



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 6, 2025 – 12:57 PM JST

PDB ID : 8YTV  
Title : The M19 variant of Mipa-Petase from Micromonospora pattaloongensis  
Authors : Hong, H.; Seo, H.; Park, J.; Kim, K.-J.  
Deposited on : 2024-03-26  
Resolution : 1.89 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

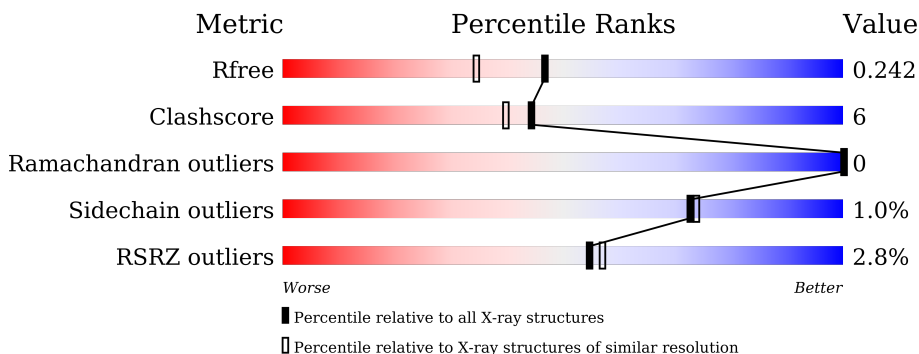
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	265	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	265	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3984 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 cutinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	4	0
			1921	1203	343	357	18			
1	B	249	Total	C	N	O	S	0	3	0
			1880	1180	334	348	18			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MET	-	initiating methionine	UNP A0A1H3QT72
A	46	GLN	GLU	variant	UNP A0A1H3QT72
A	49	CYS	LEU	variant	UNP A0A1H3QT72
A	61	CYS	SER	variant	UNP A0A1H3QT72
A	67	GLN	ALA	variant	UNP A0A1H3QT72
A	90	ALA	PRO	variant	UNP A0A1H3QT72
A	147	THR	SER	variant	UNP A0A1H3QT72
A	179	CYS	ASP	variant	UNP A0A1H3QT72
A	197	LYS	THR	variant	UNP A0A1H3QT72
A	198	CYS	SER	variant	UNP A0A1H3QT72
A	201	CYS	ARG	variant	UNP A0A1H3QT72
A	203	CYS	THR	variant	UNP A0A1H3QT72
A	215	THR	GLY	variant	UNP A0A1H3QT72
A	221	GLN	SER	variant	UNP A0A1H3QT72
A	228	GLN	THR	variant	UNP A0A1H3QT72
A	229	CYS	GLY	variant	UNP A0A1H3QT72
A	231	CYS	ALA	variant	UNP A0A1H3QT72
A	241	CYS	ALA	variant	UNP A0A1H3QT72
A	251	ASP	ALA	variant	UNP A0A1H3QT72
A	286	CYS	SER	variant	UNP A0A1H3QT72
A	295	LEU	-	expression tag	UNP A0A1H3QT72
A	296	GLU	-	expression tag	UNP A0A1H3QT72
A	297	HIS	-	expression tag	UNP A0A1H3QT72
A	298	HIS	-	expression tag	UNP A0A1H3QT72
A	299	HIS	-	expression tag	UNP A0A1H3QT72

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Chain	Residue	Modelled	Actual	Comment	Reference
A	300	HIS	-	expression tag	UNP A0A1H3QT72
A	301	HIS	-	expression tag	UNP A0A1H3QT72
A	302	HIS	-	expression tag	UNP A0A1H3QT72
B	38	MET	-	initiating methionine	UNP A0A1H3QT72
B	46	GLN	GLU	variant	UNP A0A1H3QT72
B	49	CYS	LEU	variant	UNP A0A1H3QT72
B	61	CYS	SER	variant	UNP A0A1H3QT72
B	67	GLN	ALA	variant	UNP A0A1H3QT72
B	90	ALA	PRO	variant	UNP A0A1H3QT72
B	147	THR	SER	variant	UNP A0A1H3QT72
B	179	CYS	ASP	variant	UNP A0A1H3QT72
B	197	LYS	THR	variant	UNP A0A1H3QT72
B	198	CYS	SER	variant	UNP A0A1H3QT72
B	201	CYS	ARG	variant	UNP A0A1H3QT72
B	203	CYS	THR	variant	UNP A0A1H3QT72
B	215	THR	GLY	variant	UNP A0A1H3QT72
B	221	GLN	SER	variant	UNP A0A1H3QT72
B	228	GLN	THR	variant	UNP A0A1H3QT72
B	229	CYS	GLY	variant	UNP A0A1H3QT72
B	231	CYS	ALA	variant	UNP A0A1H3QT72
B	241	CYS	ALA	variant	UNP A0A1H3QT72
B	251	ASP	ALA	variant	UNP A0A1H3QT72
B	286	CYS	SER	variant	UNP A0A1H3QT72
B	295	LEU	-	expression tag	UNP A0A1H3QT72
B	296	GLU	-	expression tag	UNP A0A1H3QT72
B	297	HIS	-	expression tag	UNP A0A1H3QT72
B	298	HIS	-	expression tag	UNP A0A1H3QT72
B	299	HIS	-	expression tag	UNP A0A1H3QT72
B	300	HIS	-	expression tag	UNP A0A1H3QT72
B	301	HIS	-	expression tag	UNP A0A1H3QT72
B	302	HIS	-	expression tag	UNP A0A1H3QT72

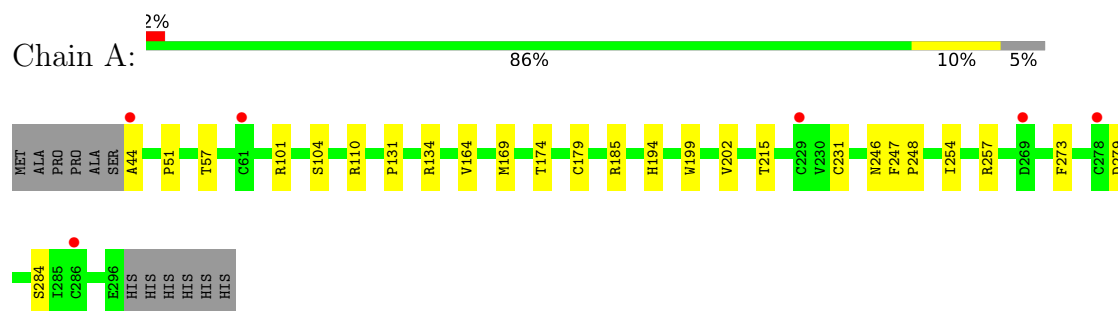
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	121	Total O 121 121	0	0
2	B	62	Total O 62 62	0	0

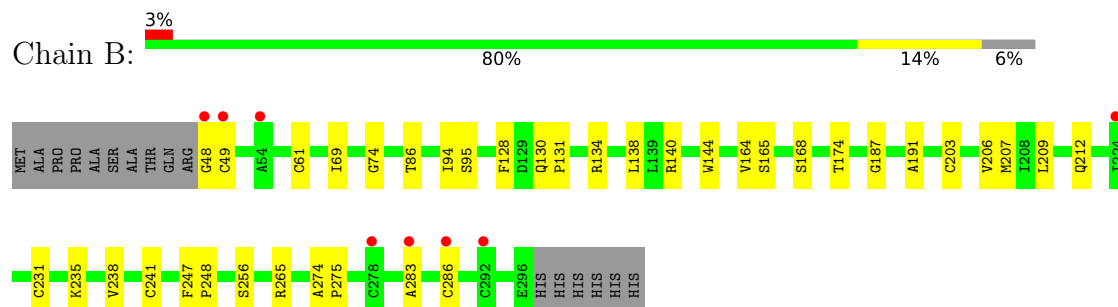
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: cutinase



#### • Molecule 1: cutinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.62Å 51.36Å 107.65Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	38.56 – 1.89 38.56 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.56-1.89) 99.7 (38.56-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, $R_{free}$	0.188 , 0.241 0.197 , 0.242	Depositor DCC
$R_{free}$ test set	1930 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3984	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 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [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	A	0.39	0/1972	0.69	0/2690
1	B	0.35	0/1931	0.64	0/2635
All	All	0.37	0/3903	0.67	0/5325

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	134	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	265	ARG	Sidechain

### 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	1921	0	1830	14	0
1	B	1880	0	1794	28	0
2	A	121	0	0	3	0
2	B	62	0	0	5	0
All	All	3984	0	3624	41	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 6.

The worst 5 of 41 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:B:49:CYS:HB2	1:B:61:CYS:SG	1.79	1.23
1:B:203[B]:CYS:SG	2:B:429:HOH:O	2.15	1.02
1:B:49:CYS:HB2	1:B:61:CYS:HG	1.40	0.83
1:A:254:ILE:HD11	1:A:284:SER:HB3	1.62	0.82
1:B:49:CYS:CB	1:B:61:CYS:SG	2.72	0.71

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	256/265 (97%)	253 (99%)	3 (1%)	0	100	100
1	B	251/265 (95%)	244 (97%)	7 (3%)	0	100	100
All	All	507/530 (96%)	497 (98%)	10 (2%)	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 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	202/207 (98%)	199 (98%)	3 (2%)	60	59
1	B	198/207 (96%)	197 (100%)	1 (0%)	86	88
All	All	400/414 (97%)	396 (99%)	4 (1%)	73	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	SER
1	A	215	THR
1	A	231	CYS
1	B	231	CYS

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

Mol	Chain	Res	Type
1	B	67	GLN
1	B	180	GLN
1	B	212	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 oligosaccharides 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	253/265 (95%)	-0.03	6 (2%) 59 61	7, 27, 40, 54	4 (1%)
1	B	249/265 (93%)	0.48	8 (3%) 50 52	10, 39, 55, 81	3 (1%)
All	All	502/530 (94%)	0.22	14 (2%) 55 57	7, 31, 52, 81	7 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	49	CYS	3.4
1	B	286	CYS	3.0
1	A	229	CYS	2.7
1	B	283	ALA	2.6
1	B	48	GLY	2.6

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.