

# Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 09:02 am BST

PDB ID : 8BKE

Title: Crystal structure of the Klebsiella phage KP34p57 capsular depolymerase

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Deposited on : 2022-11-09

Resolution : 2.00 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:

MolProbity : FAILED Xtriage (Phenix) : 1.13

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)
oteins) : Engh & Huber (2001)

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

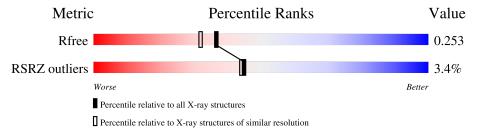
Validation Pipeline (wwPDB-VP) : 2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.00 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.



$egin{array}{ccc}  ext{Whole archive} \ (\# ext{Entries}) \end{array}$		Similar resolution $(\#\text{Entries, resolution range}(\mathring{A}))$		
$R_{free}$	130704	8085 (2.00-2.00)		
RSRZ outliers	127900	7900 (2.00-2.00)		

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.



## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6893 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 Uncharacterized protein 57.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	AAA	428	Total 3237	C 2033	N 573	O 620	S 11	0	0	0
1	BBB	428	Total 3240	C 2034	N 573	O 622	S 11	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	631	LYS	-	expression tag	UNP D1L302
AAA	632	GLY	-	expression tag	UNP D1L302
AAA	633	HIS	-	expression tag	UNP D1L302
AAA	634	HIS	_	expression tag	UNP D1L302
AAA	635	HIS	-	expression tag	UNP D1L302
AAA	636	HIS	-	expression tag	UNP D1L302
AAA	637	HIS	-	expression tag	UNP D1L302
AAA	638	HIS	-	expression tag	UNP D1L302
BBB	631	LYS	-	expression tag	UNP D1L302
BBB	632	GLY	-	expression tag	UNP D1L302
BBB	633	HIS	-	expression tag	UNP D1L302
BBB	634	HIS	-	expression tag	UNP D1L302
BBB	635	HIS	-	expression tag	UNP D1L302
BBB	636	HIS	-	expression tag	UNP D1L302
BBB	637	HIS	-	expression tag	UNP D1L302
BBB	638	HIS	-	expression tag	UNP D1L302

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	254	Total O 254 254	0	0
2	BBB	162	Total O 162 162	0	0



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# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	38.34Å 140.99Å 81.92Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $102.63^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	15.00 - 2.00	Depositor
Resolution (A)	15.00 - 2.00	EDS
% Data completeness	78.5 (15.00-2.00)	Depositor
(in resolution range)	78.7 (15.00-2.00)	EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.13  (at  2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
D.D.	0.204 , 0.247	Depositor
$R, R_{free}$	0.211 , $0.253$	DCC
$R_{free}$ test set	746 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38, 46.3	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6893	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.94% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 4 Model quality (i)

#### 4.1 Standard geometry (i)

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#### 4.2 Too-close contacts (i)

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#### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

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#### 4.3.2 Protein sidechains (i)

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#### 4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

There are no ligands in this entry.

### 4.7 Other polymers (i)

There are no such residues in this entry.



## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



### 5 Fit of model and data (i)

#### 5.1 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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	AAA	428/638 (67%)	-0.14	10 (2%) 60 59	18, 28, 42, 71	6 (1%)
1	BBB	428/638 (67%)	0.15	19 (4%) 34 33	21, 35, 53, 77	2 (0%)
All	All	856/1276 (67%)	0.00	29 (3%) 45 44	18, 31, 50, 77	8 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	27	VAL	5.8
1	BBB	151	ASP	5.6
1	AAA	454	LEU	5.2
1	BBB	28	PHE	4.3
1	BBB	286	GLN	3.6
1	BBB	290	SER	3.5
1	BBB	454	LEU	3.2
1	AAA	279	ILE	3.1
1	AAA	27	VAL	3.1
1	BBB	316	GLN	3.0
1	AAA	317	GLY	2.8
1	BBB	89	GLN	2.8
1	BBB	291	THR	2.7
1	BBB	309	ASN	2.7
1	BBB	317	GLY	2.7
1	BBB	130	SER	2.7
1	BBB	292	ASN	2.5
1	AAA	130	SER	2.5
1	BBB	345	SER	2.5
1	BBB	165	VAL	2.5
1	AAA	28	PHE	2.5
1	AAA	90	GLY	2.3
1	BBB	418	THR	2.3
1	BBB	287	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	321	SER	2.2
1	AAA	89	GLN	2.1
1	AAA	321	SER	2.0
1	AAA	316	GLN	2.0
1	BBB	318	VAL	2.0

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

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

### 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.4 Ligands (i)

There are no ligands in this entry.

### 5.5 Other polymers (i)

There are no such residues in this entry.

