

wwPDB EM Validation Summary Report (i)

Feb 12, 2024 – 04:42 AM EST

PDB ID : 3H3W

EMDB ID : EMD-1048

Title : Fitting of the gp6 crystal structure into 3D cryo-EM reconstruction of bacte-

riophage T4 dome-shaped baseplate

Authors : Aksyuk, A.A.; Leiman, P.G.; Shneider, M.M.; Mesyanzhinov, V.V.; Rossmann,

M.G.

Deposited on : 2009-04-17

Resolution : 12.00 Å(reported)

Based on initial model : 3H2T

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 (i)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev70

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)

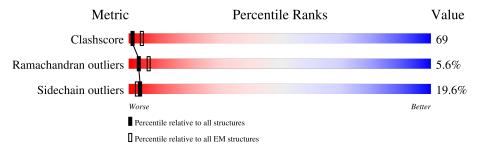
Validation Pipeline (wwPDB-VP) : 2.36

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 12.00 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	
			32%		
1	A	335	36%	46%	14% • •
			18%		
1	В	335	35%	44%	17% • •
			17%		
1	С	335	36%	46%	14% ••
	_		31%		_
1	D	335	34%	44%	17% • •
			32%		
1	Ε	335	35%	47%	14% • •
	_		17%		_
1	F	335	34%	44%	16% • •
	~	225	32%		
1	G	335	35%	47%	14% • •
			18%		_
1	Н	335	35%	44%	16% • •



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Mol	Chain	Length	Quality of chain					
			32%					
1	I	335	35%	47%	14% • •			
			17%					
1	J	335	35%	44%	16% • •			
			32%					
1	K	335	35%	47%	13% • •			
			17%					
1	$ box{L}$	335	35%	44%	16% • •			



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 31380 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 Baseplate structural protein Gp6.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
1	A	326	Total	С	N	О	S	0	0
1	A	320	2622	1667	424	528	3	0	U
1	В	204	Total	С	N	О	S	0	0
1	D	324	2608	1658	422	525	3	0	U
1	С	326	Total	С	N	О	S	0	0
1		320	2622	1667	424	528	3		U
1	D	324	Total	С	N	О	S	0	0
1	ע	324	2608	1658	422	525	3		U
1	Е	326	Total	С	N	О	S	0	0
1	12	320	2622	1667	424	528	3	0	U
1	F	324	Total	С	N	О	S	0	0
1	Г	324	2608	1658	422	525	3	0	U
1	G	326	Total	С	N	О	S	0	0
1	G	320	2622	1667	424	528	3		U
1	Н	324	Total	С	N	О	S	0	0
1	11	324	2608	1658	422	525	3	U	U
1	I	326	Total	С	Ν	Ο	S	0	0
1	1	320	2622	1667	424	528	3	U	U
1	J	324	Total	С	N	Ο	S	0	0
1		324	2608	1658	422	525	3		U
1	K	326	Total	С	N	О	S	0	0
1	117	320	2622	1667	424	528	3	<u> </u>	
1	L	324	Total	С	N	О	S	0	0
1		924	2608	1658	422	525	3	U	U

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	661	LEU	-	expression tag	UNP P19060
A	662	GLU	-	expression tag	UNP P19060
A	663	HIS	-	expression tag	UNP P19060
A	664	HIS	-	expression tag	UNP P19060
A	665	HIS	-	expression tag	UNP P19060
A	666	HIS	-	expression tag	UNP P19060



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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
A	667	HIS	-	expression tag	UNP P19060
A	668	HIS	_	expression tag	UNP P19060
В	661	LEU	-	expression tag	UNP P19060
В	662	GLU	-	expression tag	UNP P19060
В	663	HIS	-	expression tag	UNP P19060
В	664	HIS	-	expression tag	UNP P19060
В	665	HIS	-	expression tag	UNP P19060
В	666	HIS	-	expression tag	UNP P19060
В	667	HIS	-	expression tag	UNP P19060
В	668	HIS	-	expression tag	UNP P19060
С	661	LEU	-	expression tag	UNP P19060
С	662	GLU	-	expression tag	UNP P19060
С	663	HIS	-	expression tag	UNP P19060
С	664	HIS	-	expression tag	UNP P19060
С	665	HIS	-	expression tag	UNP P19060
С	666	HIS	-	expression tag	UNP P19060
С	667	HIS	-	expression tag	UNP P19060
С	668	HIS	-	expression tag	UNP P19060
D	661	LEU	-	expression tag	UNP P19060
D	662	GLU	-	expression tag	UNP P19060
D	663	HIS	-	expression tag	UNP P19060
D	664	HIS	-	expression tag	UNP P19060
D	665	HIS	-	expression tag	UNP P19060
D	666	HIS	-	expression tag	UNP P19060
D	667	HIS	-	expression tag	UNP P19060
D	668	HIS	-	expression tag	UNP P19060
Е	661	LEU	-	expression tag	UNP P19060
Е	662	GLU	-	expression tag	UNP P19060
Е	663	HIS	-	expression tag	UNP P19060
Е	664	HIS	-	expression tag	UNP P19060
Е	665	HIS	-	expression tag	UNP P19060
Е	666	HIS	-	expression tag	UNP P19060
Е	667	HIS	-	expression tag	UNP P19060
Е	668	HIS	-	expression tag	UNP P19060
F	661	LEU	-	expression tag	UNP P19060
F	662	GLU	-	expression tag	UNP P19060
F	663	HIS		expression tag	UNP P19060
F	664	HIS	-	expression tag	UNP P19060
F	665	HIS		expression tag	UNP P19060
F	666	HIS	-	expression tag	UNP P19060
F	667	HIS	-	expression tag	UNP P19060
F	668	HIS	-	expression tag	UNP P19060



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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
G	661	LEU	-	expression tag	UNP P19060
G	662	GLU	-	expression tag	UNP P19060
G	663	HIS	-	expression tag	UNP P19060
G	664	HIS	-	expression tag	UNP P19060
G	665	HIS	-	expression tag	UNP P19060
G	666	HIS	-	expression tag	UNP P19060
G	667	HIS	-	expression tag	UNP P19060
G	668	HIS	-	expression tag	UNP P19060
Н	661	LEU	-	expression tag	UNP P19060
Н	662	GLU	-	expression tag	UNP P19060
Н	663	HIS	-	expression tag	UNP P19060
Н	664	HIS	-	expression tag	UNP P19060
Н	665	HIS	_	expression tag	UNP P19060
Н	666	HIS	-	expression tag	UNP P19060
Н	667	HIS	-	expression tag	UNP P19060
Н	668	HIS	-	expression tag	UNP P19060
I	661	LEU	-	expression tag	UNP P19060
I	662	GLU	-	expression tag	UNP P19060
I	663	HIS	-	expression tag	UNP P19060
I	664	HIS	-	expression tag	UNP P19060
I	665	HIS	-	expression tag	UNP P19060
I	666	HIS	-	expression tag	UNP P19060
I	667	HIS	-	expression tag	UNP P19060
I	668	HIS	-	expression tag	UNP P19060
J	661	LEU	-	expression tag	UNP P19060
J	662	GLU	-	expression tag	UNP P19060
J	663	HIS	-	expression tag	UNP P19060
J	664	HIS	-	expression tag	UNP P19060
J	665	HIS	-	expression tag	UNP P19060
J	666	HIS	-	expression tag	UNP P19060
J	667	HIS	-	expression tag	UNP P19060
J	668	HIS	-	expression tag	UNP P19060
K	661	LEU	-	expression tag	UNP P19060
K	662	GLU	-	expression tag	UNP P19060
K	663	HIS	-	expression tag	UNP P19060
K	664	HIS	-	expression tag	UNP P19060
K	665	HIS		expression tag	UNP P19060
K	666	HIS	-	expression tag	UNP P19060
K	667	HIS	-	expression tag	UNP P19060
K	668	HIS	-	expression tag	UNP P19060
L	661	LEU	-	expression tag	UNP P19060
L	662	GLU	-	expression tag	UNP P19060



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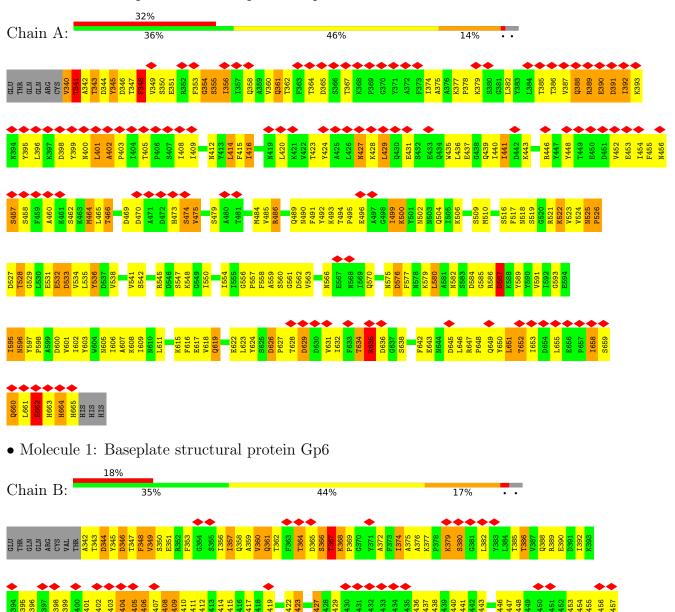
Chain	Residue	Modelled	Actual	Comment	Reference
L	663	HIS	-	expression tag	UNP P19060
L	664	HIS	-	expression tag	UNP P19060
L	665	HIS	-	expression tag	UNP P19060
L	666	HIS	-	expression tag	UNP P19060
L	667	HIS	-	expression tag	UNP P19060
L	668	HIS	-	expression tag	UNP P19060



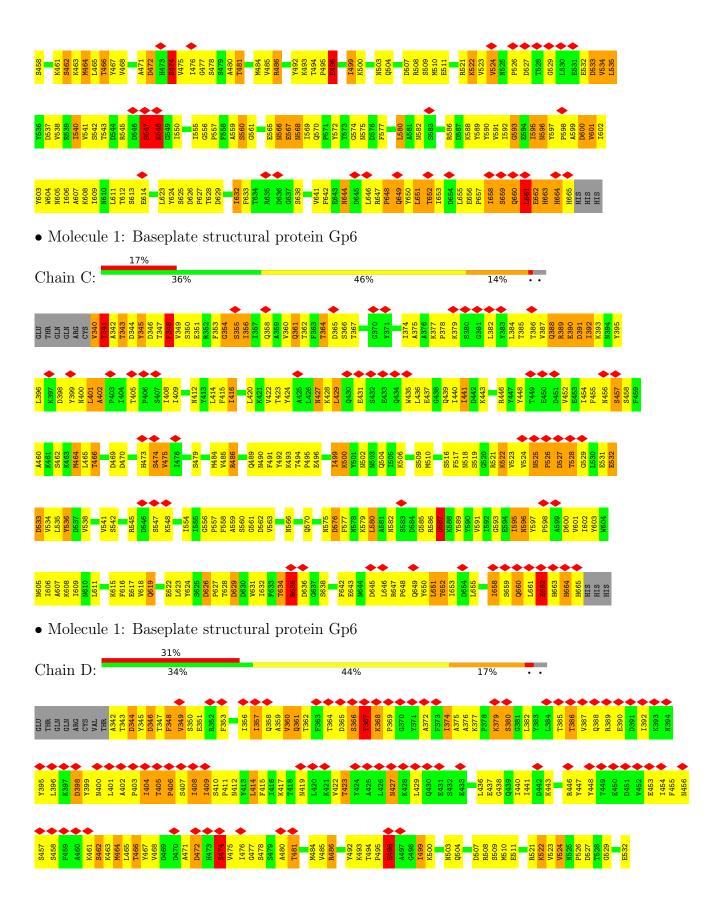
3 Residue-property plots (i)

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.

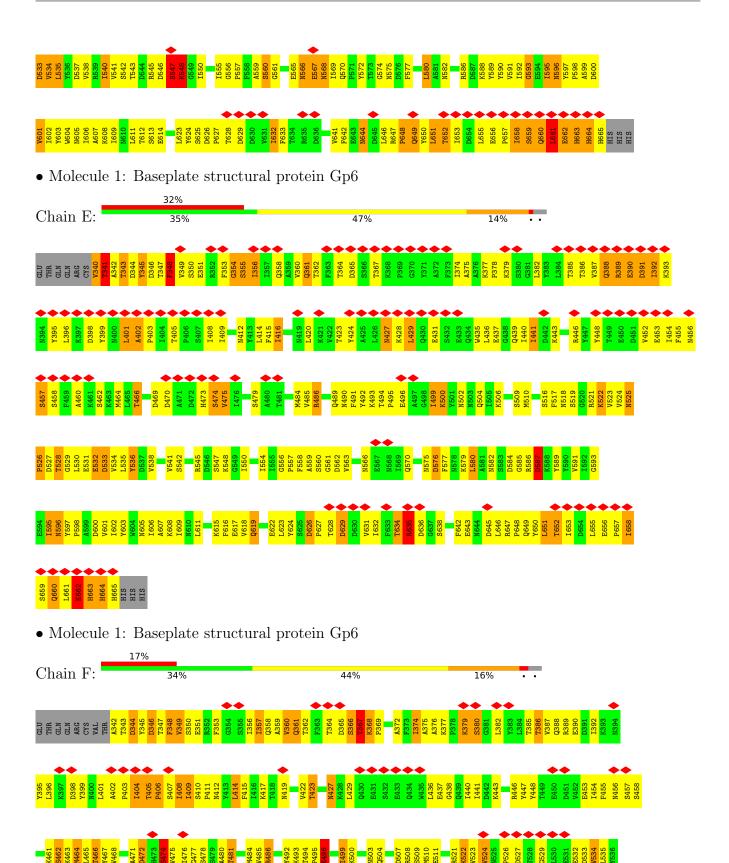
• Molecule 1: Baseplate structural protein Gp6



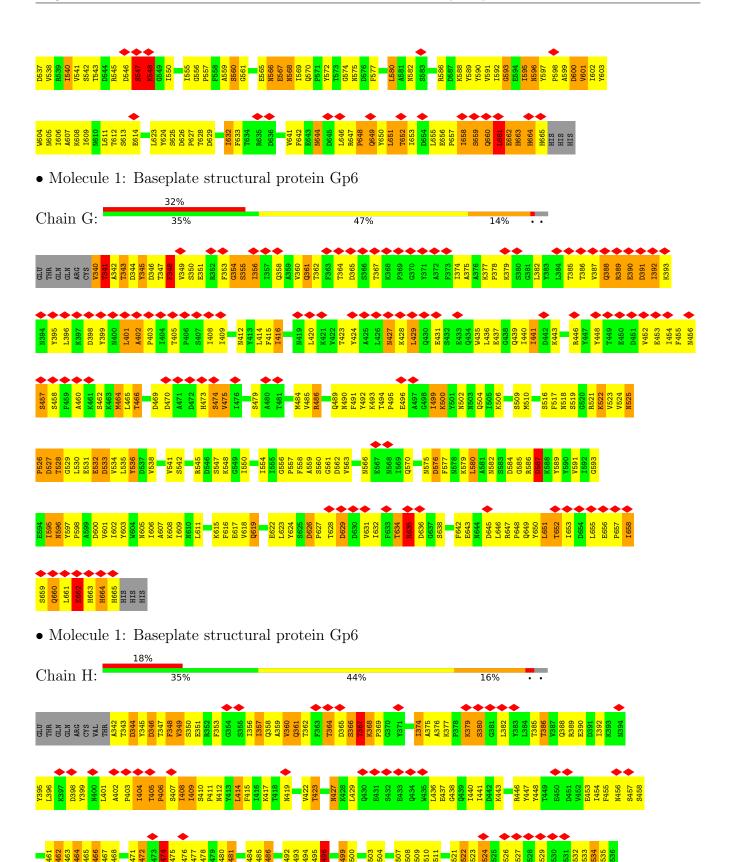




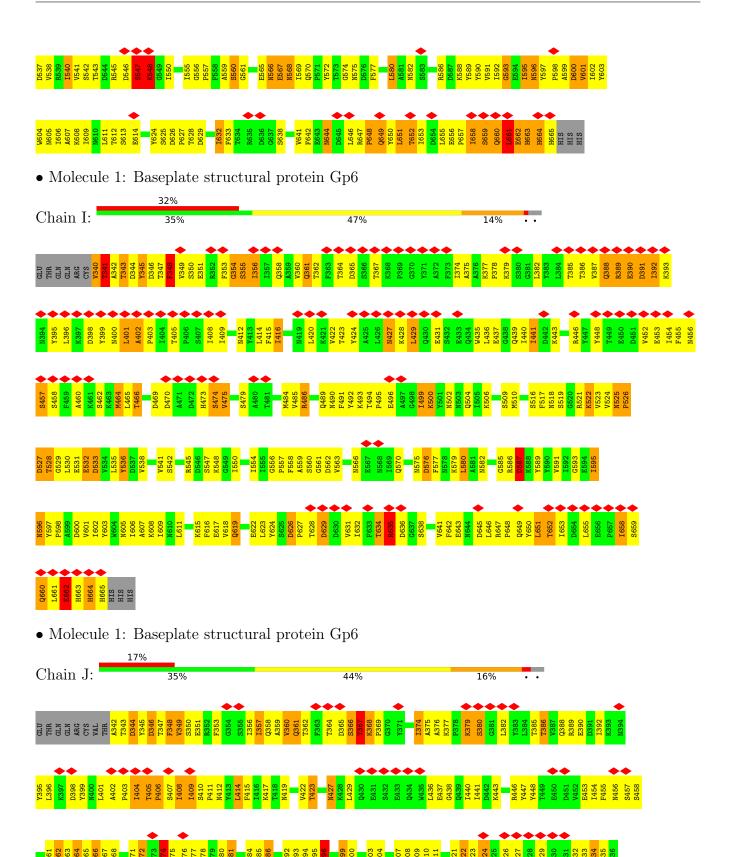




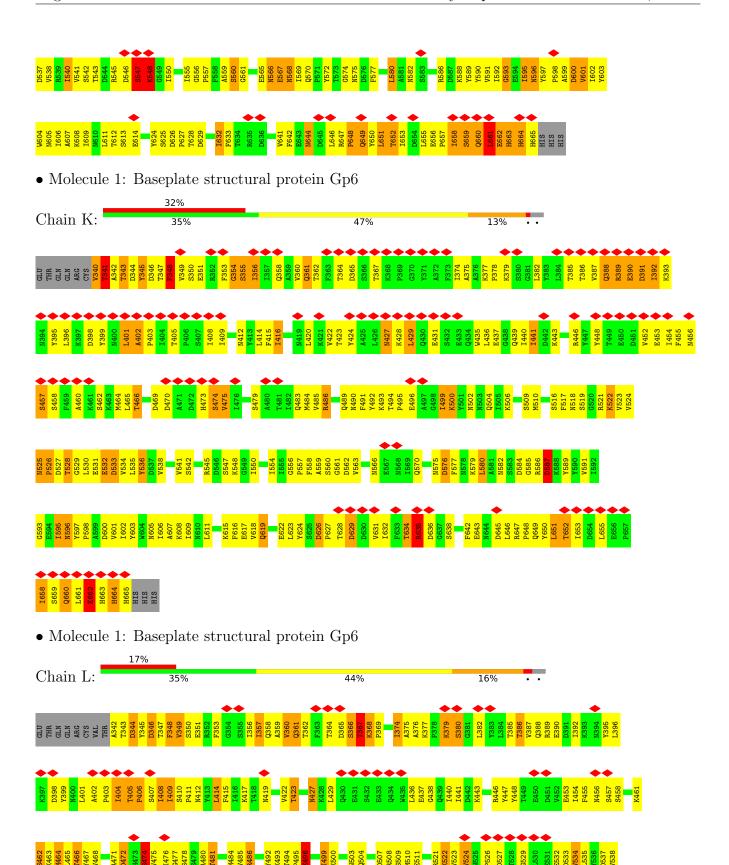




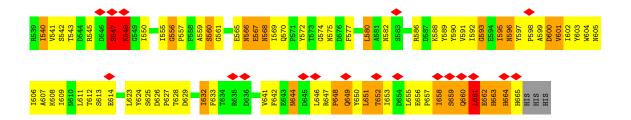














4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	945	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	47000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	10.345	Depositor
Minimum map value	-7.648	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.45	Depositor
Map size (Å)	583.8291, 583.8291, 583.8291	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.97872, 2.97872, 2.97872	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	0.50	0/2677	0.80	7/3637~(0.2%)	
1	В	0.51	0/2663	0.96	11/3617 (0.3%)	
1	С	0.50	0/2677	0.80	7/3637 (0.2%)	
1	D	0.51	0/2663	0.96	11/3617 (0.3%)	
1	Е	0.50	0/2677	0.80	7/3637 (0.2%)	
1	F	0.51	0/2663	0.96	11/3617 (0.3%)	
1	G	0.50	0/2677	0.80	7/3637 (0.2%)	
1	Н	0.51	0/2663	0.96	$11/3617 \; (0.3\%)$	
1	I	0.50	0/2677	0.80	7/3637 (0.2%)	
1	J	0.51	0/2663	0.96	11/3617~(0.3%)	
1	K	0.50	0/2677	0.80	7/3637~(0.2%)	
1	L	0.51	0/2663	0.96	11/3617 (0.3%)	
All	All	0.51	0/32040	0.88	108/43524 (0.2%)	

There are no bond length outliers.

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	J	405	THR	C-N-CD	-29.01	56.77	120.60
1	Н	405	THR	C-N-CD	-29.01	56.77	120.60
1	D	405	THR	C-N-CD	-29.01	56.78	120.60
1	F	405	THR	C-N-CD	-29.00	56.79	120.60
1	L	405	THR	C-N-CD	-29.00	56.80	120.60

There are no chirality outliers.

There are no planarity outliers.

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	2622	0	2545	394	0
1	В	2608	0	2530	369	0
1	С	2622	0	2545	396	0
1	D	2608	0	2530	375	0
1	Ε	2622	0	2543	440	0
1	F	2608	0	2530	338	0
1	G	2622	0	2543	376	0
1	Н	2608	0	2530	367	0
1	I	2622	0	2544	376	0
1	J	2608	0	2530	334	0
1	K	2622	0	2543	414	0
1	L	2608	0	2530	339	0
All	All	31380	0	30443	4266	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 4266 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:366:SER:CB	1:K:403:PRO:HB3	1.21	1.65
1:A:664:HIS:NE2	1:K:348:PHE:CZ	1.70	1.60
1:I:400:ASN:ND2	1:K:664:HIS:CE1	1.69	1.58
1:B:364:THR:CG2	1:K:401:LEU:CD1	1.79	1.58
1:E:348:PHE:CZ	1:G:664:HIS:NE2	1.68	1.57

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	Perc	entiles
1	A	324/335~(97%)	260 (80%)	47 (14%)	17 (5%)	2	19
1	В	322/335~(96%)	261 (81%)	42 (13%)	19 (6%)	1	17
1	С	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	19
1	D	322/335~(96%)	262 (81%)	41 (13%)	19 (6%)	1	17
1	E	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	19
1	F	322/335~(96%)	262 (81%)	41 (13%)	19 (6%)	1	17
1	G	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	19
1	Н	322/335 (96%)	262 (81%)	41 (13%)	19 (6%)	1	17
1	I	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	19
1	J	322/335 (96%)	261 (81%)	42 (13%)	19 (6%)	1	17
1	K	324/335 (97%)	260 (80%)	47 (14%)	17 (5%)	2	19
1	L	322/335 (96%)	261 (81%)	42 (13%)	19 (6%)	1	17
All	All	3876/4020 (96%)	3129 (81%)	531 (14%)	216 (6%)	3	19

5 of 216 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	348	PHE
1	A	354	GLY
1	A	389	ARG
1	A	390	GLU
1	A	526	PRO

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	$295/304\ (97\%)$	239 (81%)	56 (19%)	1 8
1	В	$293/304\ (96\%)$	234 (80%)	59 (20%)	1 7
1	С	295/304 (97%)	239 (81%)	56 (19%)	1 8
1	D	293/304 (96%)	234 (80%)	59 (20%)	1 7



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Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	ntile	es
1	E	295/304~(97%)	239 (81%)	56 (19%)		1	8	
1	F	293/304 (96%)	234 (80%)	59 (20%)		1	7	
1	G	295/304~(97%)	239 (81%)	56 (19%)		1	8	
1	Н	293/304 (96%)	234 (80%)	59 (20%)		1	7	
1	I	295/304~(97%)	239 (81%)	56 (19%)		1	8	
1	J	293/304 (96%)	234 (80%)	59 (20%)		1	7	
1	K	295/304~(97%)	239 (81%)	56 (19%)		1	8	
1	L	293/304 (96%)	234 (80%)	59 (20%)		1	7	
All	All	3528/3648 (97%)	2838 (80%)	690 (20%)		4	8	

5 of 690 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	345	TYR
1	J	661	LEU
1	I	414	LEU
1	I	343	THR
1	J	361	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	596	ASN
1	L	394	ASN
1	L	596	ASN
1	Е	596	ASN
1	Е	504	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.



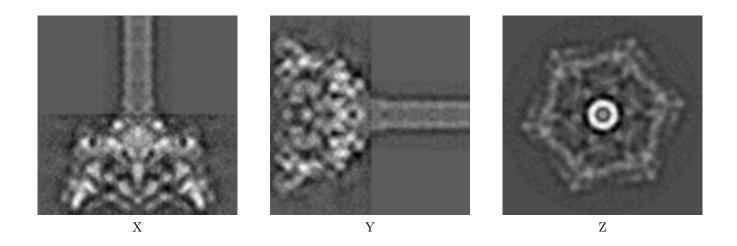
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1048. 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)

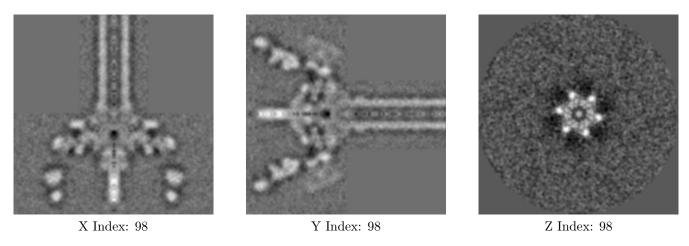
6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map

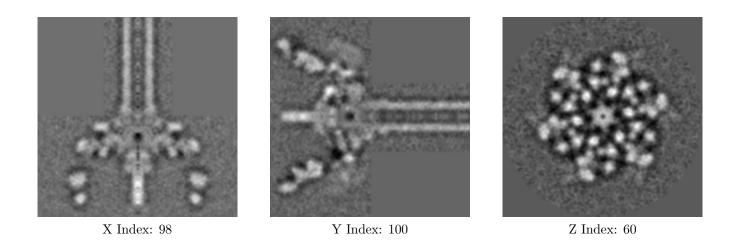




The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

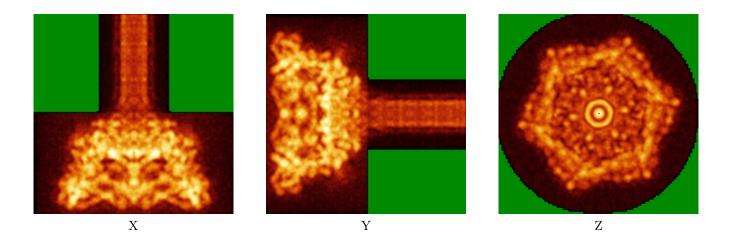
6.3.1 Primary map



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

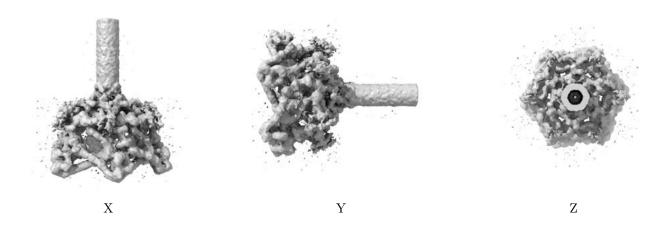


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 1.45. 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)

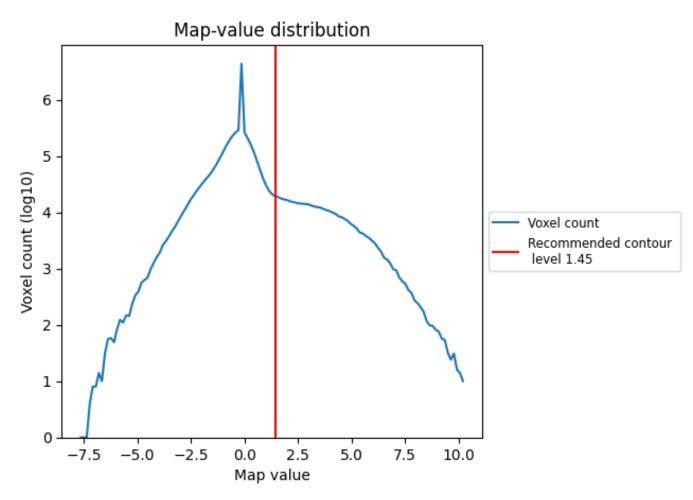
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

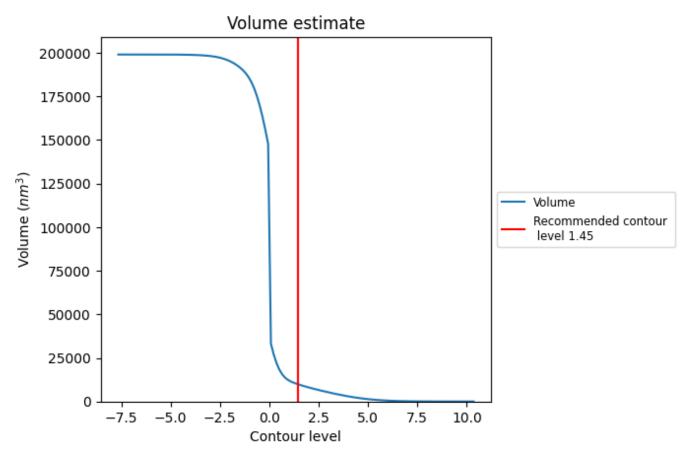
7.1 Map-value distribution (i)



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)

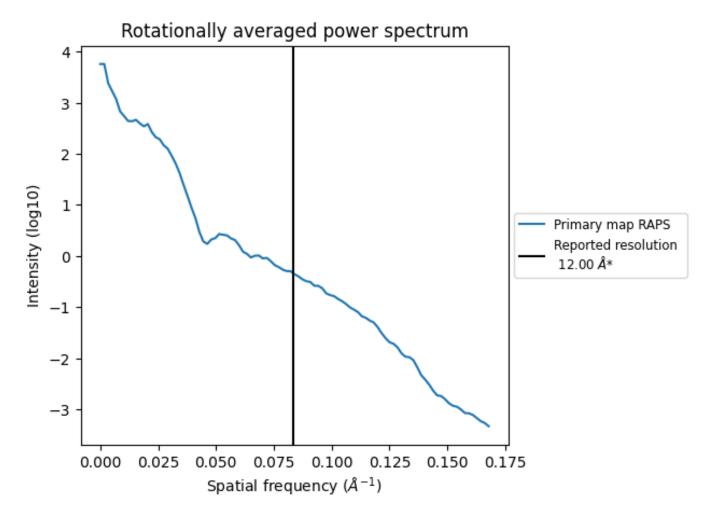


The volume at the recommended contour level is $9896~\mathrm{nm^3}$; this corresponds to an approximate mass of $8939~\mathrm{kDa}$.

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 0.083 $\rm \mathring{A}^{-1}$



8 Fourier-Shell correlation (i)

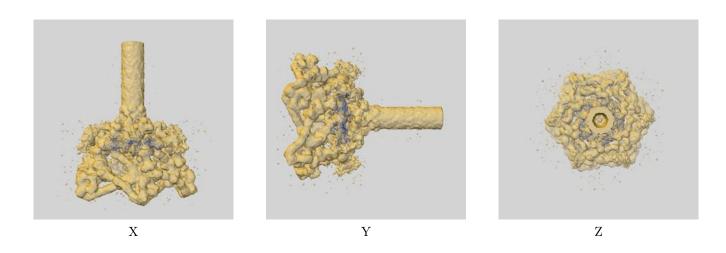
This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1048 and PDB model 3H3W. Per-residue inclusion information can be found in section 3 on page 8.

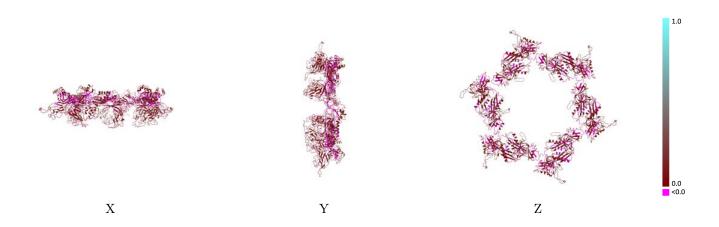
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 1.45 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.

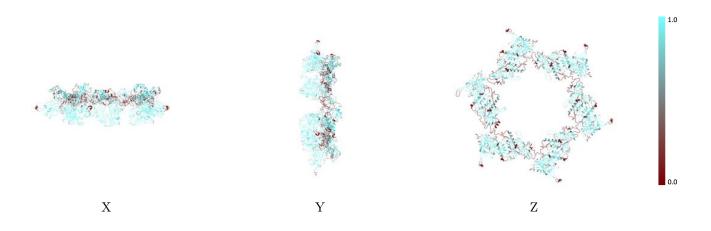


9.2 Q-score mapped to coordinate model (i)



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.

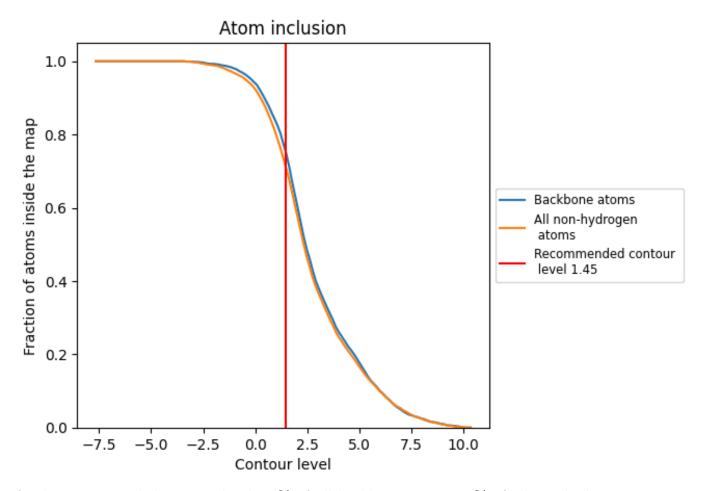
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.45).



9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (1.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.0680
A	0.6560	0.0630
В	0.7730	0.0750
С	0.7700	0.0760
D	0.6550	0.0630
E	0.6540	0.0630
F	0.7800	0.0730
G	0.6550	0.0600
Н	0.7730	0.0740
I	0.6540	0.0630
J	0.7740	0.0720
K	0.6540	0.0640
ho	0.7800	0.0750



