



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 11:33 PM UTC

PDB ID : 1VGN / pdb_00001vgn
Title : Structure-based design of the irreversible inhibitors to metallo-lactamase (IMP-1)
Authors : Kurosaki, H.; Yamaguchi, Y.; Higashi, T.; Soga, K.; Matsueda, S.; Misumi, S.; Yamagata, Y.; Arakawa, Y.; Goto, M.
Deposited on : 2004-04-27
Resolution : 2.63 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

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>.

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)
Xtriage (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

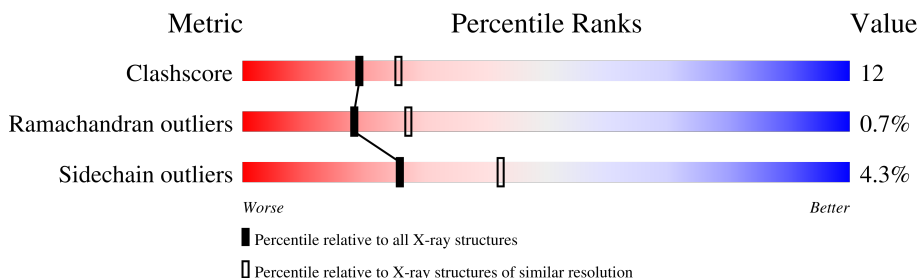
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	228	 72% 21% • 5%
1	B	228	 65% 27% • •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3513 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.

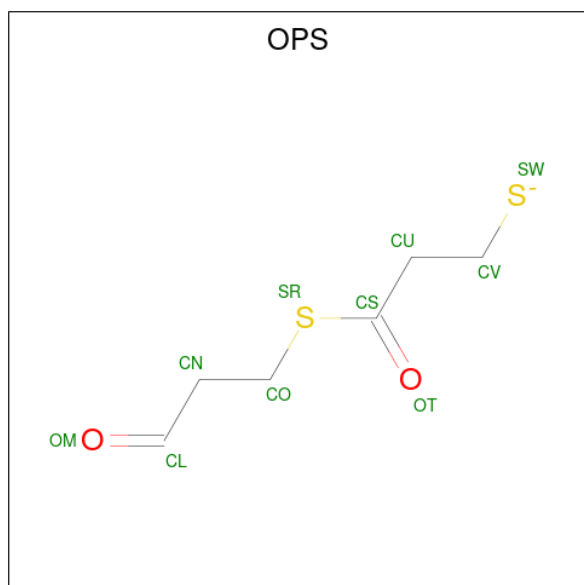
- Molecule 1 is a protein called Beta-lactamase IMP-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1697	1101	279	316	1			
1	B	218	Total	C	N	O	S	0	0	0
			1706	1107	281	317	1			

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

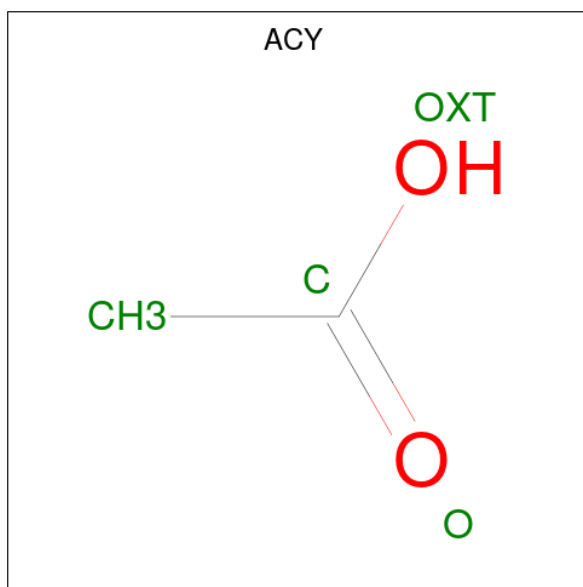
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 3-OXO-3-[(3-OXOPROPYL)SULFANYL]PROPANE-1-THIOLATE (CCD ID: OPS) (formula: C₆H₉O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 6	O 2	S 2	0	0
3	B	1	Total 10	C 6	O 2	S 2	0	0

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: $\text{C}_2\text{H}_4\text{O}_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	62	Total O 62 62	0	0
5	B	20	Total O 20 20	0	0

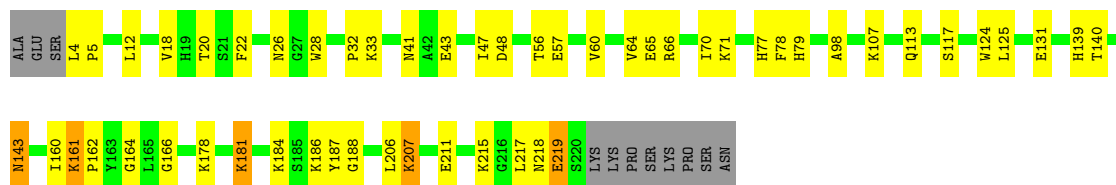
3 Residue-property plots [i](#)

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.

Note EDS was not executed.

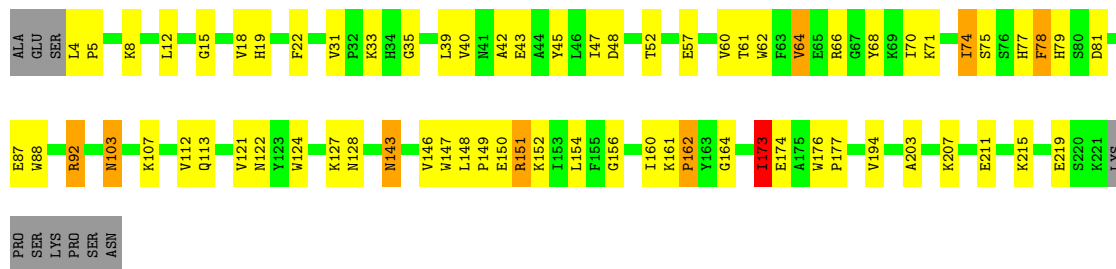
• Molecule 1: Beta-lactamase IMP-1

Chain A:  72% 21% 5%



• Molecule 1: Beta-lactamase IMP-1

Chain B:  65% 27% 8%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.99Å 53.31Å 196.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.55 – 2.63	Depositor
% Data completeness (in resolution range)	98.6 (44.55-2.63)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3513	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: OPS, 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	0.34	0/1741	0.95	6/2364 (0.3%)
1	B	0.32	0/1750	0.93	9/2375 (0.4%)
All	All	0.33	0/3491	0.94	15/4739 (0.3%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	PHE	N-CA-C	7.48	121.67	112.54
1	B	78	PHE	N-CA-C	7.34	120.33	111.82
1	A	125	LEU	N-CA-C	-7.02	103.71	111.36
1	B	64	VAL	N-CA-C	-6.03	104.47	110.62
1	B	173	ILE	N-CA-C	6.01	117.47	110.62

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	1697	0	1703	25	0
1	B	1706	0	1716	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	8	0	0
3	B	10	0	8	0	0
4	A	4	0	3	0	0
5	A	62	0	0	1	0
5	B	20	0	0	0	0
All	All	3513	0	3438	80	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 12.

The worst 5 of 80 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:92:ARG:HH11	1:B:92:ARG:HB3	1.19	1.01
1:B:215:LYS:O	1:B:219:GLU:HB2	1.76	0.85
1:A:60:VAL:HG13	1:A:70:ILE:HG13	1.65	0.79
1:B:92:ARG:HB3	1:B:92:ARG:NH1	1.98	0.78
1:B:156:GLY:HA3	1:B:160:ILE:HG13	1.68	0.75

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%)	202 (94%)	11 (5%)	2 (1%)	14	21
1	B	216/228 (95%)	196 (91%)	19 (9%)	1 (0%)	24	36
All	All	431/456 (94%)	398 (92%)	30 (7%)	3 (1%)	18	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	219	GLU
1	B	203	ALA

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%)	178 (96%)	8 (4%)	26	42
1	B	187/196 (95%)	179 (96%)	8 (4%)	26	42
All	All	373/392 (95%)	357 (96%)	16 (4%)	26	42

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151	ARG
1	B	143	ASN
1	B	8	LYS
1	B	103	ASN
1	A	219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	ASN
1	B	167	ASN
1	B	218	ASN
1	B	212	GLN
1	B	113	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	OPS	B	1161	2,1	7,9,9	0.78	0	7,9,9	2.45	3 (42%)
3	OPS	A	1161	2,1	7,9,9	1.20	1 (14%)	7,9,9	2.28	3 (42%)
4	ACY	A	401	-	3,3,3	1.10	0	3,3,3	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OPS	B	1161	2,1	-	3/7/8/8	-
3	OPS	A	1161	2,1	-	2/7/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1161	OPS	CU-CS	2.23	1.53	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	1161	OPS	CU-CS-SR	5.21	119.61	113.40
3	A	1161	OPS	CU-CS-SR	4.89	119.23	113.40
3	B	1161	OPS	OT-CS-CU	-3.00	120.52	123.98
3	A	1161	OPS	OT-CS-CU	-2.61	120.96	123.98
3	A	1161	OPS	OT-CS-SR	-2.27	119.80	122.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1161	OPS	CN-CO-SR-CS
3	B	1161	OPS	CN-CO-SR-CS
3	A	1161	OPS	CL-CN-CO-SR
3	B	1161	OPS	SR-CS-CU-CV
3	B	1161	OPS	OT-CS-CU-CV

There are no ring outliers.

No monomer is involved in short contacts.

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.