



## Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 02:19 PM JST

PDB ID : 8KGE / pdb\_00008kge  
EMDB ID : EMD-37218  
Title : Dimeric tail tube protein gpVs of bacteriophage lambda  
Authors : Wang, J.W.  
Deposited on : 2023-08-18  
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](mailto: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>.

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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 Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

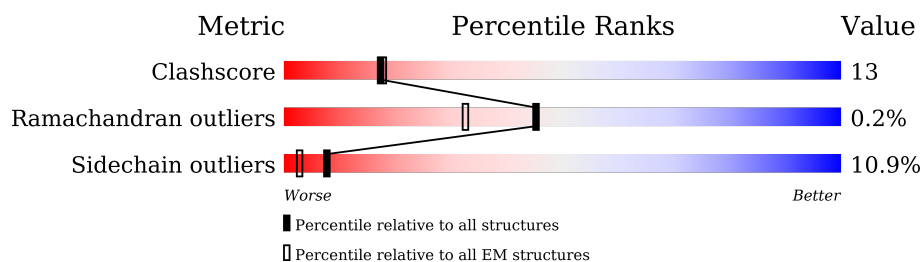
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	V	246	
1	v	246	

## 2 Entry composition

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.

- Molecule 1 is a protein called Tail tube protein.

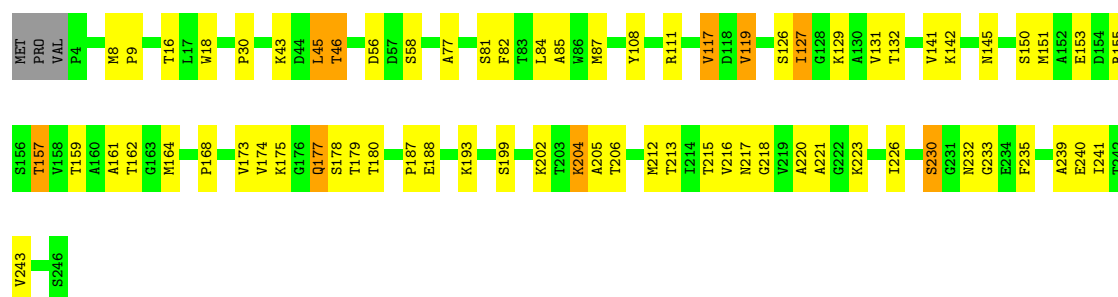
Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		
1	v	243	Total	C	N	O	S	0	0
			1792	1119	302	366	5		

### 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.

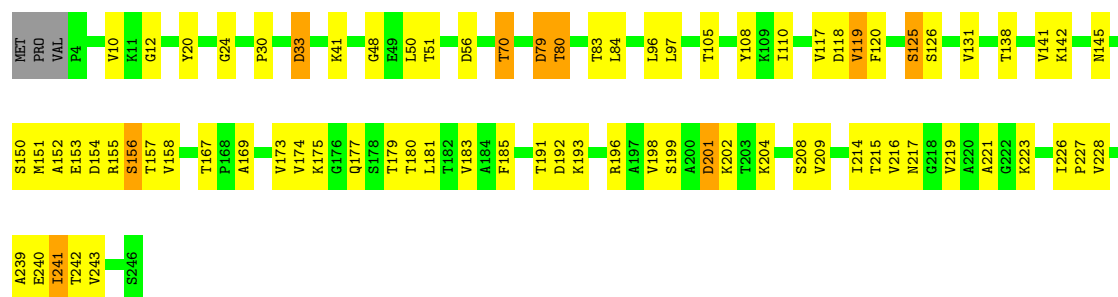
- Molecule 1: Tail tube protein

Chain V: 



- Molecule 1: Tail tube protein

Chain v: 



## 4 Experimental information

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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	V	0.17	0/1827	0.50	2/2494 (0.1%)
1	v	0.13	0/1827	0.42	0/2494
All	All	0.16	0/3654	0.46	2/4988 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	168	PRO	N-CD-CG	-6.87	92.89	103.20
1	V	168	PRO	CA-N-CD	-5.26	104.64	112.00

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	V	1792	0	1760	50	0
1	v	1792	0	1760	48	0
All	All	3584	0	3520	95	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 13.

All (95) 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:v:173:VAL:HG21	1:v:241:ILE:HG23	1.61	0.82
1:V:199:SER:HA	1:V:226:ILE:HG22	1.64	0.78
1:v:208:SER:HB3	1:v:215:THR:HB	1.65	0.78
1:V:177:GLN:NE2	1:V:216:VAL:O	2.21	0.73
1:V:151:MET:HA	1:V:151:MET:HE3	1.76	0.68
1:V:180:THR:OG1	1:V:213:THR:OG1	2.10	0.67
1:V:173:VAL:HB	1:V:177:GLN:HG2	1.76	0.66
1:V:177:GLN:HB3	1:V:217:ASN:HA	1.78	0.66
1:v:30:PRO:HB2	1:v:117:VAL:HG21	1.78	0.65
1:V:8:MET:HG3	1:V:9:PRO:HD2	1.79	0.65
1:V:129:LYS:NZ	1:v:118:ASP:OD2	2.30	0.64
1:V:126:SER:HB3	1:V:142:LYS:HB3	1.78	0.64
1:v:174:VAL:HG22	1:v:175:LYS:HG2	1.80	0.63
1:V:205:ALA:HA	1:V:218:GLY:HA2	1.81	0.63
1:v:96:LEU:HD11	1:v:141:VAL:HG21	1.80	0.62
1:v:201:ASP:OD2	1:v:204:LYS:N	2.30	0.61
1:V:178:SER:HA	1:V:216:VAL:O	2.00	0.61
1:V:30:PRO:HB2	1:V:117:VAL:HG21	1.81	0.61
1:v:173:VAL:HG13	1:v:177:GLN:HG2	1.83	0.60
1:v:151:MET:O	1:v:155:ARG:NH2	2.35	0.60
1:V:221:ALA:HA	1:V:243:VAL:HB	1.84	0.60
1:V:240:GLU:O	1:V:241:ILE:HD13	2.01	0.60
1:V:45:LEU:HD23	1:V:82:PHE:HB3	1.83	0.60
1:V:108:TYR:OH	1:V:145:ASN:OD1	2.18	0.59
1:V:177:GLN:HE22	1:V:179:THR:HG22	1.66	0.59
1:v:126:SER:HB3	1:v:142:LYS:HB3	1.82	0.59
1:V:212:MET:HA	1:V:212:MET:HE3	1.84	0.58
1:v:221:ALA:HA	1:v:243:VAL:O	2.04	0.57
1:v:199:SER:HA	1:v:226:ILE:HG22	1.87	0.57
1:v:226:ILE:HD12	1:v:226:ILE:O	2.04	0.56
1:v:201:ASP:O	1:v:202:LYS:HG2	2.06	0.55
1:v:177:GLN:NE2	1:v:179:THR:OG1	2.34	0.54
1:v:48:GLY:N	1:v:80:THR:OG1	2.33	0.54
1:v:118:ASP:HB3	1:v:120:PHE:HE1	1.73	0.54
1:V:127:ILE:O	1:v:50:LEU:N	2.41	0.53
1:v:108:TYR:OH	1:v:145:ASN:ND2	2.42	0.53
1:v:173:VAL:HB	1:v:243:VAL:HA	1.92	0.52
1:V:164:MET:HE1	1:V:230:SER:HB3	1.93	0.51
1:V:174:VAL:HG12	1:V:175:LYS:N	2.26	0.51
1:v:181:LEU:HB2	1:v:214:ILE:HB	1.92	0.51
1:V:177:GLN:HE22	1:V:179:THR:H	1.59	0.51
1:V:162:THR:HA	1:V:235:PHE:CZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:10:VAL:HG13	1:v:12:GLY:H	1.76	0.50
1:V:161:ALA:HB3	1:V:187:PRO:HG3	1.94	0.50
1:V:119:VAL:HG13	1:V:150:SER:HB3	1.93	0.50
1:v:151:MET:HE3	1:v:152:ALA:H	1.76	0.50
1:v:173:VAL:HG11	1:v:243:VAL:HG22	1.94	0.49
1:V:226:ILE:HD12	1:V:226:ILE:O	2.13	0.49
1:v:150:SER:OG	1:v:155:ARG:NH2	2.35	0.49
1:v:119:VAL:HG13	1:v:150:SER:HB3	1.96	0.48
1:V:151:MET:HB3	1:V:153:GLU:HG2	1.95	0.48
1:V:204:LYS:HA	1:V:220:ALA:HB3	1.95	0.48
1:V:178:SER:CA	1:V:216:VAL:O	2.62	0.47
1:V:178:SER:H	1:V:217:ASN:HA	1.79	0.47
1:V:202:LYS:NZ	1:V:202:LYS:HB3	2.29	0.47
1:V:177:GLN:HB3	1:V:178:SER:H	1.60	0.46
1:V:16:THR:OG1	1:V:18:TRP:NE1	2.45	0.46
1:v:41:LYS:HD2	1:v:41:LYS:HA	1.68	0.46
1:v:20:TYR:OH	1:v:24:GLY:N	2.49	0.46
1:V:43:LYS:H	1:V:84:LEU:HA	1.82	0.45
1:v:125:SER:O	1:v:125:SER:OG	2.34	0.45
1:V:206:THR:HG23	1:V:217:ASN:OD1	2.16	0.45
1:v:209:VAL:HG22	1:v:214:ILE:HD12	1.98	0.45
1:V:177:GLN:HE21	1:V:216:VAL:C	2.25	0.44
1:V:233:GLY:HA3	1:v:196:ARG:NH2	2.32	0.44
1:v:185:PHE:HB2	1:v:191:THR:HG21	1.98	0.44
1:V:223:LYS:NZ	1:V:223:LYS:HB2	2.33	0.44
1:V:173:VAL:HG12	1:V:177:GLN:OE1	2.18	0.44
1:V:226:ILE:HD11	1:V:239:ALA:HB3	1.98	0.44
1:v:151:MET:HE3	1:v:151:MET:HA	2.00	0.44
1:V:155:ARG:H	1:V:155:ARG:HG3	1.52	0.43
1:v:33:ASP:OD2	1:v:33:ASP:N	2.51	0.43
1:v:192:ASP:OD1	1:v:192:ASP:N	2.52	0.43
1:V:85:ALA:HB3	1:V:87:MET:HE3	2.00	0.43
1:v:198:VAL:O	1:v:227:PRO:HD2	2.19	0.43
1:v:153:GLU:O	1:v:156:SER:OG	2.36	0.43
1:v:153:GLU:OE1	1:v:153:GLU:N	2.51	0.43
1:V:111:ARG:HE	1:V:111:ARG:HB3	1.75	0.42
1:V:177:GLN:NE2	1:V:179:THR:H	2.15	0.42
1:V:46:THR:HG23	1:V:81:SER:HB2	2.01	0.42
1:v:56:ASP:HA	1:v:70:THR:HG22	2.00	0.42
1:v:196:ARG:HD3	1:v:196:ARG:C	2.44	0.42
1:V:187:PRO:O	1:V:188:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:226:ILE:HD11	1:v:239:ALA:HB3	2.02	0.42
1:v:223:LYS:HG3	1:v:242:THR:HG22	2.02	0.41
1:v:79:ASP:N	1:v:79:ASP:OD1	2.53	0.41
1:v:177:GLN:HB3	1:v:217:ASN:HA	2.01	0.41
1:v:240:GLU:O	1:v:241:ILE:HD13	2.19	0.41
1:V:155:ARG:O	1:V:157:THR:OG1	2.38	0.41
1:v:173:VAL:HA	1:v:177:GLN:CD	2.46	0.41
1:V:177:GLN:NE2	1:V:179:THR:HG22	2.34	0.41
1:v:241:ILE:HD13	1:v:241:ILE:HA	1.89	0.41
1:V:56:ASP:OD1	1:V:58:SER:OG	2.37	0.40
1:v:154:ASP:OD1	1:v:154:ASP:N	2.51	0.40
1:V:77:ALA:HB3	1:V:145:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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
1	v	241/246 (98%)	218 (90%)	22 (9%)	1 (0%)	30	63
All	All	482/492 (98%)	436 (90%)	45 (9%)	1 (0%)	45	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	v	169	ALA

### 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	V	193/196 (98%)	177 (92%)	16 (8%)	9	32
1	v	193/196 (98%)	167 (86%)	26 (14%)	3	18
All	All	386/392 (98%)	344 (89%)	42 (11%)	8	22

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	45	LEU
1	V	46	THR
1	V	117	VAL
1	V	119	VAL
1	V	127	ILE
1	V	131	VAL
1	V	132	THR
1	V	141	VAL
1	V	157	THR
1	V	159	THR
1	V	177	GLN
1	V	193	LYS
1	V	204	LYS
1	V	215	THR
1	V	230	SER
1	V	232	ASN
1	v	33	ASP
1	v	51	THR
1	v	70	THR
1	v	79	ASP
1	v	80	THR
1	v	83	THR
1	v	84	LEU
1	v	97	LEU
1	v	105	THR
1	v	110	ILE
1	v	119	VAL

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Mol	Chain	Res	Type
1	v	125	SER
1	v	131	VAL
1	v	138	THR
1	v	156	SER
1	v	157	THR
1	v	158	VAL
1	v	167	THR
1	v	180	THR
1	v	183	VAL
1	v	193	LYS
1	v	201	ASP
1	v	216	VAL
1	v	219	VAL
1	v	228	VAL
1	v	241	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	177	GLN
1	V	232	ASN
1	v	72	GLN
1	v	94	GLN
1	v	101	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.