



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:20 AM UTC

PDB ID : 6EU4 / pdb_00006eu4
Title : Structure of Acinetobacter phage vb_AbaP_AS12 gp42 tailspike
Authors : Taylor, N.M.I.; Shneider, M.M.; Leiman, P.G.
Deposited on : 2017-10-27
Resolution : 1.79 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

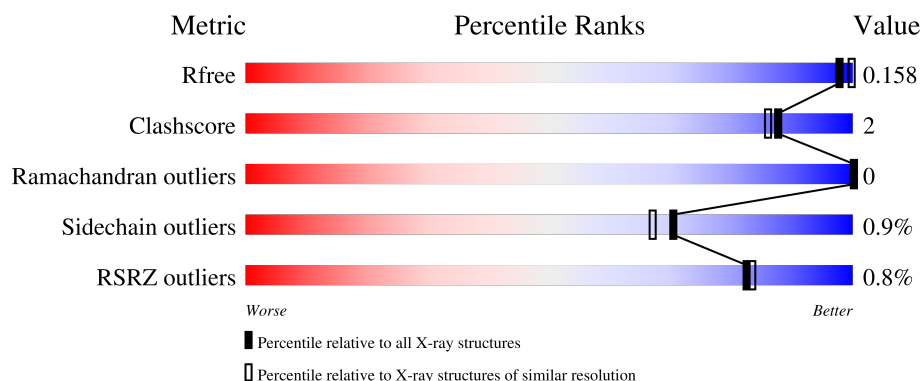
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	716	% 77% 5% 18%
1	B	716	78% • 18%
1	C	716	% 77% 5% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28742 atoms, of which 13118 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 spike protein.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	587	Total	C	H	N	O	S	Se		0	14	0
			8899	2860	4387	746	884	11	11				
1	B	587	Total	C	H	N	O	S	Se		0	12	0
			8857	2848	4362	744	881	11	11				
1	C	587	Total	C	H	N	O	S	Se		0	12	0
			8866	2850	4369	743	882	11	11				

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A218KRF6
A	2	SER	-	expression tag	UNP A0A218KRF6
A	3	GLY	-	expression tag	UNP A0A218KRF6
A	4	SER	-	expression tag	UNP A0A218KRF6
A	5	THR	-	expression tag	UNP A0A218KRF6
B	1	GLY	-	expression tag	UNP A0A218KRF6
B	2	SER	-	expression tag	UNP A0A218KRF6
B	3	GLY	-	expression tag	UNP A0A218KRF6
B	4	SER	-	expression tag	UNP A0A218KRF6
B	5	THR	-	expression tag	UNP A0A218KRF6
C	1	GLY	-	expression tag	UNP A0A218KRF6
C	2	SER	-	expression tag	UNP A0A218KRF6
C	3	GLY	-	expression tag	UNP A0A218KRF6
C	4	SER	-	expression tag	UNP A0A218KRF6
C	5	THR	-	expression tag	UNP A0A218KRF6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	710	Total 710	O 710	0	0
3	B	723	Total 723	O 723	0	0
3	C	686	Total 686	O 686	0	0

T326	ALA	TYR
	ILE	SER
N336	ALA	GLU
	LEU	LEU
E344	LYS	ASN
	GLY	CYS
G385	LEU	PHE
	GLU	VAL
E410	ASN	VAL
	ALA	ALA
E420	ARG	GLY
	TYR	ILE
Y454	HIS	ASP
Y455	PHE	TYR
K456	GLY	ARG
	VAL	LEU
R459	ILE	LEU
	ALA	SER
L475	ALA	LEU
	GLN	LEU
H588	ILE	GLU
Y569	MSE	ILE
R570	GLN	ILE
D571	CYS	GLN
	PHE	CYS
Y602	THR	PHE
	ASP	THR
SER	ASP	THR
ALA	GLY	TYR
ARG	LEU	GLY
LYS	ASP	LEU
LYS	TRP	ASP
SER	SER	TRP
GLU	LYS	SER
VAL	TYR	LYS
SER	GLY	TYR
GLU	ILE	GLY
LEU	ILE	ILE
THR	THR	ILE
GLU	TYR	THR
GLU	ASP	TYR
GLU	GLU	ASP
LYS	TRP	GLU
CYS	ASP	GLU
ALA	ASN	ASP
VAL	THR	ASN
ALA	GLU	THR
CYS	GLY	GLU
GLY	GLY	GLY
LYS	ILE	ILE
LEU	GLU	ILE
TYR	ALA	GLU
ARG	GLY	ALA
LYS	ASN	GLY
TYR	ILE	ASN
LYS	TYR	ILE
LEU	MSE	TYR
ASN	VAL	MSE
ASP	ARG	VAL

TYR
SER
GLU
LEU
ASN
CYS
PHE
VAL
ASN
ALA
GLY
ILE
ASP
TYR
ARG
LEU
SER
LEU
LEU
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.20Å 143.34Å 176.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.77 – 1.79 47.77 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.77-1.79) 99.5 (47.77-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.79Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.125 , 0.146 0.140 , 0.158	Depositor DCC
R_{free} test set	10966 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28742	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.34	0/4651	0.54	0/6323
1	B	0.35	0/4629	0.55	0/6294
1	C	0.34	0/4633	0.54	0/6298
All	All	0.34	0/13913	0.54	0/18915

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	4512	4387	4386	21	0
1	B	4495	4362	4352	18	0
1	C	4497	4369	4369	18	0
2	A	1	0	0	0	0
3	A	710	0	0	4	4
3	B	723	0	0	4	1
3	C	686	0	0	3	3
All	All	15624	13118	13107	53	4

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 2.

The worst 5 of 53 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:A:267[A]:ASN:ND2	3:A:901:HOH:O	1.99	0.95
1:B:292[B]:GLN:NE2	3:B:801:HOH:O	1.99	0.93
1:C:85:GLU:OE2	3:C:801:HOH:O	2.01	0.78
1:A:210:GLY:HA3	1:A:226[B]:THR:HG21	1.67	0.76
1:B:83:GLN:OE1	3:B:802:HOH:O	2.08	0.72

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1333:HOH:O	3:B:930:HOH:O[4_466]	1.98	0.22
3:A:1437:HOH:O	3:C:1316:HOH:O[3_546]	2.09	0.11
3:A:1437:HOH:O	3:C:1275:HOH:O[3_546]	2.09	0.11
3:A:1437:HOH:O	3:C:1238:HOH:O[3_546]	2.15	0.05

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 X-ray entries followed by that with respect to entries of similar resolution.

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	601/716 (84%)	585 (97%)	16 (3%)	0	100	100
1	B	598/716 (84%)	581 (97%)	17 (3%)	0	100	100
1	C	599/716 (84%)	584 (98%)	15 (2%)	0	100	100
All	All	1798/2148 (84%)	1750 (97%)	48 (3%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	493/572 (86%)	488 (99%)	5 (1%)	68	64
1	B	490/572 (86%)	486 (99%)	4 (1%)	73	70
1	C	491/572 (86%)	487 (99%)	4 (1%)	73	70
All	All	1474/1716 (86%)	1461 (99%)	13 (1%)	70	67

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	410	GLU
1	B	569	TYR
1	C	569	TYR
1	C	326	THR
1	C	410	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	461	GLN
1	C	402	ASN
1	B	532	ASN
1	C	353	GLN
1	B	353	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	577/716 (80%)	-0.83	6 (1%) 79 80	6, 20, 42, 79	13 (2%)
1	B	577/716 (80%)	-0.80	3 (0%) 87 88	5, 20, 42, 78	10 (1%)
1	C	577/716 (80%)	-0.83	4 (0%) 84 85	6, 21, 42, 78	11 (1%)
All	All	1731/2148 (80%)	-0.82	13 (0%) 82 83	5, 20, 42, 79	34 (1%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	VAL	4.4
1	B	16	VAL	4.4
1	B	30	LEU	4.1
1	A	31	THR	3.9
1	C	16	VAL	3.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	801	1/1	0.98	0.15	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.