	646	401	108	134	3		U

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	ALA	-	expression tag	UNP P0AFW8
a	0	MET	-	1	UNP P0AFW8
a	1	GLY	-	expression tag	UNP P0AFW8
b	-1	ALA	-	expression tag	UNP P0AFW8



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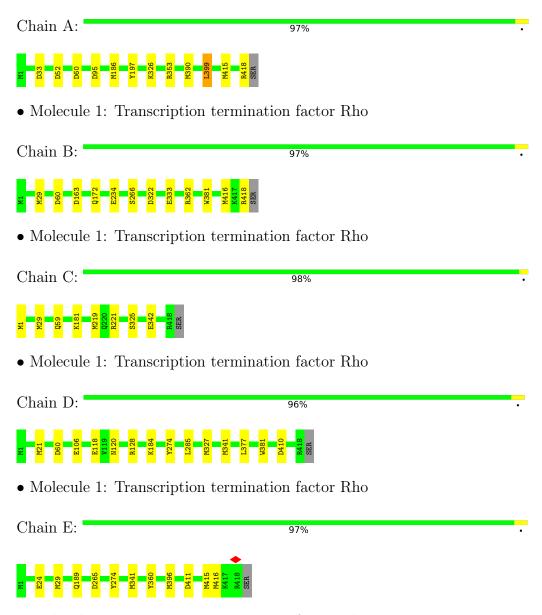
Chain	Residue	Modelled	Actual	Comment	Reference
b	0	MET	-	expression tag	UNP P0AFW8
b	1	GLY	-	expression tag	UNP P0AFW8
c	-1	ALA	-	expression tag	UNP P0AFW8
С	0	MET	-	expression tag	UNP P0AFW8
c	1	GLY	-	expression tag	UNP P0AFW8
d	-1	ALA	-	expression tag	UNP P0AFW8
d	0	MET	-	expression tag	UNP P0AFW8
d	1	GLY	-	expression tag	UNP P0AFW8
е	-1	ALA	-	expression tag	UNP P0AFW8
е	0	MET	-	expression tag	UNP P0AFW8
е	1	GLY	-	expression tag	UNP P0AFW8



## 3 Residue-property plots (i)

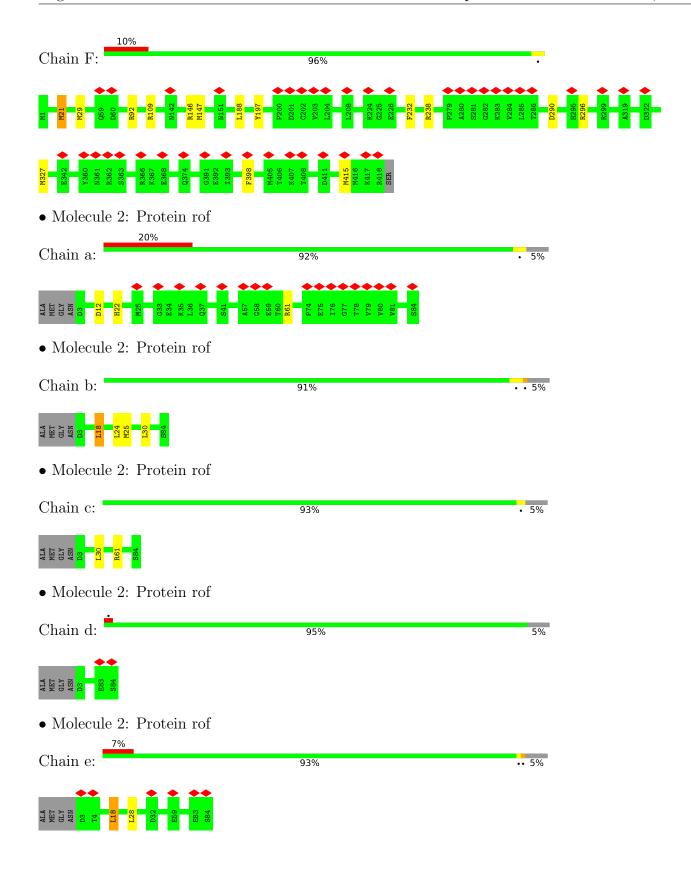
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Transcription termination factor Rho



• Molecule 1: Transcription termination factor Rho







# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.822	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.104	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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).

Mal	Mol Chain		lengths	Во	ond angles
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5
1	A	0.26	0/3340	0.57	$1/4497 \ (0.0\%)$
1	В	0.28	0/3340	0.54	1/4497 (0.0%)
1	С	0.27	0/3340	0.51	0/4497
1	D	0.27	0/3340	0.53	1/4497 (0.0%)
1	Е	0.26	0/3340	0.54	0/4497
1	F	0.25	0/3340	0.58	$2/4497 \ (0.0\%)$
2	a	0.24	0/654	0.51	0/885
2	b	0.25	0/654	0.60	1/885 (0.1%)
2	С	0.25	0/654	0.57	1/885 (0.1%)
2	d	0.25	0/654	0.52	0/885
2	е	0.27	0/654	0.55	1/885 (0.1%)
All	All	0.26	0/23310	0.55	8/31407 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	322	ASP	CB-CG-OD1	7.70	125.23	118.30
2	е	18	LEU	CA-CB-CG	6.59	130.46	115.30
2	b	18	LEU	CA-CB-CG	6.29	129.78	115.30
2	c	30	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	399	LEU	CA-CB-CG	6.13	129.40	115.30
1	F	21	MET	CA-CB-CG	5.41	122.50	113.30
1	D	377	LEU	CA-CB-CG	5.28	127.45	115.30
1	F	188	LEU	CA-CB-CG	5.02	126.85	115.30

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	Perce	ntiles
1	A	$416/419 \ (99\%)$	411 (99%)	5 (1%)	0	100	100
1	В	416/419 (99%)	410 (99%)	5 (1%)	1 (0%)	47	77
1	С	416/419 (99%)	406 (98%)	10 (2%)	0	100	100
1	D	416/419 (99%)	406 (98%)	10 (2%)	0	100	100
1	E	416/419 (99%)	411 (99%)	5 (1%)	0	100	100
1	F	416/419 (99%)	411 (99%)	5 (1%)	0	100	100
2	a	80/86 (93%)	78 (98%)	2 (2%)	0	100	100
2	b	80/86 (93%)	78 (98%)	2 (2%)	0	100	100
2	c	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
2	d	80/86 (93%)	79 (99%)	1 (1%)	0	100	100
2	e	80/86 (93%)	78 (98%)	2 (2%)	0	100	100
All	All	2896/2944 (98%)	2845 (98%)	50 (2%)	1 (0%)	100	100

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	266	SER

#### 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.

$\mathbf{M}$	ol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	=	A	358/359 (100%)	346 (97%)	12 (3%)	37 65	



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	В	$358/359 \ (100\%)$	348 (97%)	10 (3%)	43	70
1	С	358/359 (100%)	350 (98%)	8 (2%)	52	74
1	D	358/359 (100%)	345 (96%)	13 (4%)	35	63
1	E	358/359 (100%)	347 (97%)	11 (3%)	40	67
1	F	358/359 (100%)	344 (96%)	14 (4%)	32	62
2	a	74/76 (97%)	71 (96%)	3 (4%)	30	61
2	b	74/76 (97%)	70 (95%)	4 (5%)	22	53
2	c	74/76 (97%)	73 (99%)	1 (1%)	67	82
2	d	74/76 (97%)	74 (100%)	0	100	100
2	e	74/76 (97%)	72 (97%)	2 (3%)	44	71
All	All	2518/2534 (99%)	2440 (97%)	78 (3%)	43	67

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	52	ASP
1	A	60	ASP
1	A	95	ASP
1	A	186	MET
1	A	197	TYR
1	A	326	LYS
1	A	353	ARG
1	A	390	MET
1	A	399	LEU
1	A	415	MET
1	A	418	ARG
1	В	29	MET
1	В	60	ASP
1	В	163	ASP
1	В	172	GLN
1	В	234	GLU
1	В	333	GLU
1	В	362	ARG
1	В	381	TRP
1	В	416	MET
1	В	418	ARG
1	С	1	MET



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Mol	$\sim$ 1 .		
	Chain	Res	Type
1	С	29	MET
1	С	59	GLN
1	С	181	LYS
1	С	219	MET
1	С	221	ARG
1	C C C C C D	325	SER
1	С	342	GLU
1	D	21	MET
1	D	60	ASP
1	D	106	GLU
1	D	118	GLU
1	D	120	ASN
1	D	128	ARG
1	D	184	LYS
1	D	274	TYR
1	D	285	LEU
1	D	327	MET
1	D	341	MET
1	D	381	TRP
1	D	410	ASP
1	Ε	24	GLU
1	Е	29	MET
1	Е	189	GLN
1	Ε	265	ASP
1	Ε	274	TYR
1	Ε	341	MET
1	Е	360	TYR
1	Ε	396	MET
1	Ε	411	ASP
1	Ε	415	MET
1	Ε	416	MET
1	F	21	MET
1	F	29	MET
1	F	92	ARG
1	F	109	ARG
1	F	146	ARG
1	F	147	ARG MET
1	F	197	TYR
1	F	232	PHE
1	F	238	ARG
1	F	290	ASP
1	F	296	ARG



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	J	1	1 3
Mol	Chain	Res	Type
1	F	327	MET
1	F	398	PHE
1	F	415	MET
2	a	12	ASP
2	a	22	HIS
2	a	61	ARG
2	b	18	LEU
2	b	24	LEU
2	b	25	MET
2	b	30	LEU
2	c	61	ARG
2	е	18	LEU
2	е	28	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	С	25	ASN
1	С	306	ASN
1	D	190	ASN
1	D	378	GLN
1	Ε	340	ASN
1	F	374	GLN
2	е	22	HIS

#### 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.



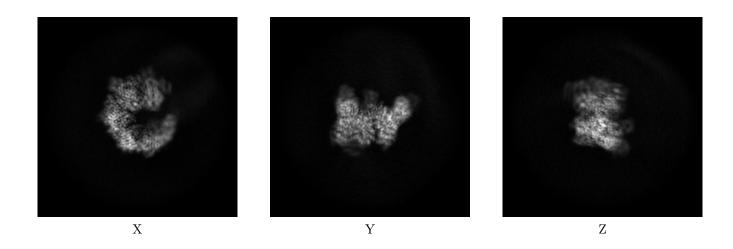
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17875. These allow visual inspection of the internal detail of the map and identification of artifacts.

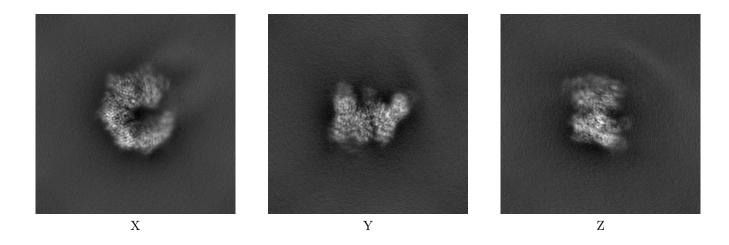
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



#### 6.1.2 Raw map

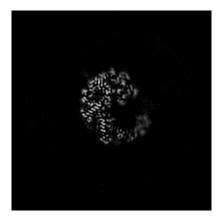


The images above show the map projected in three orthogonal directions.



### 6.2 Central slices (i)

#### 6.2.1 Primary map





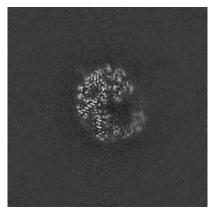


Y Index: 192

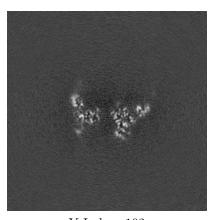


Z Index: 192

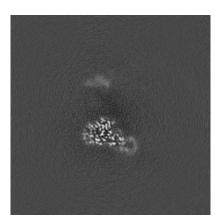
#### 6.2.2 Raw map



X Index: 192



Y Index: 192



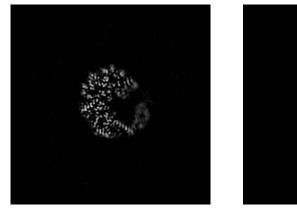
Z Index: 192

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

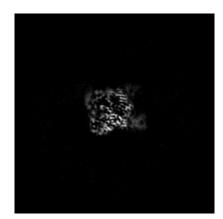


### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map





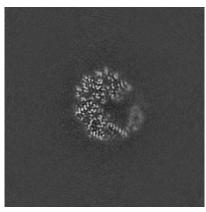


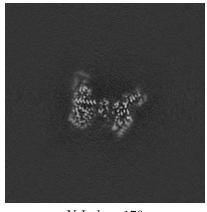
X Index: 188

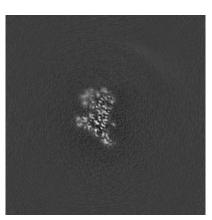
Y Index: 176

Z Index: 136

#### 6.3.2 Raw map







X Index: 188

Y Index: 176

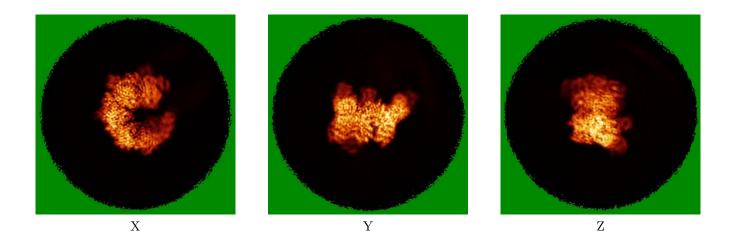
Z Index: 229

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

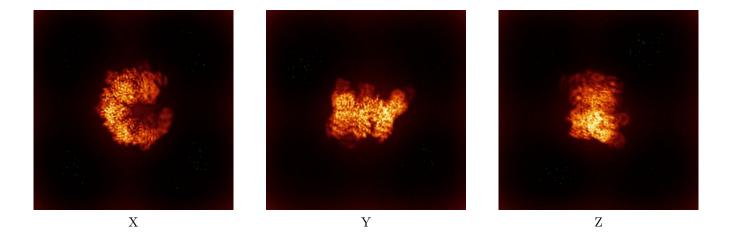


### 6.4 Orthogonal standard-deviation projections (False-color) (i)

#### 6.4.1 Primary map



#### 6.4.2 Raw map

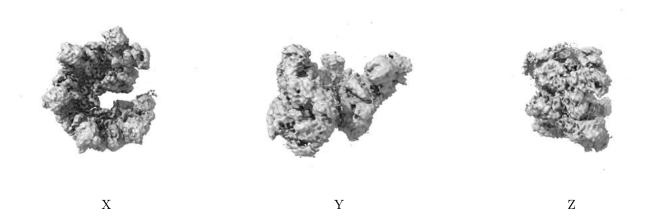


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



### 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 0.104. 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)

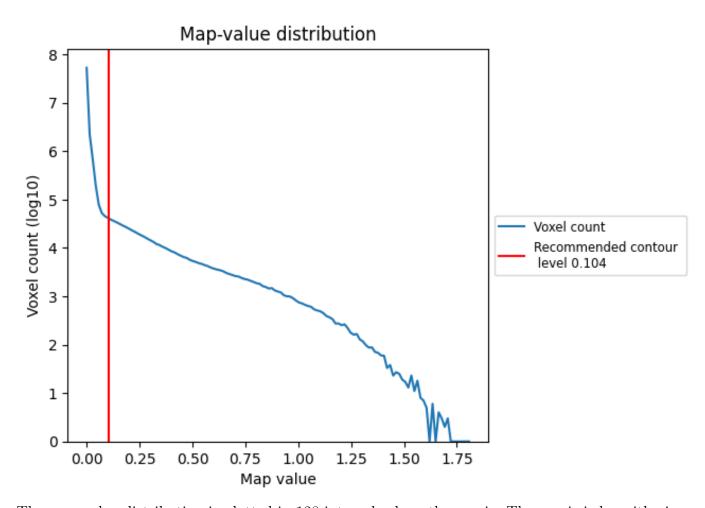
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

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

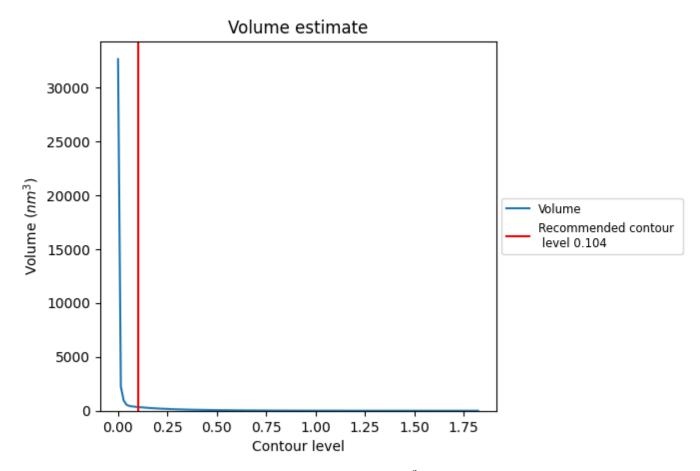
### 7.1 Map-value distribution (i)



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)

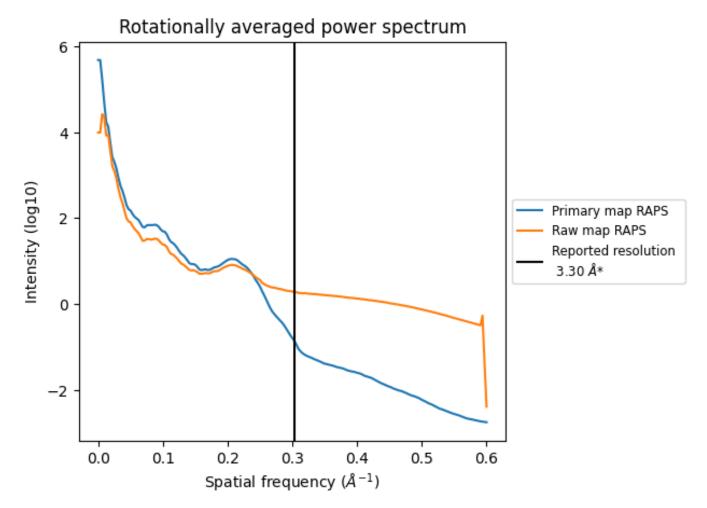


The volume at the recommended contour level is  $342~\mathrm{nm}^3$ ; this corresponds to an approximate mass of  $309~\mathrm{kDa}$ .

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)



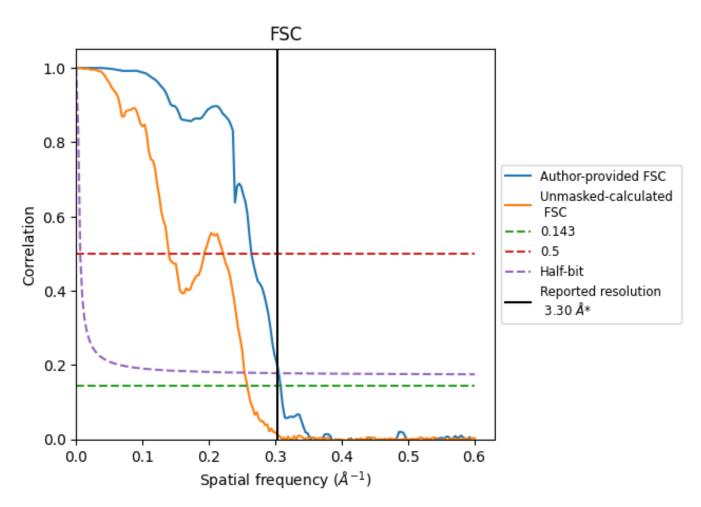
<sup>\*</sup>Reported resolution corresponds to spatial frequency of 0.303  $\rm \mathring{A}^{-1}$ 



## 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 0.303  $\rm \mathring{A}^{-1}$ 



### 8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
rtesolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.79	3.27
Unmasked-calculated*	3.88	7.15	3.94

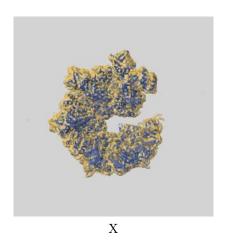
<sup>\*</sup>Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.3 by more than 10 %

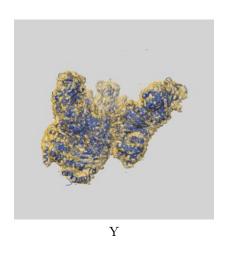


## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17875 and PDB model 8PTN. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay (i)



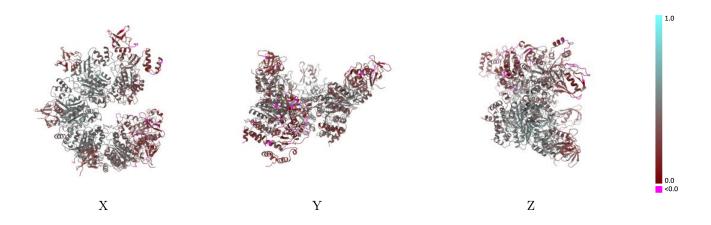




The images above show the 3D surface view of the map at the recommended contour level 0.104 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

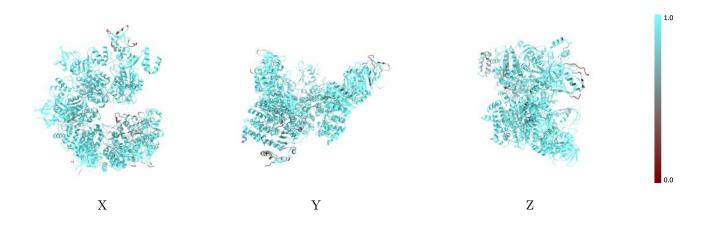


### 9.2 Q-score mapped to coordinate model (i)



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.

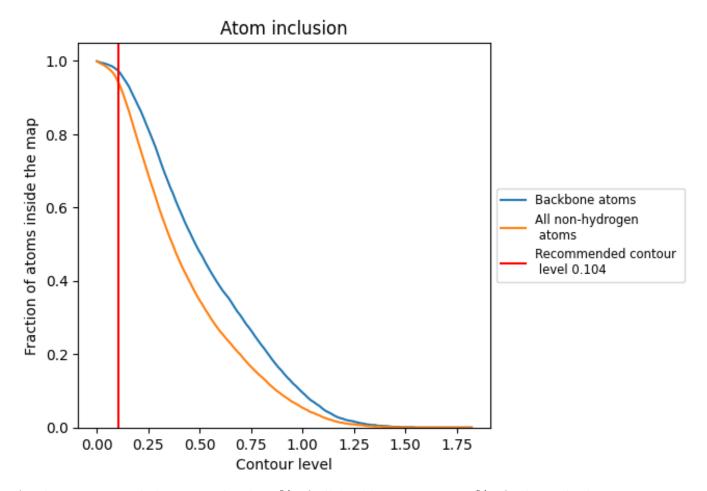
### 9.3 Atom inclusion mapped to coordinate model (i)



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 (0.104).



### 9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



### 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.104) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.3750
A	0.9780	0.3520
В	0.9900	0.4640
С	0.9910	0.4870
D	0.9810	0.4620
E	0.9500	0.3840
F	0.8170	0.2040
a	0.7080	0.1920
b	0.9860	0.3220
c	0.9730	0.3250
d	0.9360	0.2870
e	0.8450	0.2180



