



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:34 AM UTC

PDB ID : 2EC5 / pdb\_00002ec5  
Title : Crystal structures reveal a thiol-protease like catalytic triad in the C-terminal region of Pasteurella multocida toxin  
Authors : Kitadokoro, K.; Horiguchi, Y.; Kamitani, S.  
Deposited on : 2007-02-09  
Resolution : 2.60 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 : 4-5-2 with Phenix2.0  
Xtrriage (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

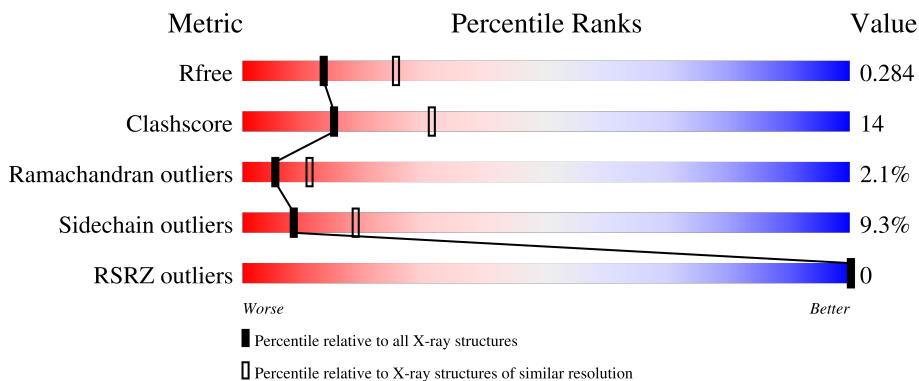
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	746	 68% 23% • 5%
1	B	746	 66% 25% • 5%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11528 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 Dermonecrotic toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	711	5643	3603	939	1075	26	0	0	0
1	B	711	5643	3603	939	1075	26	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	MET	-	cloning artifact	UNP P17452
A	541	GLY	-	cloning artifact	UNP P17452
A	542	HIS	-	expression tag	UNP P17452
A	543	HIS	-	expression tag	UNP P17452
A	544	HIS	-	expression tag	UNP P17452
A	545	HIS	-	expression tag	UNP P17452
A	546	HIS	-	expression tag	UNP P17452
A	547	HIS	-	expression tag	UNP P17452
A	548	ASP	-	cloning artifact	UNP P17452
A	549	TYR	-	cloning artifact	UNP P17452
A	550	ASP	-	cloning artifact	UNP P17452
A	551	ILE	-	cloning artifact	UNP P17452
A	552	PRO	-	cloning artifact	UNP P17452
A	553	THR	-	cloning artifact	UNP P17452
A	554	THR	-	cloning artifact	UNP P17452
A	555	GLU	-	cloning artifact	UNP P17452
A	556	ASN	-	cloning artifact	UNP P17452
A	557	LEU	-	cloning artifact	UNP P17452
A	558	TYR	-	cloning artifact	UNP P17452
A	559	PHE	-	cloning artifact	UNP P17452
A	560	GLN	-	cloning artifact	UNP P17452
A	561	GLY	-	cloning artifact	UNP P17452
A	562	ALA	-	cloning artifact	UNP P17452
A	563	HIS	-	cloning artifact	UNP P17452
A	564	MET	-	cloning artifact	UNP P17452

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Chain	Residue	Modelled	Actual	Comment	Reference
A	565	GLY	-	cloning artifact	UNP P17452
A	566	ILE	-	cloning artifact	UNP P17452
A	567	GLN	-	cloning artifact	UNP P17452
A	568	ARG	-	cloning artifact	UNP P17452
A	1159	SER	CYS	engineered mutation	UNP P17452
B	540	MET	-	cloning artifact	UNP P17452
B	541	GLY	-	cloning artifact	UNP P17452
B	542	HIS	-	expression tag	UNP P17452
B	543	HIS	-	expression tag	UNP P17452
B	544	HIS	-	expression tag	UNP P17452
B	545	HIS	-	expression tag	UNP P17452
B	546	HIS	-	expression tag	UNP P17452
B	547	HIS	-	expression tag	UNP P17452
B	548	ASP	-	cloning artifact	UNP P17452
B	549	TYR	-	cloning artifact	UNP P17452
B	550	ASP	-	cloning artifact	UNP P17452
B	551	ILE	-	cloning artifact	UNP P17452
B	552	PRO	-	cloning artifact	UNP P17452
B	553	THR	-	cloning artifact	UNP P17452
B	554	THR	-	cloning artifact	UNP P17452
B	555	GLU	-	cloning artifact	UNP P17452
B	556	ASN	-	cloning artifact	UNP P17452
B	557	LEU	-	cloning artifact	UNP P17452
B	558	TYR	-	cloning artifact	UNP P17452
B	559	PHE	-	cloning artifact	UNP P17452
B	560	GLN	-	cloning artifact	UNP P17452
B	561	GLY	-	cloning artifact	UNP P17452
B	562	ALA	-	cloning artifact	UNP P17452
B	563	HIS	-	cloning artifact	UNP P17452
B	564	MET	-	cloning artifact	UNP P17452
B	565	GLY	-	cloning artifact	UNP P17452
B	566	ILE	-	cloning artifact	UNP P17452
B	567	GLN	-	cloning artifact	UNP P17452
B	568	ARG	-	cloning artifact	UNP P17452
B	1159	SER	CYS	engineered mutation	UNP P17452

- Molecule 2 is water.

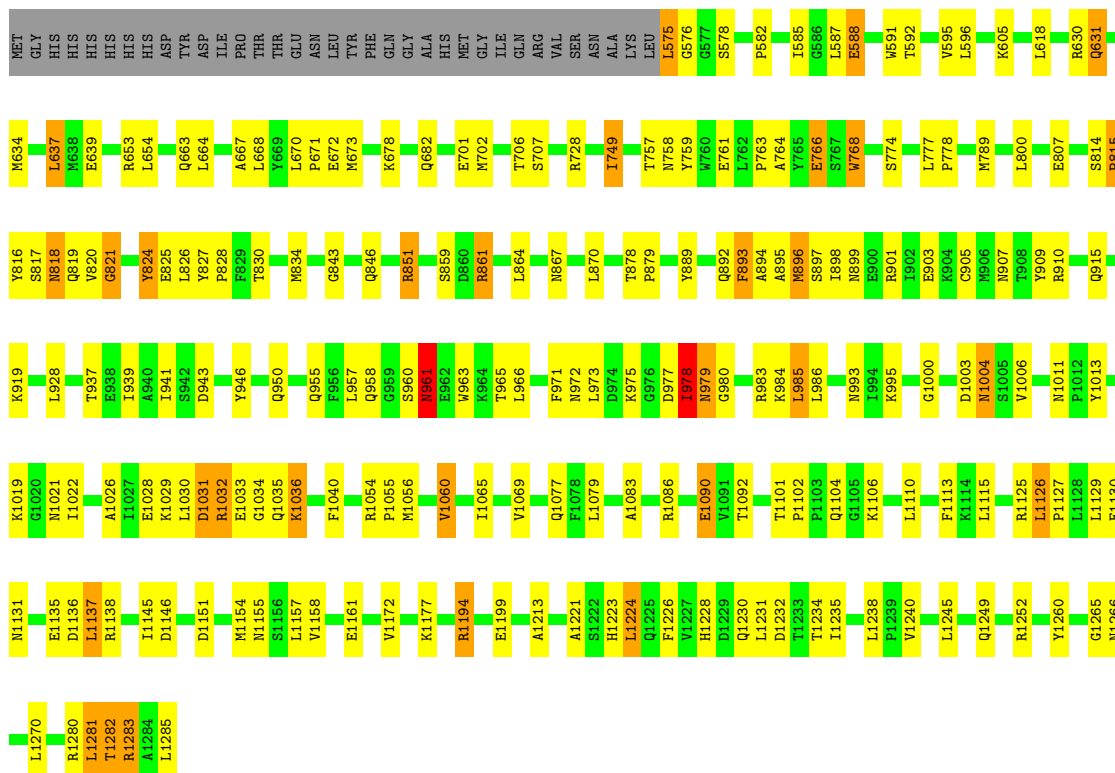
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	119	Total O 119 119	0	0
2	B	123	Total O 123 123	0	0

### 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.

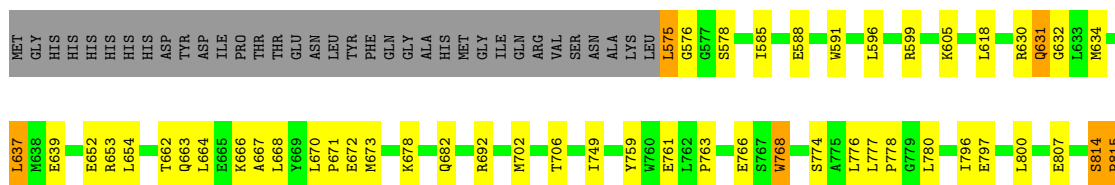
- Molecule 1: Dermonecrotic toxin

Chain A:  68% 23% 5%



- Molecule 1: Dermonecrotic toxin

Chain B:  66% 25% 5%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	197.36Å 132.82Å 82.55Å 90.00° 114.74° 90.00°	Depositor
Resolution (Å)	44.81 – 2.60 44.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.81-2.60) 96.9 (44.81-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.232 , 0.286 0.230 , 0.284	Depositor DCC
$R_{free}$ test set	2921 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.478 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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	0.51	0/5769	0.87	4/7811 (0.1%)
1	B	0.56	4/5769 (0.1%)	0.86	5/7811 (0.1%)
All	All	0.54	4/11538 (0.0%)	0.86	9/15622 (0.1%)

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	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926	ASN	CG-ND2	9.26	1.52	1.33
1	B	926	ASN	CG-OD1	7.77	1.38	1.23
1	B	922	ASP	C-O	5.91	1.31	1.24
1	B	1073	ASP	CG-OD2	5.47	1.35	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	654	LEU	N-CA-C	8.42	120.08	111.07
1	A	825	GLU	N-CA-C	6.71	118.51	110.19
1	A	1102	PRO	CA-C-N	6.45	126.20	119.05
1	A	1102	PRO	C-N-CA	6.45	126.20	119.05
1	A	654	LEU	N-CA-C	6.16	117.80	111.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	824	TYR	Peptide
1	B	824	TYR	Peptide

## 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	5643	0	5575	145	0
1	B	5643	0	5575	164	0
2	A	119	0	0	6	0
2	B	123	0	0	5	0
All	All	11528	0	11150	307	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 14.

The worst 5 of 307 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:1129:LEU:CB	1:B:1130:GLU:HA	1.66	1.22
1:B:1129:LEU:HB3	1:B:1130:GLU:CA	1.69	1.21
1:B:817:SER:CB	1:B:818:ASN:HA	1.72	1.18
1:B:817:SER:HB3	1:B:818:ASN:HA	1.27	1.15
1:A:893:PHE:HA	1:A:894:ALA:HB2	1.30	1.10

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	709/746 (95%)	647 (91%)	49 (7%)	13 (2%)	6	14
1	B	709/746 (95%)	629 (89%)	63 (9%)	17 (2%)	4	9
All	All	1418/1492 (95%)	1276 (90%)	112 (8%)	30 (2%)	5	11

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	961	ASN
1	A	978	ILE
1	B	814	SER
1	B	815	PRO
1	B	1133	VAL

### 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	616/646 (95%)	557 (90%)	59 (10%)	8	17
1	B	616/646 (95%)	561 (91%)	55 (9%)	9	20
All	All	1232/1292 (95%)	1118 (91%)	114 (9%)	8	18

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1282	THR
1	B	1224	LEU
1	B	768	TRP
1	B	1194	ARG
1	B	1129	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	663	GLN
1	B	927	ASN
1	B	785	GLN
1	B	907	ASN
1	B	961	ASN

### 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	711/746 (95%)	-1.08	0 100 100	45, 60, 77, 99	0
1	B	711/746 (95%)	-1.17	0 100 100	38, 52, 69, 95	0
All	All	1422/1492 (95%)	-1.12	0 100 100	38, 57, 75, 99	0

There are no RSRZ outliers to report.

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.