

Apr 18, 2024 – 03:23 pm BST

PDB ID : 8PTP EMDB ID : EMD-17877 Title : Structure of Rho pentamer in complex with Rof Said, N.; Hilal, T.; Wahl, M.C. Authors : Deposited on 2023-07-14 : 3.00 Å(reported) Resolution : 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. dev 92
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)	:	2.36

1 Overall quality at a glance (i)

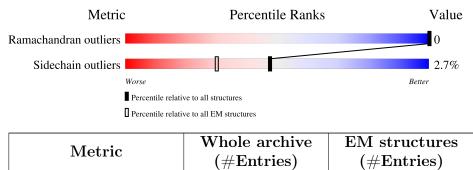
The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.00 Å.

Ramachandran outliers

Sidechain outliers

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.



154571

154315

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.

4023

3826

Mol	Chain	Length	Quality of chain	
1	А	419	97%	·
1	В	419	99%	•
1	С	419	98%	•
1	D	419	99%	·
1	Е	419	5% 96%	.
2	a	86	20%	5% 5%
2	b	86	94%	• 5%
2	с	86	91%	5% 5%
2	d	86	92%	• 5%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19039 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Λ	418	Total	С	Ν	0	S	0	0
	A	410	3291	2071	585	618	17	0	0
1	В	410	Total	С	Ν	0	S	0	0
	D	418	3291	2071	585	618	17	0	0
1	C	410	Total	С	Ν	0	S	0	0
	C	418	3291	2071	585	618	17	0	0
1	D	418	Total	С	Ν	0	S	0	0
	D	410	3291	2071	585	618	17	0	0
1	E	418	Total	С	Ν	0	S	0	0
	Ľ	410	3291	2071	585	618	17	U	0

• Molecule 1 is a protein called Transcription termination factor Rho.

• Molecule 2 is a protein called Protein rof.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	- 00	82	Total	С	Ν	0	S	0	0
	a	02	646	401	108	134	3	0	0
2	h	82	Total	С	Ν	0	S	0	0
	b	02	646	401	108	134	3	0	U
2	0	00	Total	С	Ν	0	S	0	0
	с	82	646	401	108	134	3	0	0
2	d	80	Total	С	Ν	0	S	0	0
	2 a	82	646	401	108	134	3	U	U

There are 12 discrepancies between the modelled and reference sequences:

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

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

Continued from previous page...



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





K417 R418 SER		
• Molecule 2: Protein rof		
Chain a:	91%	5% 5%
ALA MET CLV ASU ASU ASU ASE B32 B32 B32 B32 B32 B32 C33 C33 C33 C33 C33 C33 C33 C33 C33 C	K39 A57 A57 G58 B61 F71 E83 E83 S84	
• Molecule 2: Protein rof		
Chain b:	94%	• 5%
ALA MET GLY D3 D3 C2 S84		
• Molecule 2: Protein rof		
Chain c:	91%	5% 5%
ALA MET GLV GLV ASN ASN 844 846 846 846 846 846 846 846 846		
• Molecule 2: Protein rof		
Chain d:	92%	• 5%
AL A MET GLY ASN D3 M25 K3 K3 K3 K3 K3 S84		



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285647	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)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.849	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.0982	Depositor
Map size (Å)	319.488, 319.488, 319.488	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles $(^{\circ})$	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).

Mol	Chain	Bond	lengths	Bond angles		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/3340	0.53	0/4497	
1	В	0.27	0/3340	0.52	0/4497	
1	С	0.27	0/3340	0.52	0/4497	
1	D	0.27	0/3340	0.51	0/4497	
1	Е	0.26	0/3340	0.53	1/4497~(0.0%)	
2	а	0.24	0/654	0.53	0/885	
2	b	0.26	0/654	0.63	0/885	
2	с	0.28	0/654	0.63	0/885	
2	d	0.24	0/654	0.48	0/885	
All	All	0.27	0/19316	0.53	1/26025~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Е	396	MET	CA-CB-CG	5.67	122.94	113.30

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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	А	416/419~(99%)	410 (99%)	6 (1%)	0	100	100
1	В	416/419~(99%)	406 (98%)	10 (2%)	0	100	100
1	\mathbf{C}	416/419~(99%)	411 (99%)	5 (1%)	0	100	100
1	D	416/419~(99%)	410 (99%)	6 (1%)	0	100	100
1	Ε	416/419~(99%)	414 (100%)	2(0%)	0	100	100
2	a	80/86~(93%)	77~(96%)	3~(4%)	0	100	100
2	b	80/86~(93%)	77~(96%)	3~(4%)	0	100	100
2	с	80/86~(93%)	74 (92%)	6 (8%)	0	100	100
2	d	80/86~(93%)	80 (100%)	0	0	100	100
All	All	2400/2439~(98%)	2359~(98%)	41 (2%)	0	100	100

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

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	358/359~(100%)	345~(96%)	13~(4%)	35	70
1	В	358/359~(100%)	353~(99%)	5(1%)	67	88
1	С	358/359~(100%)	351~(98%)	7~(2%)	55	83
1	D	358/359~(100%)	353~(99%)	5(1%)	67	88
1	Ε	358/359~(100%)	343~(96%)	15~(4%)	30	66
2	а	74/76~(97%)	70~(95%)	4 (5%)	22	57
2	b	74/76~(97%)	73~(99%)	1 (1%)	67	88
2	с	74/76~(97%)	70~(95%)	4 (5%)	22	57
2	d	74/76~(97%)	71~(96%)	3~(4%)	30	67
All	All	2086/2099~(99%)	2029~(97%)	57 (3%)	48	77



Mol	Chain	Res	Type
1	А	7	LYS
1	А	21	MET
1	А	69	ASP
1	А	92	ARG
1	А	105	LYS
1	А	218	GLU
1	А	238	ARG
1	А	266	SER
1	А	360	TYR
1	А	366	ARG
1	А	381	TRP
1	А	413	PHE
1	А	415	MET
1	В	26	LEU
1	В	29	MET
1	В	48	ASP
1	В	325	SER
1	В	334	GLU
1	С	1	MET
1	С	56	GLU
1	С	109	ARG
1	C C C C C	181	LYS
1	С	193	GLN
1	С	275	ASN
1	С	418	ARG
1	D	219	MET
1	D	322	ASP
1	D	381	TRP
1	D	394	ASP
1	D	416	MET
1	Е	29	MET
1	Е	62	PHE
1	Е	142	ASN
1	Е	147	MET
1	Е	257	LYS
1	Е	274	TYR
1	Е	343	LEU
1	Е	356	PRO
1	Е	359	ASP
1	Е	362	ARG
1	Е	375	GLU
1	Е	396	MET
-	Continue		

All (57) residues with a non-rotameric sidechain are listed below:

Continued on next page...



Mol	Chain	Res	Type
1	Е	398	PHE
1	Е	405	MET
1	Е	416	MET
2	a	24	LEU
2	a	35	LYS
2	a	39	LYS
2	a	71	PHE
2	b	72	SER
2	с	42	ASP
2	с	43	LEU
2	с	45	SER
2	с	47	LYS
2	d	25	MET
2	d	31	LYS
2	d	39	LYS

Continued from previous page...

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such side chains are listed below:

Mol	Chain	Res	Type
1	А	401	ASN
1	В	85	GLN
1	В	120	ASN
1	В	193	GLN
1	Е	344	HIS
2	b	37	GLN
2	с	21	GLN
2	с	73	HIS
2	d	37	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-17877. These allow visual inspection of the internal detail of the map and identification of artifacts.

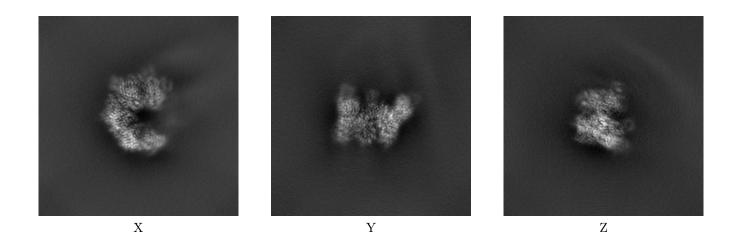
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

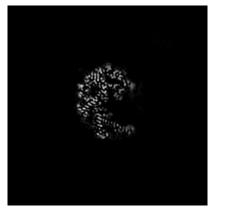


The images above show the map projected in three orthogonal directions.



6.2 Central slices (i)

6.2.1 Primary map



X Index: 192

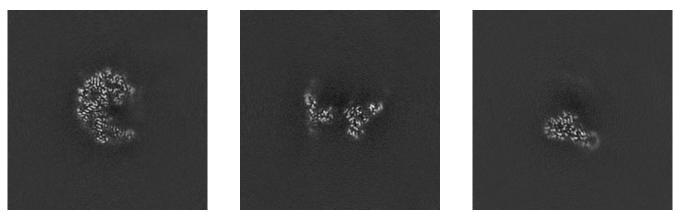


Y Index: 192



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: 192



Y Index: 178



Z Index: 230

6.3.2 Raw map



X Index: 187

Y Index: 178

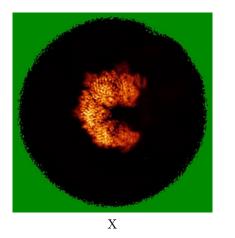


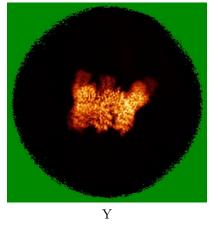
The images above show the largest variance slices of the map in three orthogonal directions.

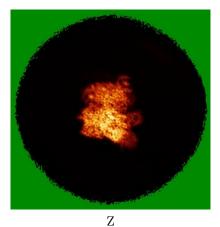


6.4 Orthogonal standard-deviation projections (False-color) (i)

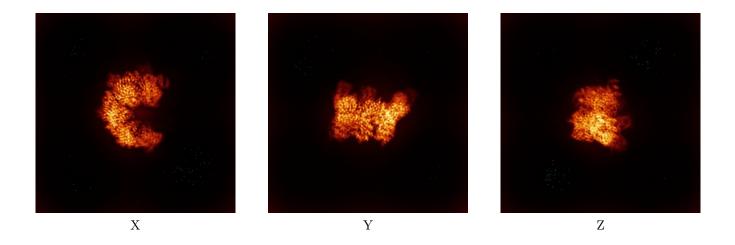
6.4.1 Primary map







6.4.2 Raw map

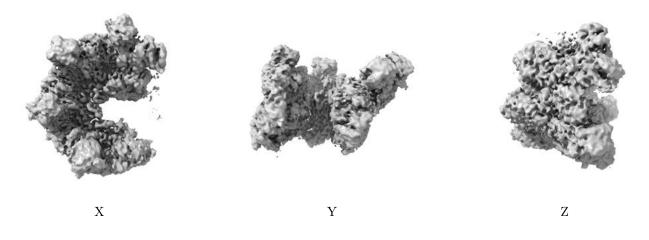


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



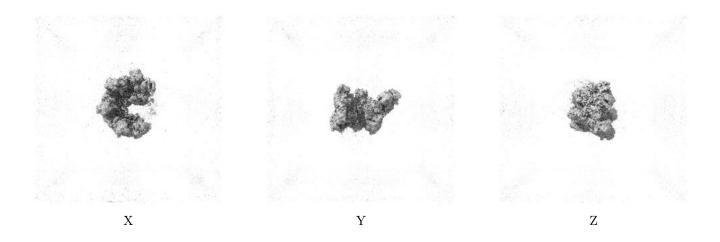
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0982. 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)

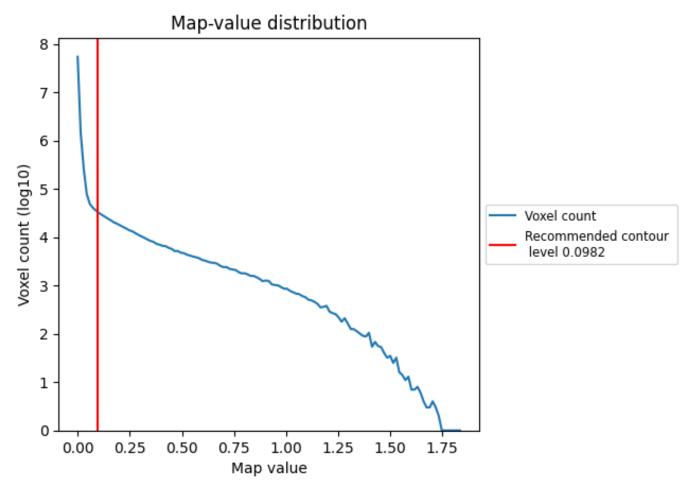
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

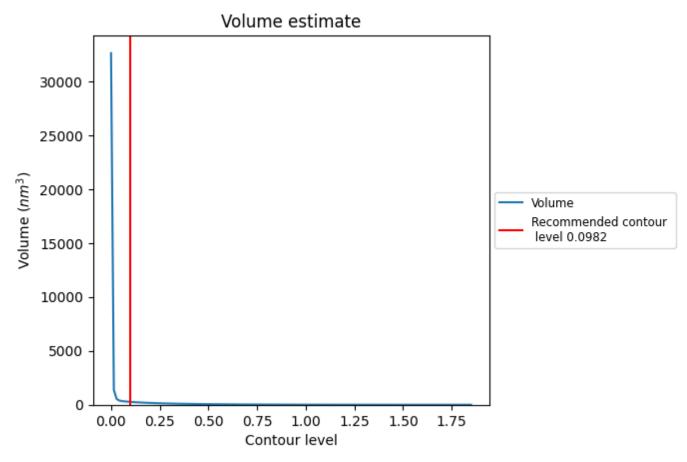
7.1 Map-value distribution (i)



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)

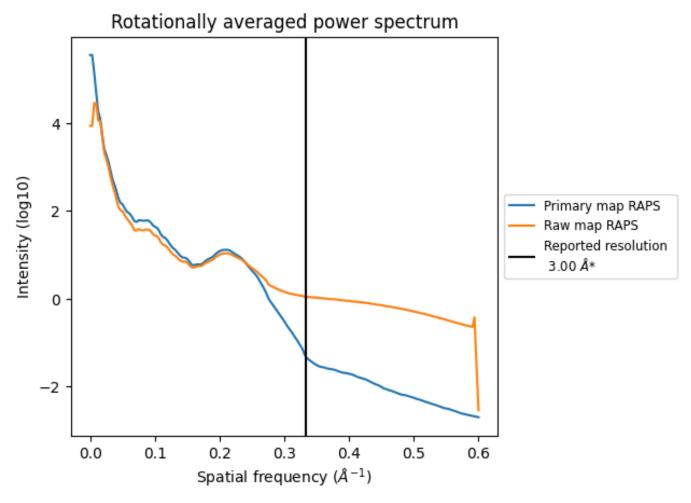


The volume at the recommended contour level is 271 nm^3 ; this corresponds to an approximate mass of 245 kDa.

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)



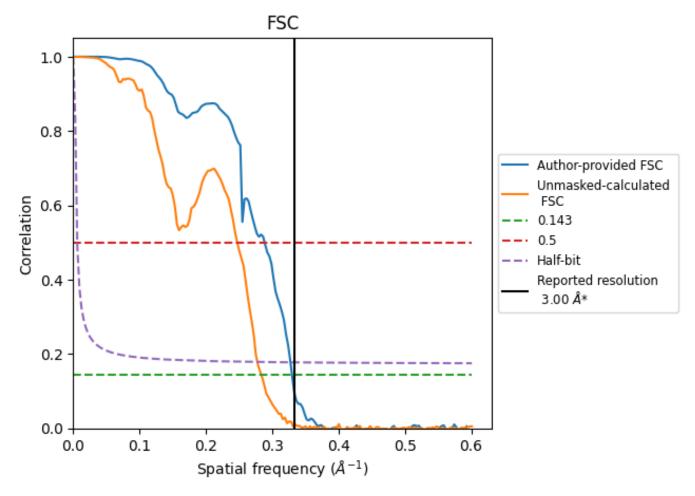
*Reported resolution corresponds to spatial frequency of 0.333 ${\rm \AA^{-1}}$



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 0.333 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.03	3.47	3.05
Unmasked-calculated*	3.52	4.04	3.60

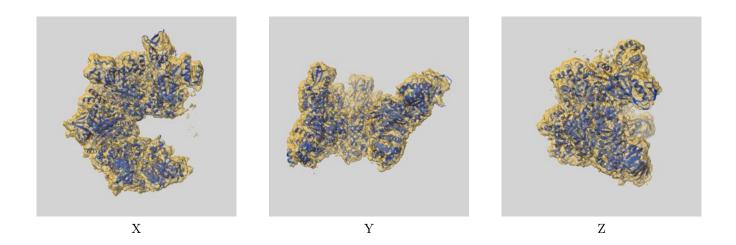
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.52 differs from the reported value 3.0 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17877 and PDB model 8PTP. Per-residue inclusion information can be found in section 3 on page 5.

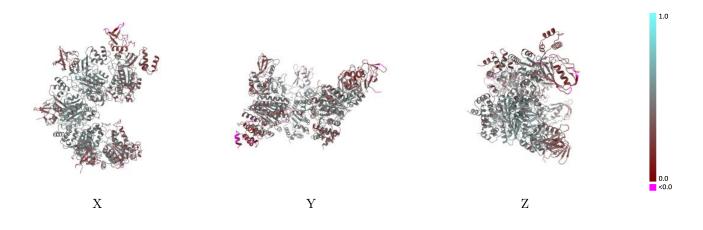
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0982 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.

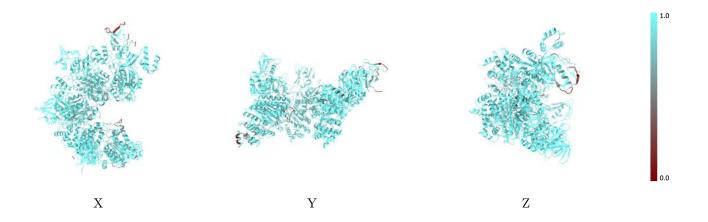


9.2 Q-score mapped to coordinate model (i)



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.

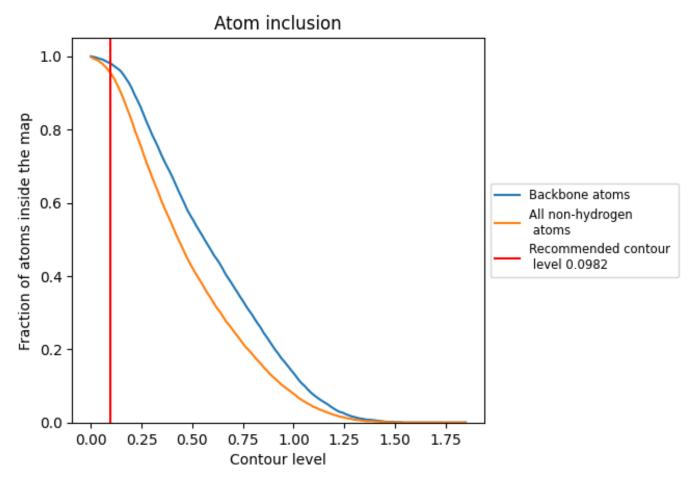
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0982).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.



Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (0.0982) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	1.0
All	0.9540	0.4330	
А	0.9620	0.4040	
В	0.9810	0.5030	
С	0.9880	0.5120	
D	0.9840	0.4950	
E	0.8930	0.3430	
a	0.7080	0.2140	
b	0.9860	0.3500	
с	0.9720	0.3640	0.0 <
d	0.9560	0.3390	

