

wwPDB EM Validation Summary Report (i)

Mar 28, 2023 – 03:19 PM EDT

PDB ID : 3IZO

EMDB ID : EMD-7034

Title: Model of the fiber tail and its interactions with the penton base of human

adenovirus by cryo-electron microscopy

Authors : Liu, H. Deposited on : 2010-11-05

Resolution : 3.60 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*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.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)

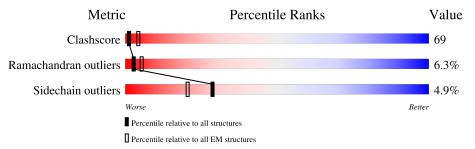
Validation Pipeline (wwPDB-VP) : 2.32.2

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 3.60 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$		
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 >=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				
			79	9%			
1	A	571	38%	36%	6%	20%	
			78	3%			
1	В	571	37%	37%	5%	20%	
			79	9%			
1	С	571	37%	37%	5%	20%	
	_		79	9%			
1	D	571	39%	36%	5%	20%	
	_		78	3%	_		
1	Е	571	38%	36%	5%	20%	
	-	X 04	•				
2	F	581	••	98%			
		F01	<u> </u>				
2	G	581	••	98%			
	TT	F01	•				
2	Н	581	••	98%			



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18537 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 Penton protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	455	Total	С	N	О	S	0	0
1	Λ	400	3642	2308	632	690	12	0	0
1	В	455	Total	С	N	О	S	0	0
1	Б	455	3642	2308	632	690	12		0
1	С	455	Total	С	N	О	S	0	0
1		455	3642	2308	632	690	12	0	
1	D	455	Total	С	N	О	S	0	0
1		455	3642	2308	632	690	12	0	
1	E	455	Total	С	N	О	S	0	0
1	Ŀ	455	3642	2308	632	690	12	U	U

• Molecule 2 is a protein called Fiber.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	F	13	Total C N O 109 70 14 25	0	0
2	G	13	Total C N O 109 70 14 25	0	0
2	Н	13	Total C N O 109 70 14 25	0	0

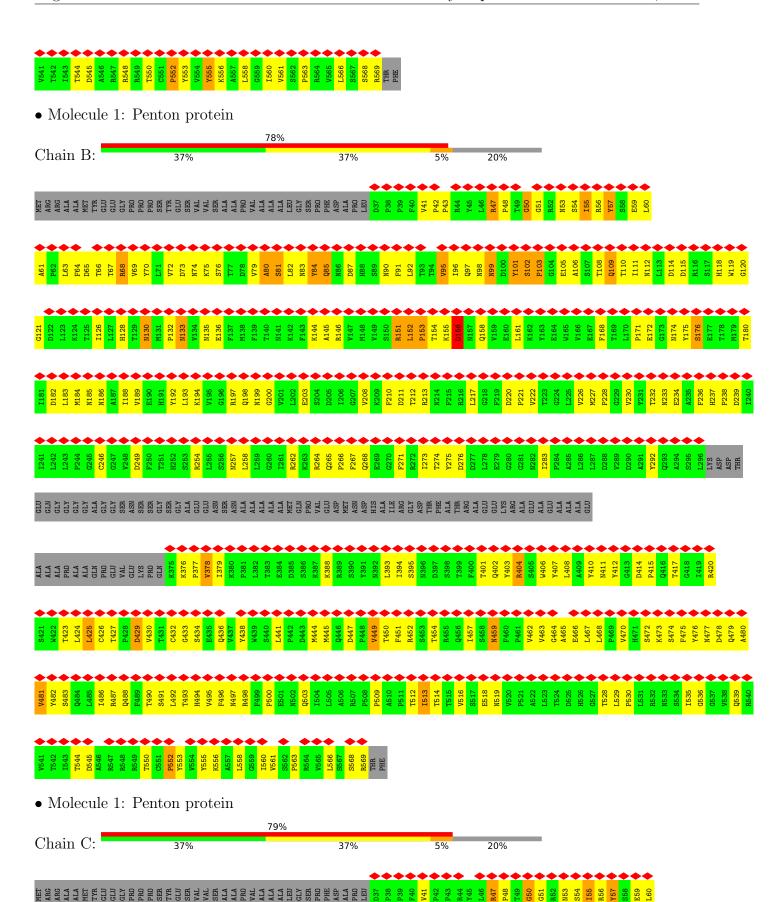


3 Residue-property plots (i)

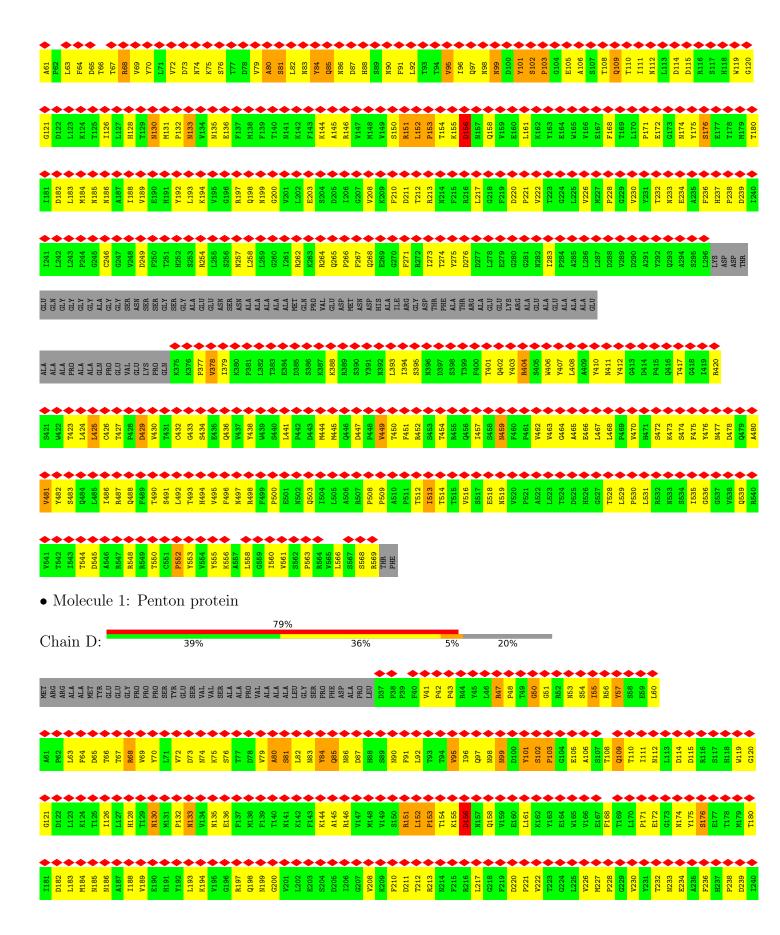
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Penton protein 79% Chain A: 36%

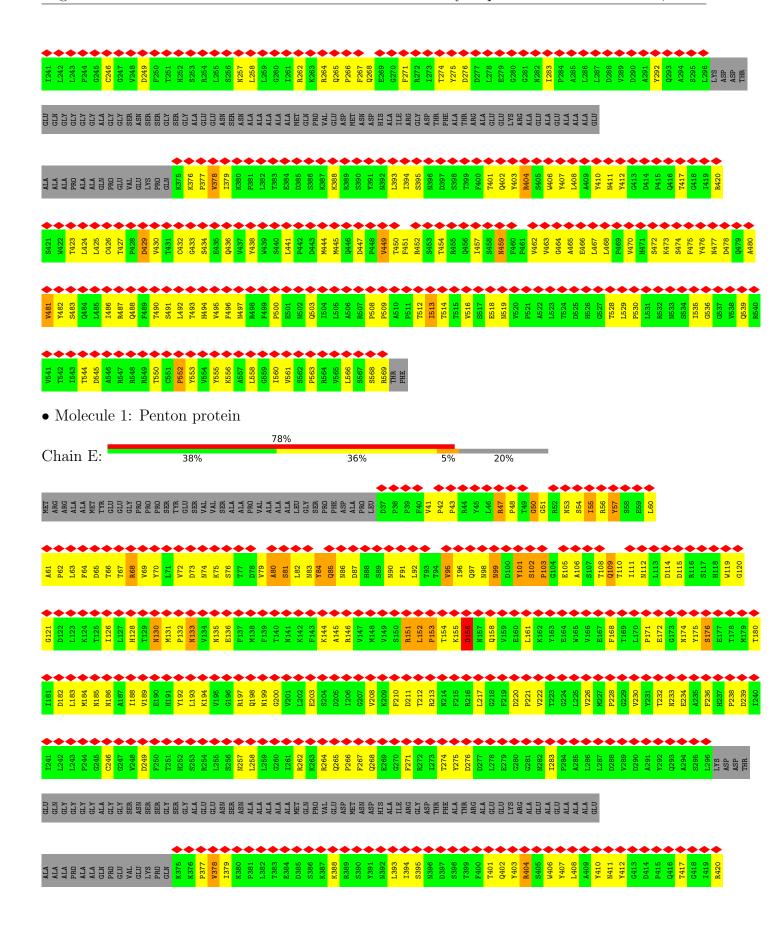




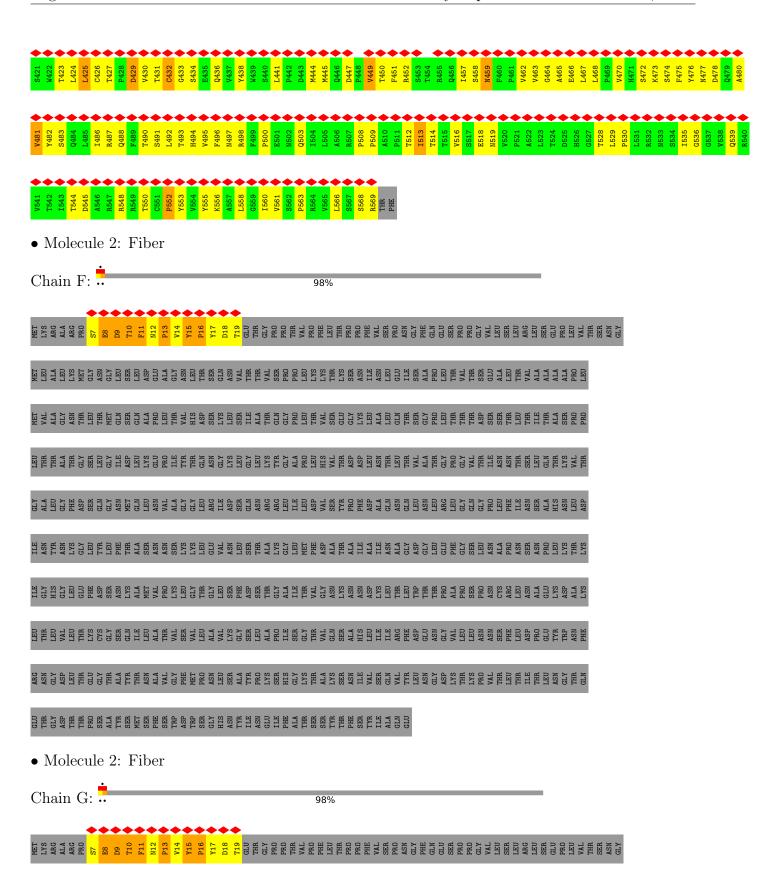




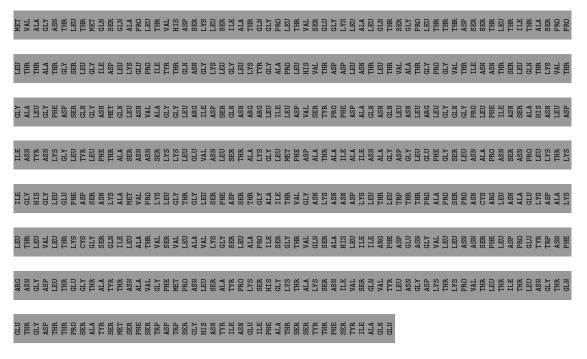






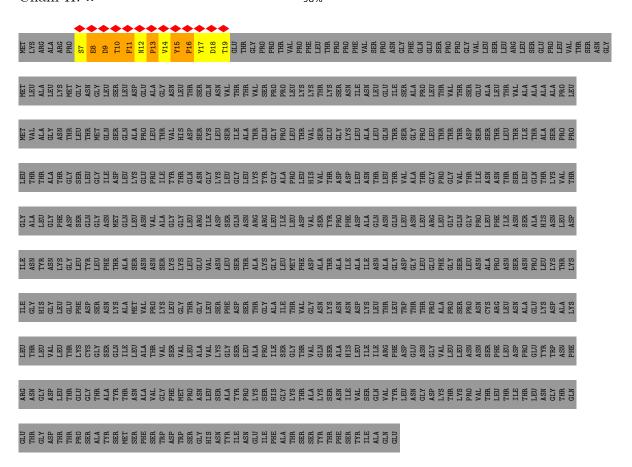






• Molecule 2: Fiber

Chain H: ... 98%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	31815	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	16.748	Depositor
Minimum map value	-11.582	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.876	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	1088.0, 1088.0, 1088.0	wwPDB
Map dimensions	1280, 1280, 1280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.33	0/3733	0.54	0/5088
1	В	0.33	0/3733	0.55	0/5088
1	С	0.33	0/3733	0.55	0/5088
1	D	0.33	0/3733	0.55	0/5088
1	Е	0.33	0/3733	0.54	0/5088
2	F	0.22	0/113	0.39	0/156
2	G	0.22	0/113	0.39	0/156
2	Н	0.22	0/113	0.39	0/156
All	All	0.33	0/19004	0.54	0/25908

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	В	0	2
1	С	0	2
1	D	0	2
1	Е	0	2
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	68	ARG	Sidechain
1	В	47	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	В	68	ARG	Sidechain
1	С	47	ARG	Sidechain

5.2 Too-close contacts (i)

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	3642	0	3571	777	0
1	В	3642	0	3571	780	0
1	С	3642	0	3571	757	0
1	D	3642	0	3571	735	0
1	Е	3642	0	3571	742	0
2	F	109	0	88	55	0
2	G	109	0	88	52	0
2	Н	109	0	88	55	0
All	All	18537	0	18119	2535	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 69.

The worst 5 of 2535 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:D:410:TYR:CE2	1:D:425:LEU:HD12	1.34	1.62	
1:D:425:LEU:HD13	1:E:172:GLU:CB	1.27	1.59	
1:A:267:PHE:CZ	1:B:80:ALA:HA	1.34	1.58	
1:C:450:THR:HG23	1:D:57:TYR:CE1	1.41	1.54	
1:A:450:THR:HG23	1:B:57:TYR:CE1	1.45	1.51	

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	451/571 (79%)	341 (76%)	84 (19%)	26 (6%)	1 18
1	В	451/571 (79%)	341 (76%)	85 (19%)	25 (6%)	2 19
1	С	451/571 (79%)	341 (76%)	85 (19%)	25 (6%)	2 19
1	D	451/571 (79%)	341 (76%)	85 (19%)	25 (6%)	2 19
1	Е	451/571 (79%)	340 (75%)	85 (19%)	26 (6%)	1 18
2	F	11/581 (2%)	3 (27%)	2 (18%)	6 (54%)	0 0
2	G	11/581 (2%)	3 (27%)	2 (18%)	6 (54%)	0 0
2	Н	11/581 (2%)	3 (27%)	2 (18%)	6 (54%)	0 0
All	All	2288/4598 (50%)	1713 (75%)	430 (19%)	145 (6%)	3 17

5 of 145 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	156	ASP
1	A	378	VAL
2	F	8	GLU
2	F	9	ASP

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	A	412/489~(84%)	391 (95%)	21 (5%)	24 58	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	В	412/489 (84%)	392 (95%)	20 (5%)	2	5	59
1	C	412/489 (84%)	392 (95%)	20 (5%)	2	5	59
1	D	412/489 (84%)	393 (95%)	19 (5%)	2	7	61
1	E	412/489 (84%)	392 (95%)	20 (5%)	2	5	59
2	F	13/489 (3%)	12 (92%)	1 (8%)	13	3	45
2	G	13/489 (3%)	12 (92%)	1 (8%)	13	3	45
2	Н	13/489 (3%)	12 (92%)	1 (8%)	13	3	45
All	All	2099/3912 (54%)	1996 (95%)	103 (5%)	2	9	59

5 of 103 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	276	ASP
1	D	133	ASN
1	Е	404	ARG
1	С	404	ARG
1	D	84	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	519	ASN
1	Е	109	GLN
1	Е	257	ASN
1	В	411	ASN
1	В	293	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.



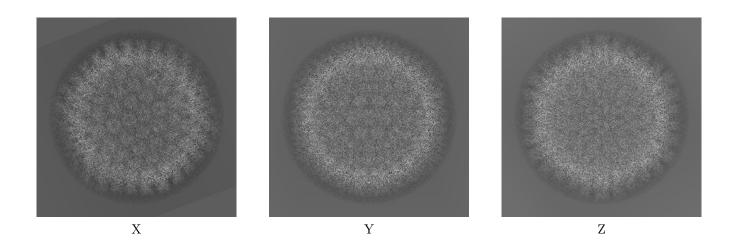
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7034. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

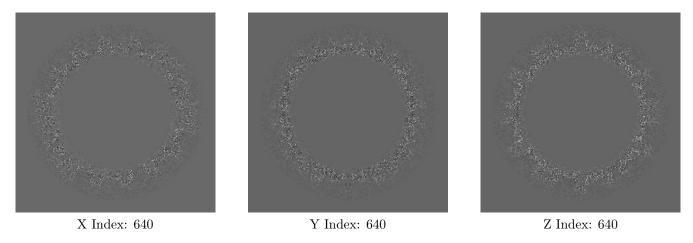
6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map

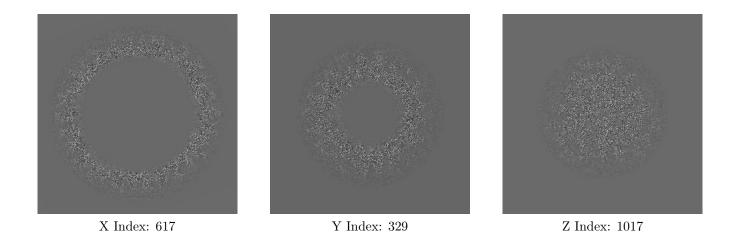




The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

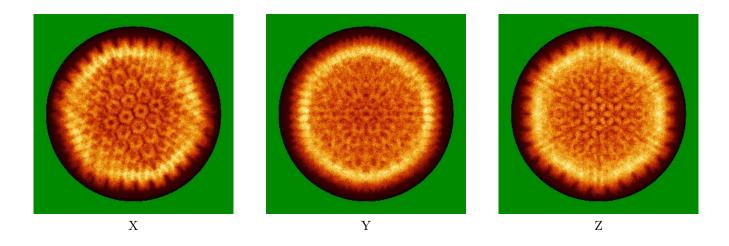
6.3.1 Primary map



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

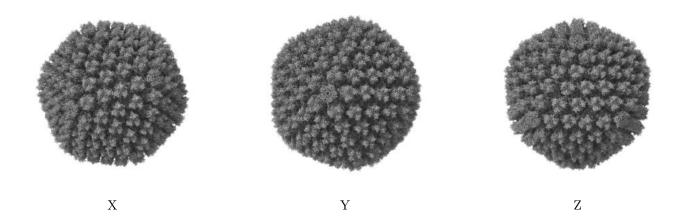


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

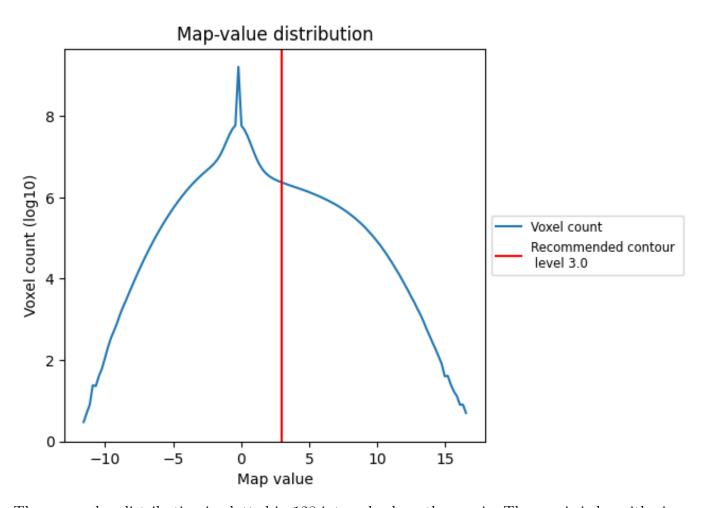
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

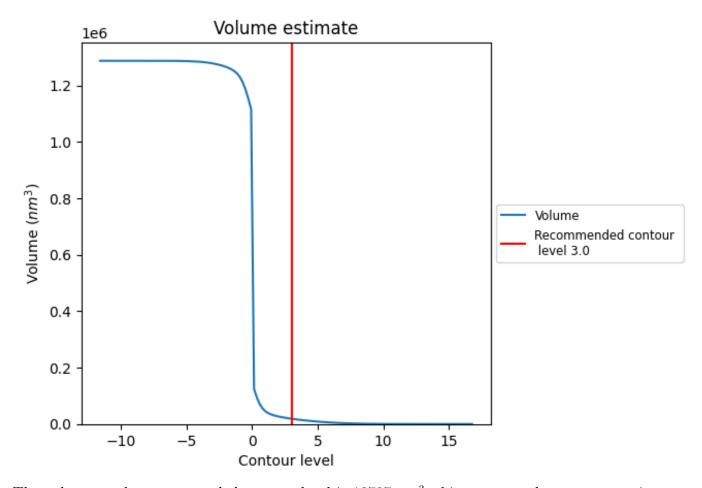
7.1 Map-value distribution (i)



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)

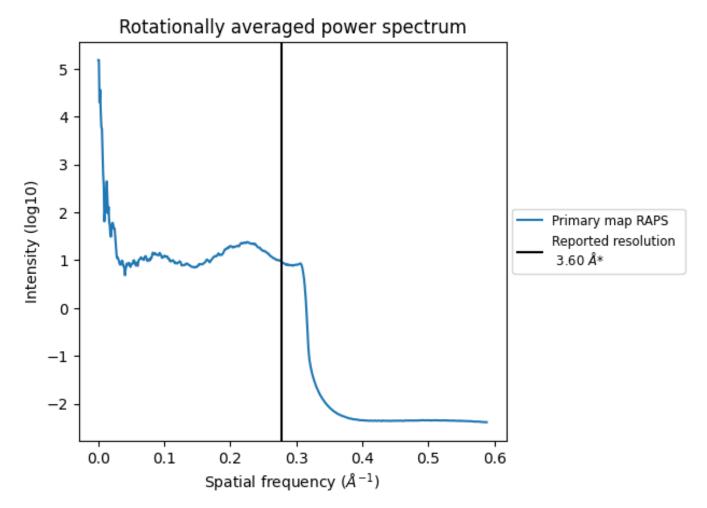


The volume at the recommended contour level is 18707 nm^3 ; this corresponds to an approximate mass of 16898 kDa.

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 0.278 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

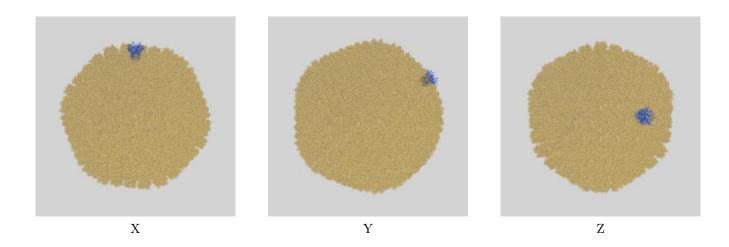
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7034 and PDB model 3IZO. Per-residue inclusion information can be found in section 3 on page 4.

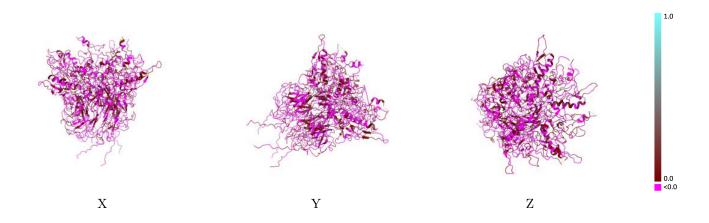
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

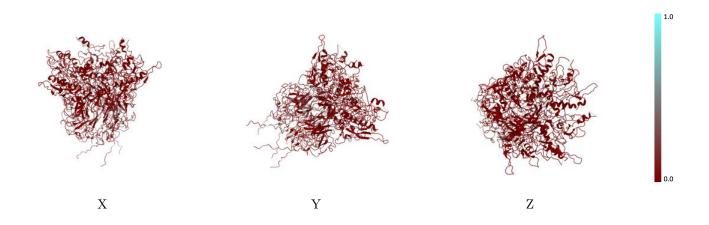


9.2 Q-score mapped to coordinate model (i)



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.

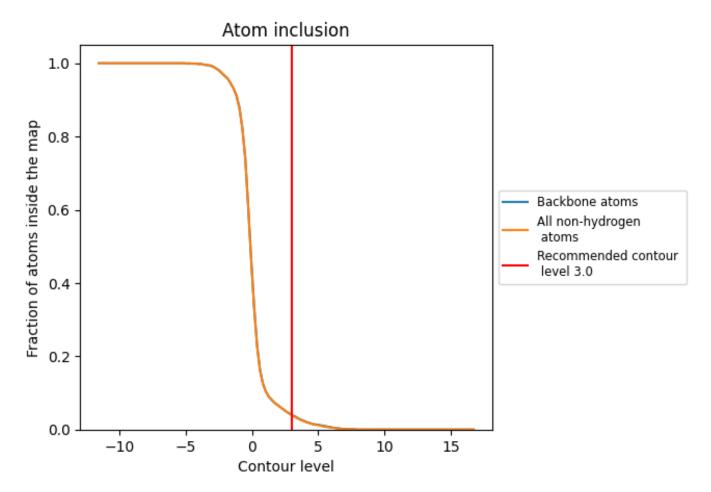
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.0).



9.4 Atom inclusion (i)



At the recommended contour level, 4% of all backbone atoms, 4% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0390	-0.0130
A	0.0300	-0.0250
В	0.0660	-0.0180
С	0.0260	-0.0010
D	0.0350	-0.0190
E	0.0440	-0.0030
F	0.0000	0.0190
G	0.0000	-0.0160
Н	0.0000	-0.1000



