



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:42 PM BST

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 wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

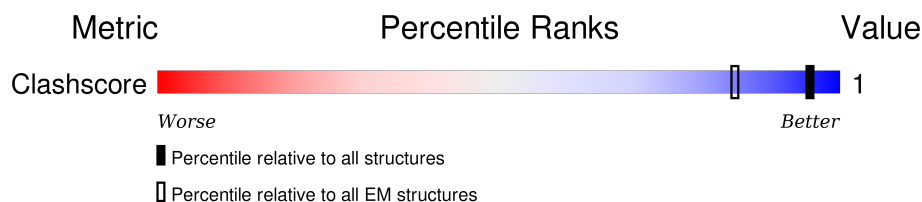
1 Overall quality at a glance

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	114402	924

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%

- Molecule 1: Fibrin

Category	Percentage
Red Segment	30%
Grey Segment	70%

- Molecule 1: Fibrin

Satisfaction Level	Percentage
Very satisfied	30%
Not very satisfied	70%

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

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

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	2727	Depositor
Resolution determination method	FSC at 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	38000	Depositor
Image detector	Not provided	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.