



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:19 AM UTC

PDB ID : 1WUP / pdb\_00001wup  
Title : Crystal structure of metallo-beta-lactamase IMP-1 mutant (D81E)  
Authors : Yamaguchi, Y.; Yamagata, Y.; Goto, M.  
Deposited on : 2004-12-08  
Resolution : 3.00 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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

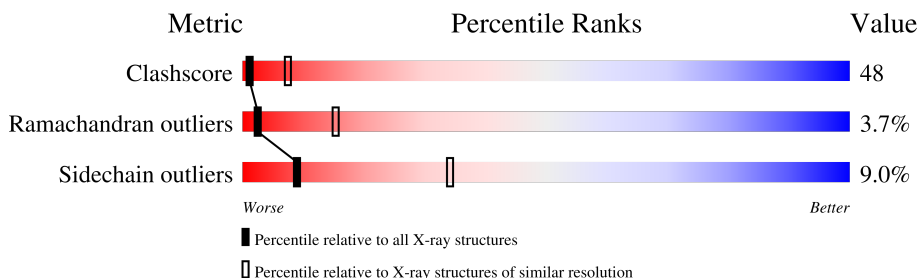
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	31% 53% 11% • 5%
1	B	228	30% 53% 11% • 5%
1	C	228	34% 48% 12% • 5%
1	D	228	30% 55% 9% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACY	A	401	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6810 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 Beta-lactamase IMP-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	1698	1102	279	316	1	0	0	0
1	B	216	1692	1099	278	314	1	0	0	0
1	C	217	1698	1102	279	316	1	0	0	0
1	D	217	1698	1102	279	316	1	0	0	0

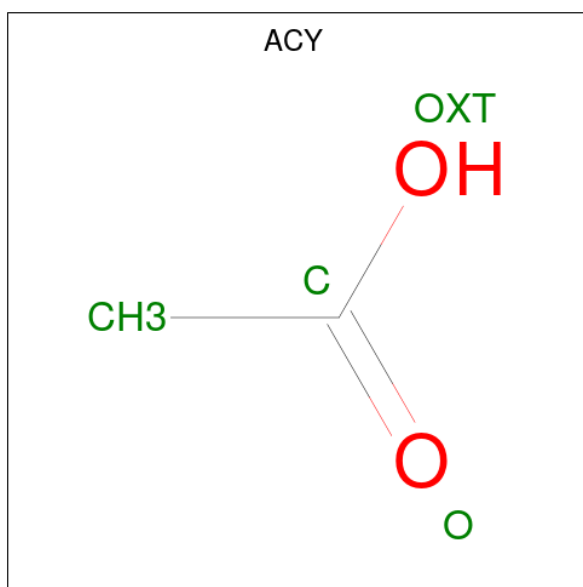
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	GLU	ASP	engineered mutation	UNP P52699
B	81	GLU	ASP	engineered mutation	UNP P52699
C	81	GLU	ASP	engineered mutation	UNP P52699
D	81	GLU	ASP	engineered mutation	UNP P52699

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.21Å 73.06Å 80.89Å 84.81° 76.10° 74.00°	Depositor
Resolution (Å)	19.73 – 3.00	Depositor
% Data completeness (in resolution range)	88.7 (19.73-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.224 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, 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	0.53	0/1742	1.12	18/2365 (0.8%)
1	B	0.52	0/1736	1.14	14/2357 (0.6%)
1	C	0.52	0/1742	1.12	14/2365 (0.6%)
1	D	0.52	0/1742	1.11	11/2365 (0.5%)
All	All	0.52	0/6962	1.12	57/9452 (0.6%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	VAL	N-CA-C	9.54	119.45	108.96
1	A	161	LYS	CA-C-N	9.45	129.20	119.56
1	A	161	LYS	C-N-CA	9.45	129.20	119.56
1	A	28	TRP	N-CA-C	-8.68	102.27	112.86
1	C	40	VAL	N-CA-C	-8.66	98.47	109.30

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	1698	0	1707	159	0
1	B	1692	0	1702	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1698	0	1707	181	0
1	D	1698	0	1707	172	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	4	0	3	5	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
3	D	4	0	3	1	0
All	All	6810	0	6835	661	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 48.

The worst 5 of 661 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:40:VAL:HG12	1:B:41:ASN:H	1.11	1.07
1:C:145:VAL:HG23	1:C:156:GLY:HA2	1.39	1.01
1:C:164:GLY:N	1:C:212:GLN:HE22	1.61	0.98
1:C:43:GLU:HB3	1:C:71:LYS:HB2	1.49	0.94
1:A:102:THR:HG22	1:A:142:ASP:OD1	1.69	0.91

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	215/228 (94%)	186 (86%)	21 (10%)	8 (4%)	2	15
1	B	214/228 (94%)	179 (84%)	27 (13%)	8 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	215/228 (94%)	180 (84%)	27 (13%)	8 (4%)	2	15
1	D	215/228 (94%)	184 (86%)	23 (11%)	8 (4%)	2	15
All	All	859/912 (94%)	729 (85%)	98 (11%)	32 (4%)	2	15

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	LYS
1	C	26	ASN
1	C	41	ASN
1	C	203	ALA
1	A	127	LYS

### 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	186/196 (95%)	173 (93%)	13 (7%)	14	44
1	B	185/196 (94%)	166 (90%)	19 (10%)	7	28
1	C	186/196 (95%)	164 (88%)	22 (12%)	5	22
1	D	186/196 (95%)	173 (93%)	13 (7%)	14	44
All	All	743/784 (95%)	676 (91%)	67 (9%)	9	34

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	74	ILE
1	D	101	LEU
1	D	212	GLN
1	B	127	LYS
1	B	121	VAL

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	D	143	ASN
1	D	90	ASN
1	C	34	HIS
1	D	34	HIS
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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACY	B	402	2	3,3,3	0.98	0	3,3,3	0.74	0
3	ACY	D	404	2	3,3,3	1.03	0	3,3,3	0.79	0
3	ACY	C	403	2	3,3,3	1.03	0	3,3,3	0.80	0
3	ACY	A	401	2	3,3,3	1.00	0	3,3,3	0.84	0

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	ACY	1	0
3	D	404	ACY	1	0
3	A	401	ACY	5	0

## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.