



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jun 4, 2019 – 06:28 PM EDT

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 wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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 ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

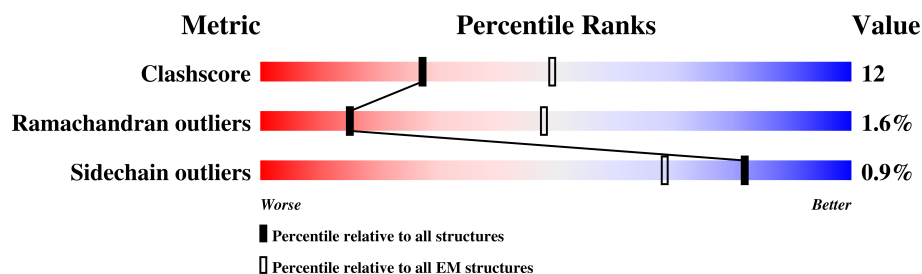
1 Overall quality at a glance

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 (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0a	309	79% 17%
1	0b	309	79% 17%
1	0c	309	79% 17%
1	0d	309	79% 17%
1	0e	309	79% 17%
1	0f	309	79% 17%
1	0g	309	79% 17%
1	0h	309	79% 17%
1	0i	309	79% 17%

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Mol	Chain	Length	Quality of chain
1	0j	309	 79% • 17%
1	0k	309	 79% • 17%
1	0l	309	 79% • 17%

2 Entry composition

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.

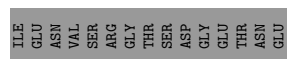
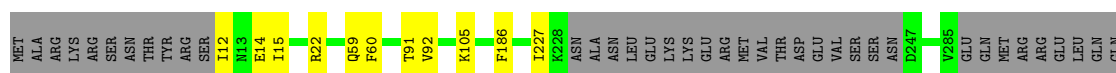
Mol	Chain	Residues	Atoms					AltConf	Trace
1	0a	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0b	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0c	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0d	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0e	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0f	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0g	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0h	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0i	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0j	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0k	256	Total 2097	C 1347	N 346	O 397	S 7	0	0
1	0l	256	Total 2097	C 1347	N 346	O 397	S 7	0	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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. 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. 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.

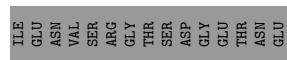
- Molecule 1: Portal protein

Chain 0a: 




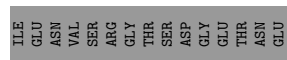
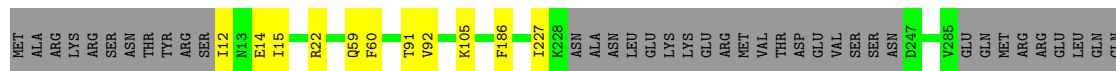
- Molecule 1: Portal protein

Chain 0b: 




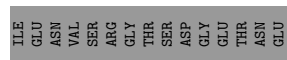
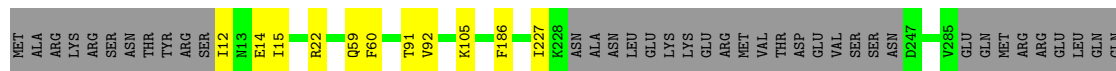
- Molecule 1: Portal protein

Chain 0c: 




- Molecule 1: Portal protein

Chain 0d: 




- Molecule 1: Portal protein

Chain 0e:  79% 17%

MET	ALA	ARG	ASN	LYS	ARG	SER	ASN	THR	TYR	ARG	SER	I112	N113	E114	I115	R222	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	ASP	GLU	ARG	MET	THR	THR	ASP	GLU	VAL	SER	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	ARG	SER	GLY	THR	SER	ASP	GLY	GLU	THR	ASN	GLU
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• Molecule 1: Portal protein

Chain 0f:  79% 17%

MET	ALA	ARG	ASN	LYS	ARG	SER	ASN	THR	TYR	ARG	SER	I112	N113	E114	I115	R222	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	ASP	GLU	ARG	MET	THR	THR	ASP	GLU	VAL	SER	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	ARG	SER	GLY	THR	SER	ASP	GLY	GLU	THR	ASN	GLU
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• Molecule 1: Portal protein

Chain 0g:  79% 17%

MET	ALA	ARG	ASN	LYS	ARG	SER	ASN	THR	TYR	ARG	SER	I112	N113	E114	I115	R222	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	ASP	GLU	ARG	MET	THR	THR	ASP	GLU	VAL	SER	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	ARG	SER	GLY	THR	SER	ASP	GLY	GLU	THR	ASN	GLU
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• Molecule 1: Portal protein

Chain 0h:  79% 17%

MET	ALA	ARG	ASN	LYS	ARG	SER	ASN	THR	TYR	ARG	SER	I112	N113	E114	I115	R222	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	ASP	GLU	ARG	MET	THR	THR	ASP	GLU	VAL	SER	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	ARG	SER	GLY	THR	SER	ASP	GLY	GLU	THR	ASN	GLU
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• Molecule 1: Portal protein

Chain 0i:  79% 17%

MET	ALA	ARG	ASN	LYS	ARG	SER	ASN	THR	TYR	ARG	SER	I112	N113	E114	I115	R222	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	ASP	GLU	ARG	MET	THR	THR	ASP	GLU	VAL	SER	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	ARG	SER	GLY	THR	SER	ASP	GLY	GLU	THR	ASN	GLU
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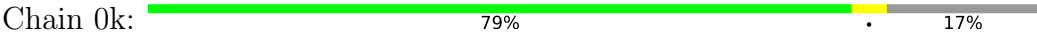
• Molecule 1: Portal protein

Chain 0j:  79% 17%

MET	ALA	ASN	LYS	ARG	ASN	THR	TYR	ASP	SER	I12	N13	E14	I15	R22	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	GLY	ARG	MET	THR	ASP	GLU	VAL	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	SER	ARG	GLY	THR	ASP	GLY	GLU	THR	ASN	GLU
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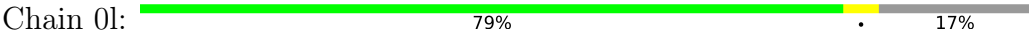
● Molecule 1: Portal protein



MET	ALA	ARG	LYS	ARG	ASN	THR	TYR	ASP	SER	I12	N13	E14	I15	R22	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	GLY	ARG	MET	THR	ASP	GLU	VAL	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	SER	ARG	GLY	THR	ASP	GLY	GLU	THR	ASN	GLU
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● Molecule 1: Portal protein



MET	ALA	ARG	LYS	ARG	ASN	THR	TYR	ASP	SER	I12	N13	E14	I15	R22	Q59	F60	T91	V92	K105	F186	I227	K228	ASN	ALA	ASN	LEU	GLU	LYS	GLY	ARG	MET	THR	ASP	GLU	VAL	SER	SER	ASN	D247	V285	GLU	GLN	MET	ARG	GLU	LEU	GLN
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ILE	GLU	ASN	VAL	SER	ARG	GLY	THR	ASP	GLY	GLU	THR	ASN	GLU
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

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	
		RMSZ	# Z >2	RMSZ	# Z >2
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	0l	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 mainchain 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	0f	0	5
1	0g	0	5
1	0h	0	5
1	0i	0	5
1	0j	0	5
1	0k	0	5
1	0l	0	5
All	All	0	60

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 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

5.2 Too-close contacts

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	0f	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
1	0k	2097	0	2047	0	0
1	0l	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

5.3.1 Protein backbone

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	0a	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0b	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0c	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0d	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0e	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0f	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0g	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0h	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0i	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0j	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0k	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
1	0l	252/309 (82%)	212 (84%)	36 (14%)	4 (2%)	11	50
All	All	3024/3708 (82%)	2544 (84%)	432 (14%)	48 (2%)	15	50

5 of 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

5.3.2 Protein sidechains

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	0a	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0b	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0c	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0d	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0e	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0f	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0g	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0h	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0i	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0j	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0k	228/277 (82%)	226 (99%)	2 (1%)	81	91
1	0l	228/277 (82%)	226 (99%)	2 (1%)	81	91
All	All	2736/3324 (82%)	2712 (99%)	24 (1%)	82	91

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0f	12	ILE
1	0g	227	ILE
1	0l	12	ILE
1	0f	227	ILE
1	0g	12	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	0f	167	ASN
1	0g	168	GLN
1	0l	88	ASN
1	0g	88	ASN
1	0h	88	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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.