

Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 08:55 pm GMT

PDB ID : 6QX7

EMDB ID : EMD-4662

Title : The cryo-EM structure of connector in bacteriophage phi29 prohead

Authors: Xu, J.; Gui, M.; Xiang, Y.

Deposited on : 2019-03-07

Resolution : 3.80 Å(reported)

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.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)

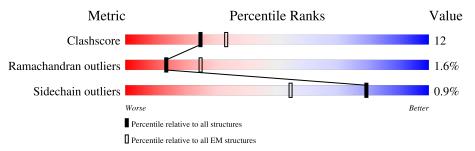
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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 $(\# ext{Entries})$	${ m EM~structures} \ (\#{ m Entries})$		
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 cha	ain
1	0a	309	79%	• 17%
1	0b	309	79%	• 17%
1	0c	309	79%	• 17%
1	0d	309	9% 79% 8%	• 17%
1	0e	309	79%	• 17%
1	Of	309	79%	• 17%
1	0g	309	79%	• 17%
1	0h	309	79%	• 17%



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Mol	Chain	Length		Quality of chair	n	
1	0i	309	9%	79%	·	17%
1	0j	309	9%	79%		17%
1	0k	309	9%	79%	•	17%
1	Ol	309	9%	79%		17%



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25164 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 Portal protein.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
1	O ₂	256	Total	С	N	О	S	0	0
1	0a	250	2097	1347	346	397	7	0	0
1	0b	256	Total	С	N	О	S	0	0
1	UD	250	2097	1347	346	397	7	0	U
1	0c	256	Total	С	N	О	S	0	0
1	00	250	2097	1347	346	397	7	0	0
1	0d	256	Total	С	N	О	S	0	0
1	- ou	250	2097	1347	346	397	7	U	0
1	0e	256	Total	С	N	О	S	0	0
1	06	250	2097	1347	346	397	7	U	U
1	Of	256	Total	С	N	О	S	0	0
1	U1	250	2097	1347	346	397	7	U	U
1	0g	256	Total	С	N	О	S	0	0
1	Ug	250	2097	1347	346	397	7	U	U
1	0h	256	Total	С	N	О	S	0	0
1	011	250	2097	1347	346	397	7	U	U
1	0i	256	Total	С	N	О	S	0	0
1	01	250	2097	1347	346	397	7	U	U
1	Oj	256	Total	\mathbf{C}	N	O	S	0	0
1	OJ .	250	2097	1347	346	397	7	0	U
1	0k	256	Total	С	N	О	S	0	0
1	UK	250	2097	1347	346	397	7		U
1	Ol	256	Total	С	N	О	S	0	0
	O1	200	2097	1347	346	397	7	U	U

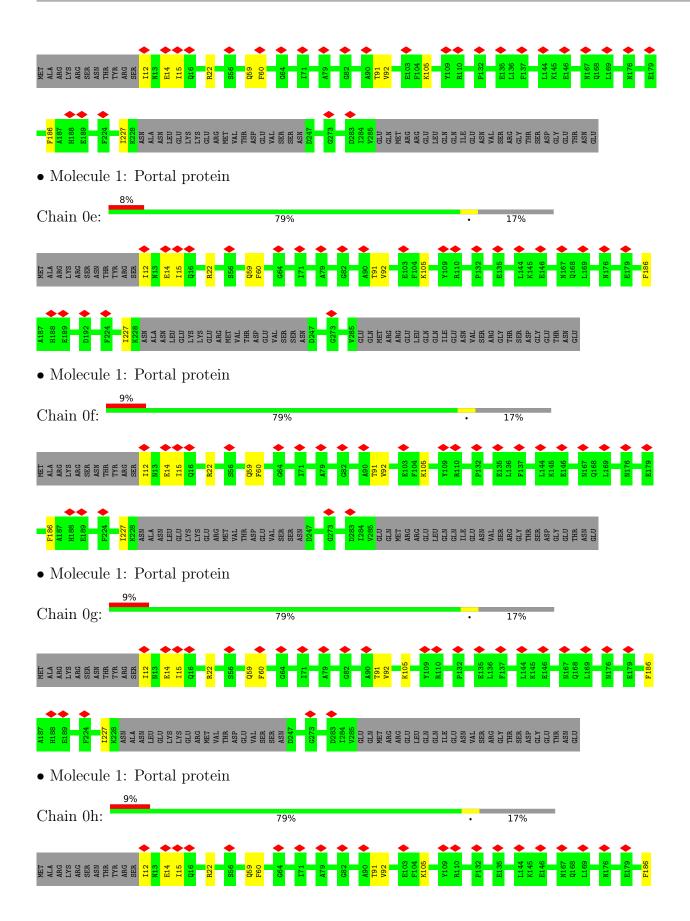


3 Residue-property plots (i)

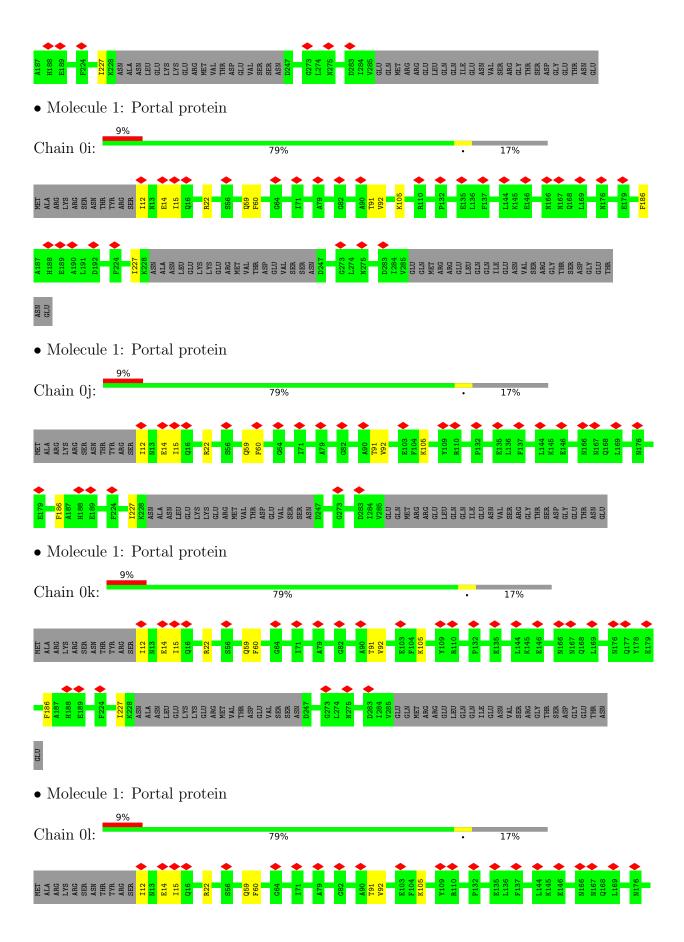
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Portal protein Chain 0a: • Molecule 1: Portal protein Chain 0b: • Molecule 1: Portal protein Chain 0c: • Molecule 1: Portal protein Chain 0d: 79% 17%















4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	30.005	Depositor
Minimum map value	-11.511	Depositor
Average map value	0.083	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	274.432, 274.432, 274.432	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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	0a	0.35	0/2144	0.58	0/2905	
1	0b	0.35	0/2144	0.58	0/2905	
1	0c	0.35	0/2144	0.58	0/2905	
1	0d	0.35	0/2144	0.58	0/2905	
1	0e	0.35	0/2144	0.58	0/2905	
1	0f	0.35	0/2144	0.58	0/2905	
1	0g	0.35	0/2144	0.58	0/2905	
1	0h	0.35	0/2144	0.58	0/2905	
1	0i	0.35	0/2144	0.58	0/2905	
1	0j	0.35	0/2144	0.58	0/2905	
1	0k	0.35	0/2144	0.58	0/2905	
1	Ol	0.35	0/2144	0.59	0/2905	
All	All	0.35	0/25728	0.58	0/34860	

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0a	0	5
1	0b	0	5
1	0c	0	5
1	0d	0	5
1	0e	0	5
1	Of	0	5
1	0g	0	5
1	0h	0	5
1	0i	0	5
1	0j	0	5
1	0k	0	5
1	Ol	0	5
All	All	0	60



There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0a	105	LYS	Peptide
1	0a	186	PHE	Peptide
1	0a	22	ARG	Peptide
1	0a	59	GLN	Peptide
1	0a	91	THR	Peptide
1	0b	105	LYS	Peptide
1	0b	186	PHE	Peptide
1	0b	22	ARG	Peptide
1	0b	59	GLN	Peptide
1	0b	91	THR	Peptide
1	0c	105	LYS	Peptide
1	0c	186	PHE	Peptide
1	0c	22	ARG	Peptide
1	0c	59	GLN	Peptide
1	0c	91	THR	Peptide
1	0d	105	LYS	Peptide
1	0d	186	PHE	Peptide
1	0d	22	ARG	Peptide
1	0d	59	GLN	Peptide
1	0d	91	THR	Peptide
1	0e	105	LYS	Peptide
1	0e	186	PHE	Peptide
1	0e	22	ARG	Peptide
1	0e	59	GLN	Peptide
1	0e	91	THR	Peptide
1	0f	105	LYS	Peptide
1	0f	186	PHE	Peptide
1	0f	22	ARG	Peptide
1	Of	59	GLN	Peptide
1	Of	91	THR	Peptide
1	0g	105	LYS	Peptide
1	0g	186	PHE	Peptide
1	0g	22	ARG	Peptide
1	0g	59	GLN	Peptide
1	0g	91	THR	Peptide
1	0h	105	LYS	Peptide
1	0h	186	PHE	Peptide



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Mol	Chain	$ hootnote{Res}$	Type	Group
1	0h	22	ARG	Peptide
1	0h	59	GLN	Peptide
1	0h	91	THR	Peptide
1	0i	105	LYS	Peptide
1	0i	186	PHE	Peptide
1	0i	22	ARG	Peptide
1	0i	59	GLN	Peptide
1	0i	91	THR	Peptide
1	0j	105	LYS	Peptide
1	0j	186	PHE	Peptide
1	0j	22	ARG	Peptide
1	0j	59	GLN	Peptide
1	0j	91	THR	Peptide
1	0k	105	LYS	Peptide
1	0k	186	PHE	Peptide
1	0k	22	ARG	Peptide
1	0k	59	GLN	Peptide
1	0k	91	THR	Peptide
1	01	105	LYS	Peptide
1	Ol	186	PHE	Peptide
1	Ol	22	ARG	Peptide
1	Ol	59	GLN	Peptide
1	Ol	91	THR	Peptide

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	0a	2097	0	2047	0	0
1	0b	2097	0	2047	0	0
1	0c	2097	0	2047	0	0
1	0d	2097	0	2047	0	0
1	0e	2097	0	2047	0	0
1	Of	2097	0	2047	0	0
1	0g	2097	0	2047	0	0
1	0h	2097	0	2047	0	0
1	0i	2097	0	2047	0	0
1	0j	2097	0	2047	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0k	2097	0	2047	0	0
1	01	2097	0	2047	0	0
All	All	25164	0	24564	0	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 12.

There are no clashes within the asymmetric unit.

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	Perce	entiles
1	0a	252/309~(82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0b	252/309~(82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0c	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0d	252/309~(82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0e	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	Of	252/309~(82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0g	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0h	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	Oi	252/309~(82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	Oj	252/309~(82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	0k	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	9	44
1	01	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	9	44
All	All	3024/3708 (82%)	2544 (84%)	432 (14%)	48 (2%)	13	44

All (48) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	0a	15	ILE
1	0b	15	ILE
1	0c	15	ILE
1	0d	15	ILE
1	0e	15	ILE
1	Of	15	ILE
1	0g	15	ILE
1	0h	15	ILE
1	0i	15	ILE
1	0j	15	ILE
1	0k	15	ILE
1	01	15	ILE
1	0a	14	GLU
1	0a	60	PHE
1	0b	14	GLU
1	0b	60	PHE
1	0c	14	GLU
1	0c	60	PHE
1	0d	14	GLU
1	0d	60	PHE
1	0e	14	GLU
1	0e	60	PHE
1	0f	14	GLU
1	Of	60	PHE
1	0g	14	GLU
1	0g	60	PHE
1	0h	14	GLU
1	0h	60	PHE
1	0i	14	GLU
1	0i	60	PHE
1	0j	14	GLU
1	0j	60	PHE
1	0k	14	GLU
1	0k	60	PHE
1	Ol	14	GLU
1	01	60	PHE
1	0a	92	VAL
1	0b	92	VAL
1	0c	92	VAL
1	0d	92	VAL
1	0e	92	VAL
1	0f	92	VAL
1	0g	92	VAL



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Mol	Chain	Res	Type
1	0h	92	VAL
1	0i	92	VAL
1	0j	92	VAL
1	0k	92	VAL
1	01	92	VAL

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	Perce	ntiles
1	0a	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0b	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0c	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0d	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0e	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	Of	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0g	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0h	228/277~(82%)	226 (99%)	2 (1%)	78	88
1	0i	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	0j	228/277~(82%)	226 (99%)	2 (1%)	78	88
1	0k	228/277 (82%)	226 (99%)	2 (1%)	78	88
1	01	228/277 (82%)	226 (99%)	2 (1%)	78	88
All	All	2736/3324 (82%)	2712 (99%)	24 (1%)	79	88

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0a	12	ILE
1	0a	227	ILE
1	0b	12	ILE
1	0b	227	ILE
1	0c	12	ILE



Continued from previous page...

Mol	Chain	Res	Type
1	0c	227	ILE
1	0d	12	ILE
1	0d	227	ILE
1	0e	12	ILE
1	0e	227	ILE
1	Of	12	ILE
1	Of	227	ILE
1	0g	12	ILE
1	0g	227	ILE
1	0h	12	ILE
1	0h	227	ILE
1	0i	12	ILE
1	0i	227	ILE
1	0j	12	ILE
1	0j	227	ILE
1	0k	12	ILE
1	0k	227	ILE
1	Ol	12	ILE
1	Ol	227	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	0a	88	ASN
1	0a	89	GLN
1	0a	167	ASN
1	0a	168	GLN
1	0a	188	HIS
1	0b	88	ASN
1	0b	89	GLN
1	0b	167	ASN
1	0b	168	GLN
1	0b	188	HIS
1	0c	88	ASN
1	0c	89	GLN
1	0c	167	ASN
1	0c	168	GLN
1	0c	188	HIS
1	0d	88	ASN
1	0d	89	GLN
1	0d	167	ASN
1	0d	168	GLN



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Mol	Chain	Res	$egin{array}{c} ext{rus } page \ ext{ } ext{ }$
1	0d	188	HIS
1	0e	88	ASN
1	0e	89	GLN
1	0e	167	ASN
1	0e	168	GLN
1	0e	188	HIS
1	Of	88	ASN
1	Of	89	GLN
1	Of	167	ASN
1	Of	168	GLN
1	Of	188	HIS
1	0g	88	ASN
1	0g	89	GLN
1	0g	167	ASN
1	0g	168	GLN
1	0g	188	HIS
1	0h	88	ASN
1	0h	89	GLN
1	0h	167	ASN
1	0h	168	GLN
1	0h	188	HIS
1	0i	88	ASN
1	0i	89	GLN
1	0i	167	ASN
1	0i	168	GLN
1	0i	188	HIS
1	0j	88	ASN
1	0j	89	GLN
1	0j	167	ASN
1	0j	168	GLN
1	0j	188	HIS
1	0k	88	ASN
1	0k	89	GLN
1	0k	167	ASN
1	0k	168	GLN
1	0k	188	HIS
1	Ol	88	ASN
1	Ol	89	GLN
1	Ol	167	ASN
1	Ol	168	GLN
1	01	188	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.



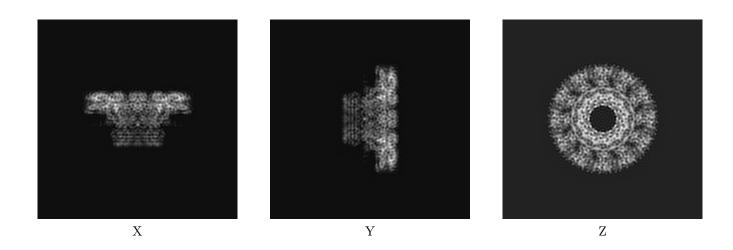
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4662. 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







Y Index: 128



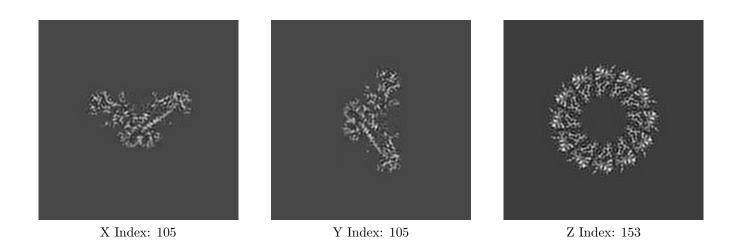
Z Index: 128



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

6.3 Largest variance slices (i)

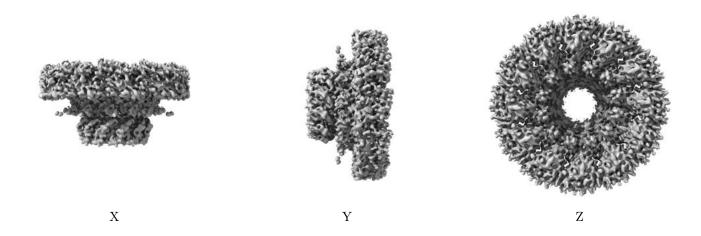
6.3.1 Primary map



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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

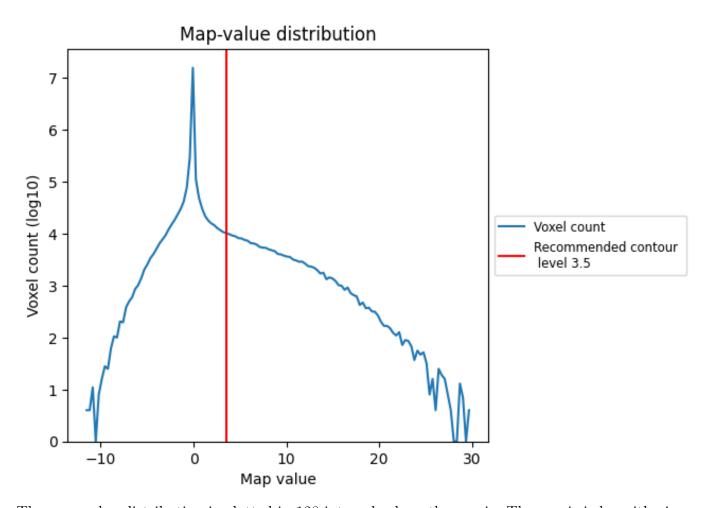
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

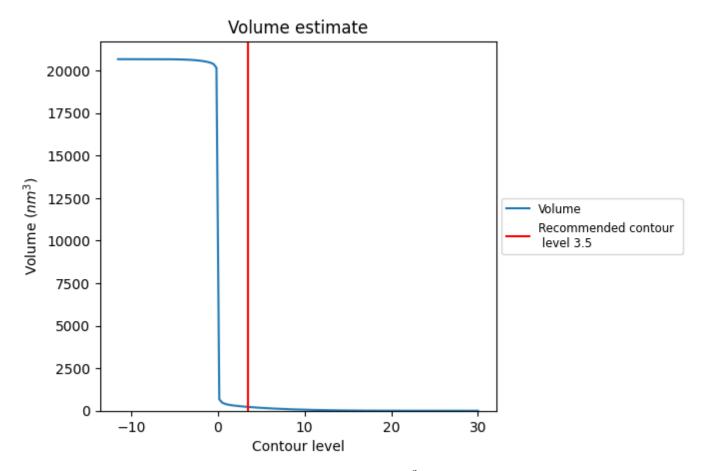
7.1 Map-value distribution (i)



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)

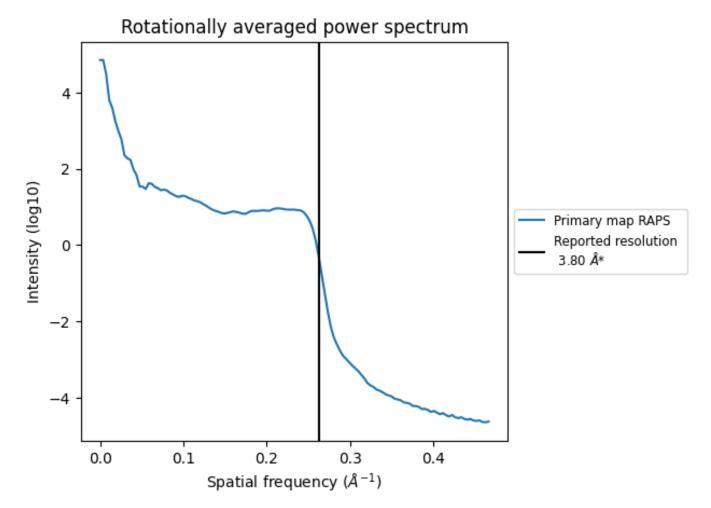


The volume at the recommended contour level is $225~\mathrm{nm}^3$; this corresponds to an approximate mass of $203~\mathrm{kDa}$.

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)



^{*}Reported resolution corresponds to spatial frequency of 0.263 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

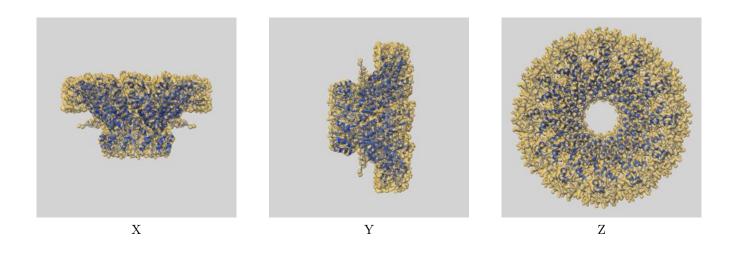
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4662 and PDB model 6QX7. Per-residue inclusion information can be found in section 3 on page 5.

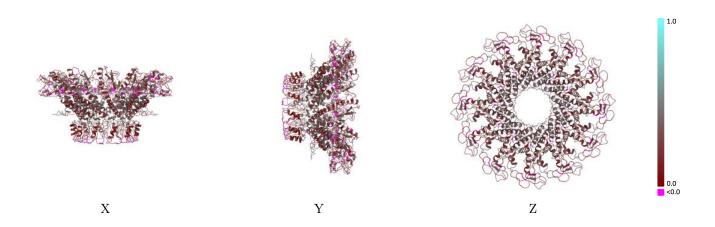
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 3.5 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.

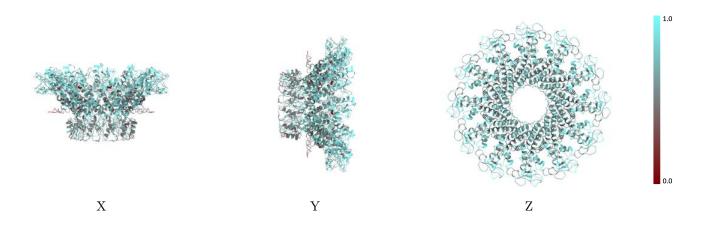


9.2 Q-score mapped to coordinate model (i)



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.

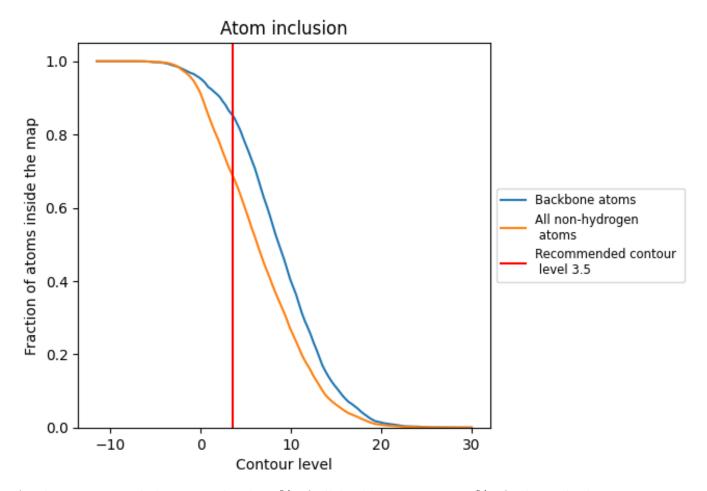
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.5).



9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 69% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6892	0.2710
0a	0.6947	0.2720
0b	0.6893	0.2700
0c	0.6888	0.2710
0d	0.6893	0.2710
0e	0.6879	0.2700
Of	0.6879	0.2690
0g	0.6913	0.2710
0h	0.6903	0.2720
0i	0.6883	0.2730
0j	0.6869	0.2700
0k	0.6883	0.2700
01	0.6869	0.2710



