

Jan 14, 2024 – 12:06 AM JST

PDB ID	:	8KGE
EMDB ID	:	EMD-37218
Title	:	Dimeric tail tube protein gpVs of bacteriophage lambda
Authors	:	Wang, J.W.
Deposited on		
Resolution	:	3.80 Å(reported)

This is a Full wwPDB EM Validation 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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.80 Å.

Sidechain outliers

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	Percentile Ranl	ks Value		
Ramachandran outliers		0.2%		
Sidechain outliers 💻	11.7%			
Worse		Better		
Percentil	le relative to all structures			
Percentil	le relative to all EM structures			
Metric	Whole archive	EM structures		
IVIEUI IC	$(\# { m Entries})$	$(\# { m Entries})$		
Ramachandran outliers	154571	4023		

154315

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 <=5%

3826

Mol	Chain	Length	Quality of chain					
1	V	246	91%	8%	·			
1	V	246	88%	11%	·			



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3584 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	243	Total 1792	C 1119		-		0	0
1		949	Total				-	0	0
1 V	243	1792	1119	302	366	5	0	0	

• Molecule 1 is a protein called Tail tube protein.



3 Residue-property plots (i)

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: Tail tube protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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		
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	V	0.28	0/1827	0.61	1/2494~(0.0%)	
1	V	0.27	0/1827	0.57	0/2494	
All	All	0.28	0/3654	0.59	1/4988~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	V	168	PRO	N-CD-CG	-6.87	92.89	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	V	241/246~(98%)	218 (90%)	23 (10%)	0	100 100		

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Mol	Chain	Analysed Favoured Allowed		Outliers	Percentiles	
1	V	241/246~(98%)	218 (90%)	22 (9%)	1 (0%)	34 70
All	All	482/492~(98%)	436 (90%)	45~(9%)	1 (0%)	50 79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	169	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Analysed Rotameric Outliers		Percentiles		
1	V	193/196~(98%)	174 (90%)	19 (10%)		8	33
1	V	193/196~(98%)	167~(86%)	26 (14%)		4	22
All	All	386/392~(98%)	341 (88%)	45 (12%)		9	27

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	23	SER
1	V	33	ASP
1	V	46	THR
1	V	59	TYR
1	V	64	ASP
1	V	84	LEU
1	V	111	ARG
1	V	121	ARG
1	V	127	ILE
1	V	131	VAL
1	V	132	THR
1	V	157	THR
1	V	177	GLN
1	V	193	LYS
1	V	196	ARG

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Mol	Chain	Res	Type
1	V	212	MET
1	V	215	THR
1	V	232	ASN
1	V	240	GLU
1	V	21	LYS
1	V	38	ARG
1	V	51	THR
1	V	70	THR
1	V	79	ASP
1	V	83	THR
1	V	84	LEU
1	V	87	MET
1	V	97	LEU
1	V	119	VAL
1	V	125	SER
1	V	138	THR
1	V	148	ARG
1	V	156	SER
1	V	157	THR
1	V	164	MET
1	V	167	THR
1	V	180	THR
1	V	183	VAL
1	V	192	ASP
1	V	193	LYS
1	V	195	PHE
1	V	196	ARG
1	V	201	ASP
1	V	210	SER
1	V	228	VAL

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	177	GLN

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 monosaccharides 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.

