



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:34 PM BST

PDB ID : 2BSG
EMDB ID: : EMD-1126
Title : The modeled structure of fibrin (gpvac) of bacteriophage T4 based on cryo-EM reconstruction of the extended tail of bacteriophage T4
Authors : Kostyuchenko, V.A.; Chipman, P.R.; Leiman, P.G.; Arisaka, F.; Mesyanzhinov, V.V.; Rossmann, M.G.
Deposited on : 2005-05-20
Resolution : 15.00 Å(reported)
Based on PDB ID : 1AA0

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

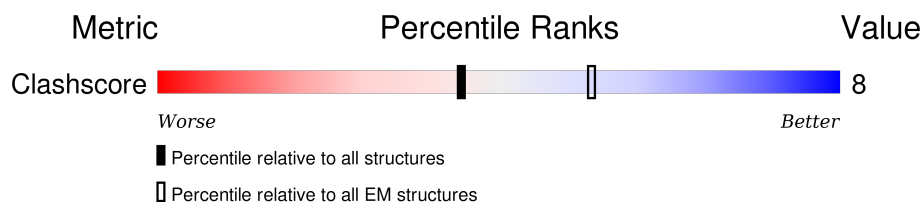
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 15.00 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	487	 74% • 25%
1	B	487	 74% • 25%
1	C	487	 74% • 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1089 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 FIBRITIN.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	363	Total 363	C 363	1	363
1	B	363	Total 363	C 363	1	363
1	C	363	Total 363	C 363	1	363

- Molecule 1: FIBRITIN

[illegible]

- Molecule 1: FIBRITIN

S348	L176	MET
I319	L194	THR
SER	SER	
LEU	GLU	980
ASN	LEU	GLY
ILE	GLU	ILE
GLY	THR	LEU
VAL	LYS	ASP
GLY	PHE	VAL
GLU	ILE	SER
ASN	GLU	GLY
THR	SER	ASP
SER	ASP	ILE
SER	VAL	GLU
GLY	GLY	ALA
L334	S208	LEU
V345	L220	ALA
GLY	GLY	GLN
THR	PRO	ILE
THR	PRO	GLY
ASP	LYS	197
SER	PRO	
SER	PRO	1130
GLY	SER	GLY
GLY	PHE	PRO
GLN	SER	PHE
PRO	GLN	ASN
SER	ASN	ALA
PRO	V231	GLU
PRO		ALA
GLY	L266	ASN
S359	GLY	SER
S370	THR	VAL
V371	PRO	TYR
S372	GLY	ARG
	ASN	THR
L483	S263	1144
SER		1155
PRO	E281	GLY
ALA	LEU	GLN
	ASN	TYR
	GLN	THR
	SER	GLY
	GLY	GLN
	GLY	ASP
	L288	ILE
		ASN
	L299	GLY
	SER	LEU
	SER	PRO
	ASP	VAL
	ASP	VAL
	ILE	GLY
	PRO	ASN
	SER	PRO
	SER	SER
	L308	GLY

- Molecule 1: FIBRITIN

S318	L319	GLU	SER	LEU	ASN	GLY	ILE	VAL	GLY	GLU	ASN	THR	SER	SER	SER	GLY	GLN	PRO	PRO	PRO	GLY	L360	L483	SER	PRO	ALA																							
M176	L1494	SER	GLU	LEU	THR	LVS	PHE	ILE	GLU	VAL	GLY	S208	L220	PRO	PRO	PRO	PHE	SER	GLN	ASN	V231	L256	THR	GLY	ASN	S263	E281	LEU	ASN	GLN	SER	GLY	GLY	L268	L299	SER	SER	ASP	ASP	ILE	PRO	SER	SER	I308					
MET	THR	D2	Q80	GLY	ILE	LEU	ASP	VAL	SER	GLY	ASP	ILE	GLU	ALA	LEU	ALA	GLN	ILE	GLY	I97	I130	GLY	PRO	PHE	ASN	ALA	GLU	ALA	ASN	VAL	THR	THR	I144	I155	GLY	GLN	THR	GLY	GLN	ASP	ILE	ASN	LEU	VAL	VAL	GLY	PRO	SER	GLY

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	PHILIPS CM300 FEG	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	3.2	Depositor
Magnification	45000	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	363	0	0	3	0
1	B	363	0	0	3	0
1	C	363	0	0	3	0
All	All	1089	0	0	9	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 8.

All (9) 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	1.56
1:A:344:ILE:CA	1:A:360:LEU:CA	1.84	1.49
1:A:318:SER:CA	1:A:334:LEU:CA	2.33	1.06
1:B:370:SER:CA	1:B:371:VAL:CA	2.54	0.85
1:B:318:SER:CA	1:B:334:LEU:CA	2.71	0.69
1:C:318:SER:CA	1:C:334:LEU:CA	2.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:CA	1:A:359:SER:CA	2.81	0.59
1:C:344:ILE:CA	1:C:360:LEU:CA	2.84	0.55
1:C:319:ILE:CA	1:C:334:LEU:CA	2.89	0.51

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 ⓘ

There are no chain breaks in this entry.