wwPDB EM Validation Summary Report (i)

May 4, 2024 – 06:46 pm BST

PDB ID	:	6QXM
EMDB ID	:	EMD-4669
Title	:	Cryo-EM structure of T7 bacteriophage portal protein, 12mer, open valve
Authors	:	Fabrega-Ferrer, M.; Cuervo, A.; Machon, C.; Fernandez, F.J.; Perez-Luque, R.; Pous, J.; Vega, M.C.; Carrascosa, J.L.; Coll, M.
Deposited on	:	2019-03-07
Resolution	:	4.10 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.10 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 37164 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	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	392	3097	1961	522	600	14	0	0
1	B	392	3097	1961	522	600	14	0	0
1	C	392	3097	1961	522	600	14	0	0
1	D	392	3097	1961	522	600	14	0	0
1	E	392	3097	1961	522	600	14	0	0
1	F	392	3097	1961	522	600	14	0	0
1	G	392	3097	1961	522	600	14	0	0
1	H	392	3097	1961	522	600	14	0	0
1	I	392	3097	1961	522	600	14	0	0
1	J	392	3097	1961	522	600	14	0	0
1	K	392	3097	1961	522	600	14	0	0
1	L	392	3097	1961	522	600	14	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	ALA	-	expression tag	UNP P03728
A	538	ALA	-	expression tag	UNP P03728
A	539	ALA	-	expression tag	UNP P03728
A	540	LEU	-	expression tag	UNP P03728
A	541	GLU	-	expression tag	UNP P03728
A	542	HIS	-	expression tag	UNP P03728

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Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP P03728
A	544	HIS	-	expression tag	UNP P03728
A	545	HIS	-	expression tag	UNP P03728
A	546	HIS	-	expression tag	UNP P03728
A	547	HIS	-	expression tag	UNP P03728
B	537	ALA	-	expression tag	UNP P03728
B	538	ALA	-	expression tag	UNP P03728
B	539	ALA	-	expression tag	UNP P03728
B	540	LEU	-	expression tag	UNP P03728
B	541	GLU	-	expression tag	UNP P03728
B	542	HIS	-	expression tag	UNP P03728
B	543	HIS	-	expression tag	UNP P03728
B	544	HIS	-	expression tag	UNP P03728
B	545	HIS	-	expression tag	UNP P03728
B	546	HIS	-	expression tag	UNP P03728
B	547	HIS	-	expression tag	UNP P03728
C	537	ALA	-	expression tag	UNP P03728
C	538	ALA	-	expression tag	UNP P03728
C	539	ALA	-	expression tag	UNP P03728
C	540	LEU	-	expression tag	UNP P03728
C	541	GLU	-	expression tag	UNP P03728
C	542	HIS	-	expression tag	UNP P03728
C	543	HIS	-	expression tag	UNP P03728
C	544	HIS	-	expression tag	UNP P03728
C	545	HIS	-	expression tag	UNP P03728
C	546	HIS	-	expression tag	UNP P03728
C	547	HIS	-	expression tag	UNP P03728
D	537	ALA	-	expression tag	UNP P03728
D	538	ALA	-	expression tag	UNP P03728
D	539	ALA	-	expression tag	UNP P03728
D	540	LEU	-	expression tag	UNP P03728
D	541	GLU	-	expression tag	UNP P03728
D	542	HIS	-	expression tag	UNP P03728
D	543	HIS	-	expression tag	UNP P03728
D	544	HIS	-	expression tag	UNP P03728
D	545	HIS	-	expression tag	UNP P03728
D	546	HIS	-	expression tag	UNP P03728
D	547	HIS	-	expression tag	UNP P03728
E	537	ALA	-	expression tag	UNP P03728
E	538	ALA	-	expression tag	UNP P03728
E	539	ALA	-	expression tag	UNP P03728
E	540	LEU	-	expression tag	UNP P03728

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Chain	Residue	Modelled	Actual	Comment	Reference
E	541	GLU	-	expression tag	UNP P03728
E	542	HIS	-	expression tag	UNP P03728
E	543	HIS	-	expression tag	UNP P03728
E	544	HIS	-	expression tag	UNP P03728
E	545	HIS	-	expression tag	UNP P03728
E	546	HIS	-	expression tag	UNP P03728
E	547	HIS	-	expression tag	UNP P03728
F	537	ALA	-	expression tag	UNP P03728
F	538	ALA	-	expression tag	UNP P03728
F	539	ALA	-	expression tag	UNP P03728
F	540	LEU	-	expression tag	UNP P03728
F	541	GLU	-	expression tag	UNP P03728
F	542	HIS	-	expression tag	UNP P03728
F	543	HIS	-	expression tag	UNP P03728
F	544	HIS	-	expression tag	UNP P03728
F	545	HIS	-	expression tag	UNP P03728
F	546	HIS	-	expression tag	UNP P03728
F	547	HIS	-	expression tag	UNP P03728
G	537	ALA	-	expression tag	UNP P03728
G	538	ALA	-	expression tag	UNP P03728
G	539	ALA	-	expression tag	UNP P03728
G	540	LEU	-	expression tag	UNP P03728
G	541	GLU	-	expression tag	UNP P03728
G	542	HIS	-	expression tag	UNP P03728
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G	544	HIS	-	expression tag	UNP P03728
G	545	HIS	-	expression tag	UNP P03728
G	546	HIS	-	expression tag	UNP P03728
G	547	HIS	-	expression tag	UNP P03728
H	537	ALA	-	expression tag	UNP P03728
H	538	ALA	-	expression tag	UNP P03728
H	539	ALA	-	expression tag	UNP P03728
H	540	LEU	-	expression tag	UNP P03728
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H	543	HIS	-	expression tag	UNP P03728
H	544	HIS	-	expression tag	UNP P03728
H	545	HIS	-	expression tag	UNP P03728
H	546	HIS	-	expression tag	UNP P03728
H	547	HIS	-	expression tag	UNP P03728
I	537	ALA	-	expression tag	UNP P03728
I	538	ALA	-	expression tag	UNP P03728

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Chain	Residue	Modelled	Actual	Comment	Reference
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I	540	LEU	-	expression tag	UNP P03728
I	541	GLU	-	expression tag	UNP P03728
I	542	HIS	-	expression tag	UNP P03728
I	543	HIS	-	expression tag	UNP P03728
I	544	HIS	-	expression tag	UNP P03728
I	545	HIS	-	expression tag	UNP P03728
I	546	HIS	-	expression tag	UNP P03728
I	547	HIS	-	expression tag	UNP P03728
J	537	ALA	-	expression tag	UNP P03728
J	538	ALA	-	expression tag	UNP P03728
J	539	ALA	-	expression tag	UNP P03728
J	540	LEU	-	expression tag	UNP P03728
J	541	GLU	-	expression tag	UNP P03728
J	542	HIS	-	expression tag	UNP P03728
J	543	HIS	-	expression tag	UNP P03728
J	544	HIS	-	expression tag	UNP P03728
J	545	HIS	-	expression tag	UNP P03728
J	546	HIS	-	expression tag	UNP P03728
J	547	HIS	-	expression tag	UNP P03728
K	537	ALA	-	expression tag	UNP P03728
K	538	ALA	-	expression tag	UNP P03728
K	539	ALA	-	expression tag	UNP P03728
K	540	LEU	-	expression tag	UNP P03728
K	541	GLU	-	expression tag	UNP P03728
K	542	HIS	-	expression tag	UNP P03728
K	543	HIS	-	expression tag	UNP P03728
K	544	HIS	-	expression tag	UNP P03728
K	545	HIS	-	expression tag	UNP P03728
K	546	HIS	-	expression tag	UNP P03728
K	547	HIS	-	expression tag	UNP P03728
L	537	ALA	-	expression tag	UNP P03728
L	538	ALA	-	expression tag	UNP P03728
L	539	ALA	-	expression tag	UNP P03728
L	540	LEU	-	expression tag	UNP P03728
L	541	GLU	-	expression tag	UNP P03728
L	542	HIS	-	expression tag	UNP P03728
L	543	HIS	-	expression tag	UNP P03728
L	544	HIS	-	expression tag	UNP P03728
L	545	HIS	-	expression tag	UNP P03728
L	546	HIS	-	expression tag	UNP P03728
L	547	HIS	-	expression tag	UNP P03728

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	32688	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 ($e^-/Å^2$)	39.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4669. 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.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

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

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

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

6 Map analysis (i)

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

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

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

8 Map-model fit (i)

This section was not generated.