

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 06:40 PM EDT

PDB ID : 1QVE

Title : Crystal structure of the truncated K122-4 pilin from Pseudomonas aeruginosa

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Deposited on : 2003-08-27

Resolution : 1.54 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS: 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

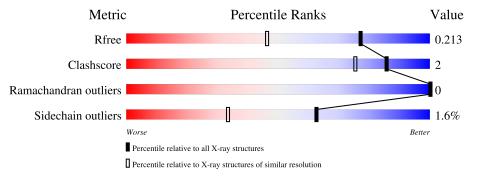
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(\mathring{A}))$
R_{free}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)

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 <=5%

Mol	Chain	Length	Quality of chain	
1	A	126	92%	7% •
1	В	126	94%	6% •



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2078 atoms, of which 0 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 Fimbrial protein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	1 Λ	A 126	Total	С	N	О	S	0	5	0
	120	902	551	150	194	7	0	9	0	
1	1 D	125	Total	С	N	О	S	0	0	0
	120	887	543	150	188	6	0	0	U	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ILE	-	expression tag	UNP P17838
A	26	SER	-	expression tag	UNP P17838
A	27	GLU	-	expression tag	UNP P17838
A	28	PHE	_	expression tag	UNP P17838
A	36	ALA	ARG	conflict	UNP P17838
В	25	ILE	-	expression tag	UNP P17838
В	26	SER	-	expression tag	UNP P17838
В	27	GLU	-	expression tag	UNP P17838
В	28	PHE	-	expression tag	UNP P17838
В	36	ALA	ARG	conflict	UNP P17838

• Molecule 2 is water.

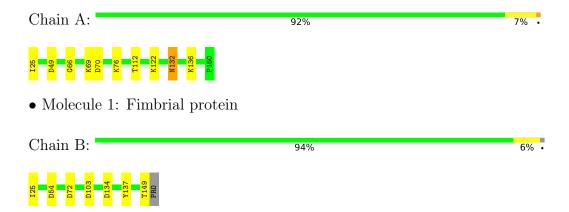
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	152	Total O 152 152	0	0
2	В	137	Total O 137 137	0	0



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: Fimbrial protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	40.18Å 38.93Å 37.23Å	Donositor
a, b, c, α , β , γ	66.39° 111.11° 93.74°	Depositor
Resolution (Å)	35.58 - 1.54	Depositor
rtesolution (A)	37.33 - 1.54	EDS
% Data completeness	93.9 (35.58-1.54)	Depositor
(in resolution range)	93.9 (37.33-1.54)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	4.86 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
D D.	0.139 , 0.179	Depositor
R, R_{free}	0.190 , 0.213	DCC
R_{free} test set	957 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 40.3	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2078	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.97% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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	A	0.61	0/932	0.84	$2/1267 \ (0.2\%)$	
1	В	0.63	0/896	0.84	4/1217 (0.3%)	
All	All	0.62	0/1828	0.84	6/2484 (0.2%)	

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	70	ASP	CB-CG-OD2	8.19	125.67	118.30
1	В	54	ASP	CB-CG-OD2	6.13	123.82	118.30
1	A	49	ASP	CB-CG-OD2	5.87	123.58	118.30
1	В	134	ASP	CB-CG-OD1	5.83	123.55	118.30
1	В	103	ASP	CB-CG-OD2	5.12	122.91	118.30
1	В	72	ASP	CB-CG-OD2	5.07	122.87	118.30

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	902	0	887	7	0
1	В	887	0	885	1	0
2	A	152	0	0	3	0
2	В	137	0	0	0	0
All	All	2078	0	1772	8	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 2.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:112:THR:H	1:A:132:ASN:ND2	2.01	0.58
1:A:112:THR:H	1:A:132:ASN:HD21	1.50	0.57
1:A:66:GLY:HA3	2:A:263:HOH:O	2.05	0.56
1:B:25:ILE:HD13	1:B:137:TYR:HA	1.95	0.49
1:A:132:ASN:HD22	1:A:132:ASN:C	2.18	0.46
1:A:76:LYS:HE2	2:A:238:HOH:O	2.19	0.42
1:A:69:LYS:HE3	2:A:292:HOH:O	2.19	0.41
1:A:25:ILE:HG12	1:A:136:LYS:HE3	2.01	0.41

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 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	129/126 (102%)	127 (98%)	2 (2%)	0	100 100
1	В	123/126 (98%)	123 (100%)	0	0	100 100
All	All	$252/252 \ (100\%)$	250 (99%)	2 (1%)	0	100 100

There are no Ramachandran outliers to report.

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 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	\mathbf{s}
1	A	100/96 (104%)	98 (98%)	2 (2%)	55 24	
1	В	95/96~(99%)	94 (99%)	1 (1%)	73 51	
All	All	195/192 (102%)	192 (98%)	3 (2%)	62 36	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	132	ASN
1	В	149	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	132	ASN
1	В	143	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.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

