



wwPDB EM Validation Summary Report ⓘ

Jun 28, 2026 – 12:31 AM JST

PDB ID : 21DI / pdb_000021di
EMDB ID : EMD-67586
Title : Cryo-EM reconstruction of the cyanophage Pam5 small terminase
Authors : Dong, D.Q.; Jiang, Y.L.; Zhou, C.Z.
Deposited on : 2025-12-09
Resolution : 3.50 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

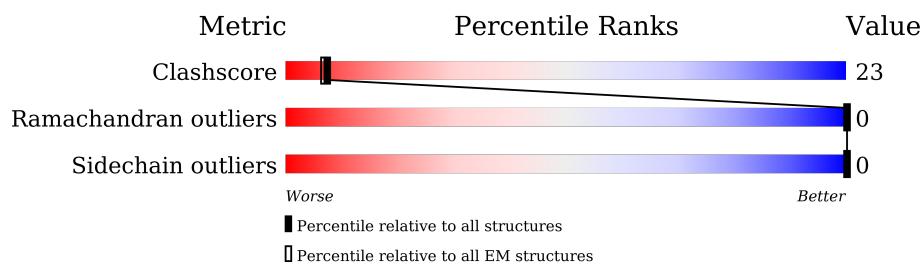
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	134	23% 16% 60%
1	B	134	23% 16% 60%
1	C	134	23% 16% 60%
1	D	134	24% 16% 60%
1	E	134	24% 16% 60%
1	F	134	25% 15% 60%
1	G	134	28% 12% 60%
1	H	134	24% 16% 60%
1	I	134	26% 13% 60%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3753 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.

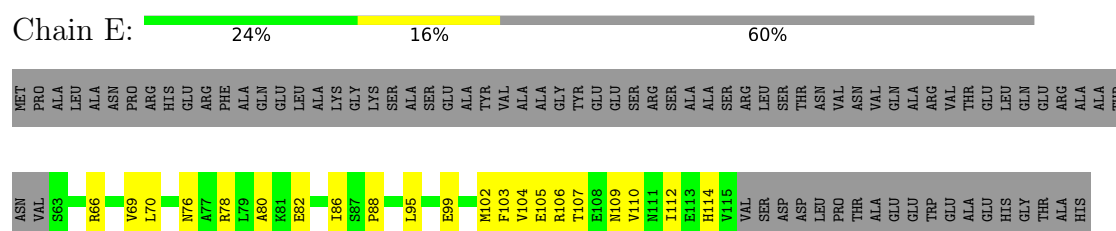
- Molecule 1 is a protein called Pam5 small terminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	A	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	B	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	C	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	D	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	F	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	G	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	H	53	Total	C	N	O	S	0	0
			417	259	74	83	1		
1	I	53	Total	C	N	O	S	0	0
			417	259	74	83	1		

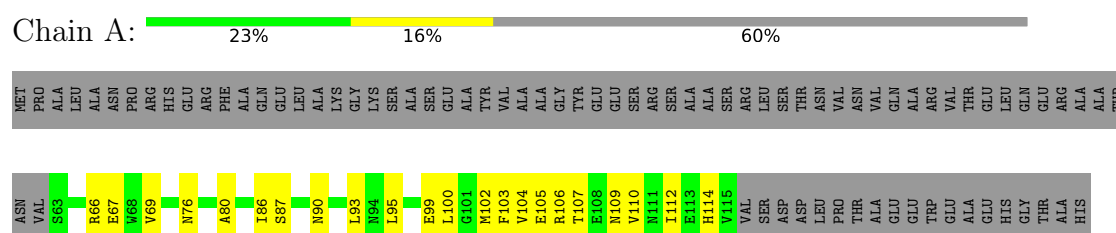
3 Residue-property plots

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

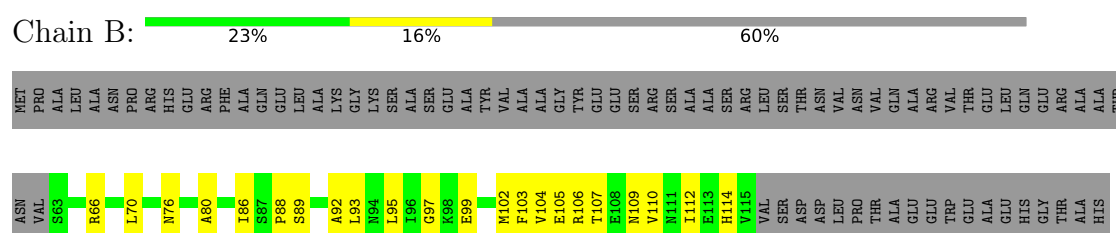
- Molecule 1: Pam5 small terminase



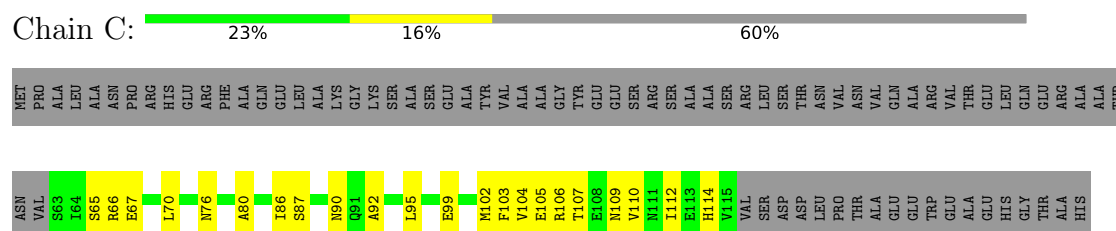
- Molecule 1: Pam5 small terminase



- Molecule 1: Pam5 small terminase



- Molecule 1: Pam5 small terminase



- Molecule 1: Pam5 small terminase

Chain D:  24% 16% 60%

MET	PRO	ALA	LEU	ALA	ASN	PRO	ARG	HIS	GLU	ARG	PHE	ALA	GLN	LEU	ALA	LYS	GLY	LYS	SER	ALA	SER	GLU	GLU	TYR	VAL	ALA	ALA	GLY	TYR	GLU	GLU	SER	SER	ARG	SER	ALA	ALA	SER	VAL	ARG	LEU	SER	SER	LEU	THR	ASN	VAL	VAL	VAL	GLN	ALA	ARG	VAL	THR	THR	GLU	LEU	GLN	GLU	ARG	ALA	ALA
ASN	VAL	S63	R66	L70	N76	A80	I86	N90	N94	L95	I96	G97	E99	L100	G101	M102	F103	V104	E105	R106	T107	E108	N109	V110	N111	I112	E113	H114	V115	VAL	SER	ASP	ASP	LEU	PRO	THR	THR	ALA	ALA	GLU	GLU	TRP	GLU	ALA	VAL	THR	GLU	HIS	THR	GLY	THR	ALA	ALA	ALA	THR							

- Molecule 1: Pam5 small terminase

Chain F:  25% 15% 60%

MET	PRO	ALA	LEU	ALA	ASN	PRO	ARG	HIS	GLU	ARG	PHE	ALA	GLN	LEU	LEU	LYS	GLY	LYS	SER	SER	ALA	GLU	ALA	TYR	VAL	ALA	ALA	GLY	TYR	GLU	GLU	SER	ARG	SER	ALA	ALA	SER	VAL	ARG	LEU	SER	SER	LEU	THR	ASN	VAL	VAL	ASN	VAL	GLN	GLU	GLU	TRP	ALA	GLU	GLU	VAL	THR	GLY	THR	ALA	ALA	HIS
ASN	VAL	S63	R66	L70	N76	A80	I86	S89	N94	L95	I96	G97	E99	M102	F103	V104	E105	R106	T107	E108	N109	V110	N111	I112	E113	H114	V115	VAL	SER	ASP	ASP	LEU	PRO	THR	THR	ALA	ASN	VAL	GLU	GLU	TRP	GLU	ALA	GLU	GLU	HIS	THR	GLU	THR	ALA	ALA	ALA	HIS										

- Molecule 1: Pam5 small terminase

Chain G:  28% 12% 60%

MET	PRO	ALA	LEU	ALA	ASN	PRO	ARG	HIS	GLU	PHE	ALA	GLN	LEU	LEU	LYS	GLY	LYS	SER	SER	ALA	GLU	ALA	ALA	ALA	GLY	TYR	GLU	GLU	SER	SER	ASP	LEU	ARG	SER	SER	ALA	ALA	SER	VAL	ARG	LEU	SER	SER	LEU	THR	ASN	VAL	VAL	ASN	VAL	GLN	GLU	GLU	VAL	THR	GLU	GLN	ARG	ALA	ALA
ASN	VAL	S63	R66	A80	I86	N90	L95	L100	G101	M102	F103	V104	E105	R106	T107	E108	N109	V110	N111	I112	E113	H114	V115	VAL	SER	ASP	ASP	LEU	THR	ALA	ALA	GLU	GLU	TRP	ALA	HIS	GLY	THR	ALA	HIS	GLU	THR	ALA	HIS																

- Molecule 1: Pam5 small terminase

Chain H:  24% 16% 60%

MET	PRO	ALA	LEU	ALA	ASN	PRO	ARG	HIS	GLU	PHE	ALA	GLN	LEU	LEU	LYS	GLY	LYS	SER	SER	ALA	GLU	ALA	TYR	VAL	ALA	ALA	GLY	TYR	GLU	GLU	SER	ARG	SER	ALA	ALA	SER	VAL	ARG	LEU	SER	SER	LEU	THR	ASN	VAL	VAL	ASN	VAL	GLN	GLU	GLU	TRP	GLU	ALA	GLU	GLU	VAL	THR	GLY	THR	GLU	GLU	GLN	ARG	VAL	THR	GLU	GLU	ARG	ALA	ALA	THR
ASN	VAL	S63	I64	S65	R66	E67		N76	A77	R78	L79	A80	R81	E82		I86		L95	I96	G97		M102	F103	V104	E105	R106	T107	E108	N109	V110	N111	I112	E113	H114	V115	VAL	SER	ASP	ASP	LEU	PRO	THR	THR	ALA	GLU	GLU	TRP	GLU	ALA	ALA	GLU	HIS	THR	GLY	THR	ALA	ALA	ALA	HIS													

- Molecule 1: Pam5 small terminase

Chain I:  26% 13% 60%

MET	PRO	ALA	LEU	ALA	ASN	PRO	ARG	HIS	GLU	PHE	ALA	GLN	LEU	LEU	LYS	GLY	LYS	SER	SER	ALA	GLU	ALA	TYR	VAL	ALA	ALA	GLY	TYR	GLU	GLU	SER	ARG	SER	ALA	ALA	SER	VAL	ARG	LEU	SER	SER	LEU	THR	ASN	VAL	VAL	ASN	VAL	GLN	GLY	THR	ALA	VAL	THR	GLU	GLN	ARG	ALA	ALA
ASN	VAL	S63	R66	L70	N76	A80	I86	L95	E99	L100	G101	M102	F103	V104	E105	R106	T107	E108	N109	V110	N111	I112	E113	H114	V115	VAL	SER	ASP	ASP	LEU	PRO	THR	THR	ALA	GLU	GLU	TRP	GLU	ALA	GLU	GLU	HIS	GLY	THR	THR	ALA	ALA	HIS											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	906838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/421	0.32	0/568
1	B	0.14	0/421	0.31	0/568
1	C	0.15	0/421	0.33	0/568
1	D	0.15	0/421	0.34	0/568
1	E	0.14	0/421	0.33	0/568
1	F	0.15	0/421	0.33	0/568
1	G	0.16	0/421	0.35	0/568
1	H	0.15	0/421	0.34	0/568
1	I	0.14	0/421	0.33	0/568
All	All	0.15	0/3789	0.33	0/5112

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 [i](#)

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	417	0	415	35	0
1	B	417	0	415	36	0
1	C	417	0	415	41	0
1	D	417	0	415	36	0
1	E	417	0	415	37	0
1	F	417	0	415	32	0
1	G	417	0	415	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	417	0	415	31	0
1	I	417	0	415	35	0
All	All	3753	0	3735	174	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 23.

The worst 5 of 174 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:E:80:ALA:HB2	1:A:86:ILE:HG21	1.63	0.80
1:B:70:LEU:HD11	1:B:99:GLU:HG2	1.61	0.79
1:E:105:GLU:HB3	1:A:107:THR:HA	1.67	0.77
1:B:80:ALA:HB2	1:C:86:ILE:HG21	1.65	0.76
1:H:80:ALA:HB2	1:I:86:ILE:HG21	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	51/134 (38%)	47 (92%)	4 (8%)	0	100	100
1	B	51/134 (38%)	45 (88%)	6 (12%)	0	100	100
1	C	51/134 (38%)	45 (88%)	6 (12%)	0	100	100
1	D	51/134 (38%)	46 (90%)	5 (10%)	0	100	100
1	E	51/134 (38%)	47 (92%)	4 (8%)	0	100	100
1	F	51/134 (38%)	47 (92%)	4 (8%)	0	100	100
1	G	51/134 (38%)	44 (86%)	7 (14%)	0	100	100
1	H	51/134 (38%)	44 (86%)	7 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	51/134 (38%)	44 (86%)	7 (14%)	0	100	100
All	All	459/1206 (38%)	409 (89%)	50 (11%)	0	100	100

There are no Ramachandran outliers to report.

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	A	46/108 (43%)	46 (100%)	0	100	100
1	B	46/108 (43%)	46 (100%)	0	100	100
1	C	46/108 (43%)	46 (100%)	0	100	100
1	D	46/108 (43%)	46 (100%)	0	100	100
1	E	46/108 (43%)	46 (100%)	0	100	100
1	F	46/108 (43%)	46 (100%)	0	100	100
1	G	46/108 (43%)	46 (100%)	0	100	100
1	H	46/108 (43%)	46 (100%)	0	100	100
1	I	46/108 (43%)	46 (100%)	0	100	100
All	All	414/972 (43%)	414 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	D	91	GLN
1	F	90	ASN
1	I	76	ASN

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 oligosaccharides 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.