



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 16, 2018 – 04:31 pm GMT

PDB ID : 3J2O
EMDB ID: : EMD-5528
Title : Model of the bacteriophage T4 fibritin based on the cryo-EM reconstruction of the contracted T4 tail containing the phage collar and whiskers
Authors : Fokine, A.; Zhang, Z.; Kanamaru, S.; Bowman, V.D.; Aksyuk, A.A.; Arisaka, F.; Rao, V.B.; Rossmann, M.G.
Deposited on : 2012-11-12
Resolution : 25.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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) : trunk30686

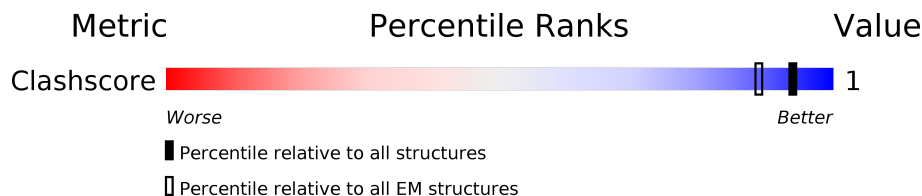
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY







The reported resolution of this entry is 25.00 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 (#Entries)	EM structures (#Entries)
Clashscore	136279	1886

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	A	486	 74% 26%
1	B	486	 74% 26%
1	C	486	 74% 26%
1	D	486	 30% 70%
1	E	486	 30% 70%
1	F	486	 30% 70%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1518 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 Fibrinin.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	362	Total 362	C 362	0	362
1	B	362	Total 362	C 362	0	362
1	C	362	Total 362	C 362	0	362
1	D	144	Total 144	C 144	0	144
1	E	144	Total 144	C 144	0	144
1	F	144	Total 144	C 144	0	144

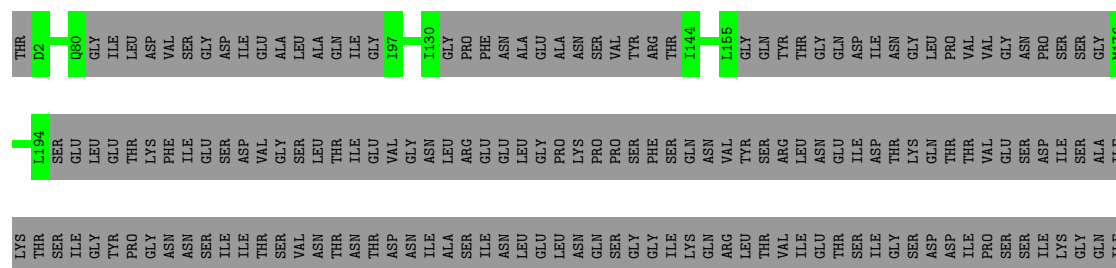
Category	Percentage
Green Segment	30%
Grey Segment	70%



Category	Percentage
Green	30%
Grey	70%



Category	Percentage
Red	30%
Grey	70%



LYS	ASP	ASN	THR	THR	SER	ILE	GLU	SER	SER	LEU	ASN	GLY	ILE	VAL	GLY	GLU	ASN	ASN	THR	SER	SER	GLY	LEU	ARG	ALA	ASN	VAL	SER	THR	LEU	ASN	GLN	ILE	ILE	VAL	GLY	GLY	GLY	GLN	PRO	PRO	SER	SER	PRO	PRO	PRO	GLY	GLY	SER	SER	LEU	LEU	ASN	ASN	ARG	VAL	VAL	SER	SER	THR	THR	ILE	GLU	GLU	THR	THR	VAL	VAL	SER	SER	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLY	LEU	ASN	ALA	ASN	VAL	GLN	ASN	LEU	GLN	VAL	GLU	ILE	GLY	ASN	ASN	SER	ALA	GLY	ILE	LYS	GLY	GLN	VAL	VAL	ALA	LEU	LEU	THR	THR	VAL	ASN	PRO	ASN	GLY	SER	THR	VAL	GLU	GLU	ARG	GLY	LEU	THR	ASN	LYS	ALA	ALA	GLU	THR	ASN	ILE	ILE	SER	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	GLN	GLU	VAL	ASN	THR	ALA	LYS	GLY	ASN	ILE	SER	SER	LEU	GLN	GLY	ASP	VAL	GLN	GLU	LEU	ALA	GLY	TYR	ILE	PRO	GLU	ALA	PRO	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	PHE	THR	PHE	LEU	SER	PRO	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	2727	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	phase flipping	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	39190	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	362	0	0	0	0
1	B	362	0	0	2	0
1	C	362	0	0	0	0
1	D	144	0	0	0	0
1	E	144	0	0	0	0
1	F	144	0	0	0	0
All	All	1518	0	0	2	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 1.

All (2) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:SER:CA	1:B:372:SER:CA	1.81	1.52
1:B:370:SER:CA	1:B:371:VAL:CA	2.54	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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.