



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 03:38 AM UTC

PDB ID : 5I63 / pdb_00005i63
Title : Crystal structure of TEM1 beta-lactamase mutant I263N in the presence of 1.2 MPa xenon
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Deposited on : 2016-02-15
Resolution : 1.95 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
Xtriage (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

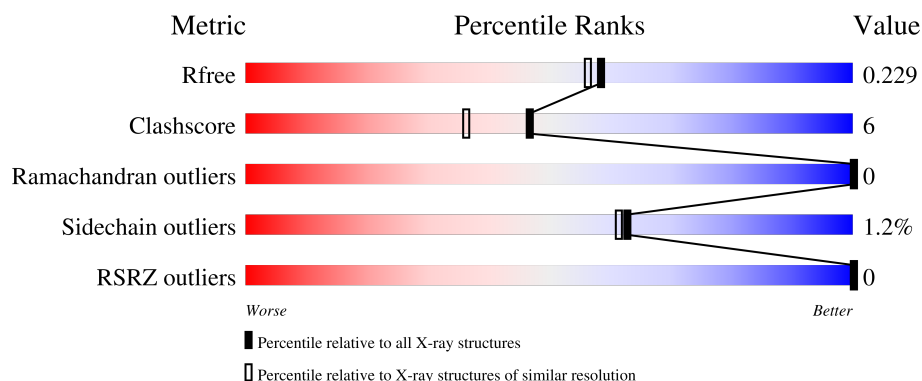
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

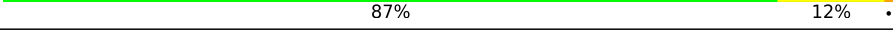
The reported resolution of this entry is 1.95 Å.

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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	263	 84% 16%
1	B	263	 89% 11%
1	C	263	 88% 10% .
1	D	263	 87% 12% .

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
2	XE	B	302	-	-	X	-
2	XE	C	302	-	-	X	-
2	XE	D	302	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8614 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 TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	2	0
			1992	1248	355	378	11			
1	B	263	Total	C	N	O	S	0	0	0
			1999	1245	356	388	10			
1	C	263	Total	C	N	O	S	0	1	0
			2002	1248	359	385	10			
1	D	263	Total	C	N	O	S	0	1	0
			2005	1252	357	386	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	THR	MET	engineered mutation	UNP P62593
A	263	ASN	ILE	engineered mutation	UNP P62593
B	182	THR	MET	engineered mutation	UNP P62593
B	263	ASN	ILE	engineered mutation	UNP P62593
C	182	THR	MET	engineered mutation	UNP P62593
C	263	ASN	ILE	engineered mutation	UNP P62593
D	182	THR	MET	engineered mutation	UNP P62593
D	263	ASN	ILE	engineered mutation	UNP P62593

- Molecule 2 is XENON (CCD ID: XE) (formula: Xe).

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

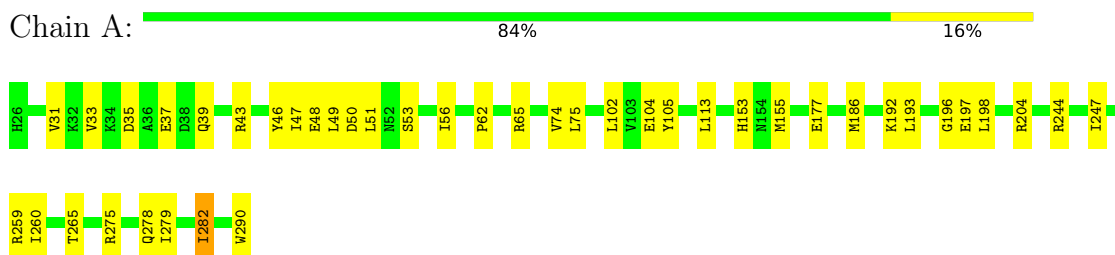
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total 149	O 149	0	0
3	B	162	Total 162	O 162	0	0
3	C	144	Total 144	O 144	0	0
3	D	153	Total 153	O 153	0	0

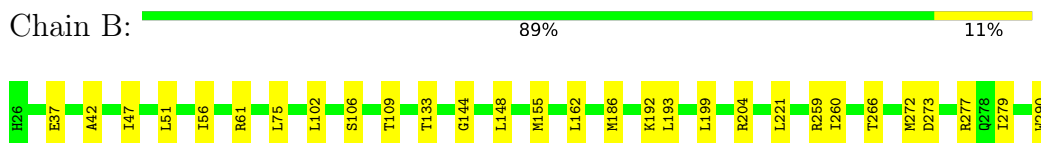
3 Residue-property plots

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.

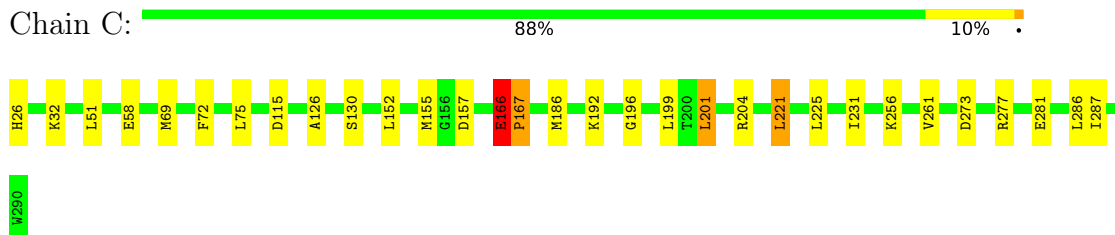
- Molecule 1: Beta-lactamase TEM



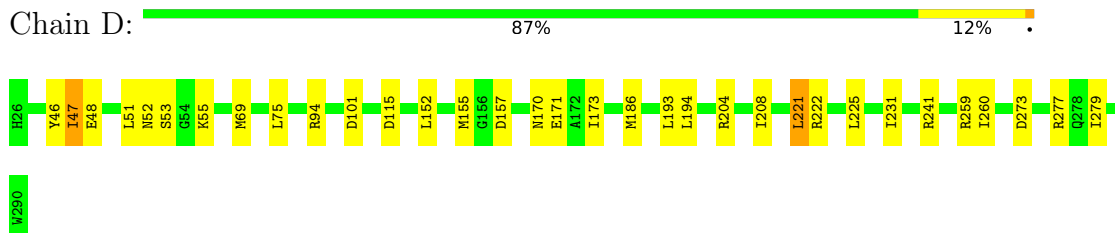
- Molecule 1: Beta-lactamase TEM



- Molecule 1: Beta-lactamase TEM



- Molecule 1: Beta-lactamase TEM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.07Å 84.20Å 96.22Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	60.07 – 1.95 60.07 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (60.07-1.95) 97.4 (60.07-1.95)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.222 (Not available) , 0.229	Depositor DCC
R_{free} test set	3405 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	1.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.396 for h,-k,-l	Xtriage
Reported twinning fraction	0.380 for h,-k,-l	Depositor
Outliers	4 of 68184 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8614	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1393e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XE

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	0.57	5/2032 (0.2%)	0.77	2/2757 (0.1%)
1	B	0.32	0/2033	0.70	2/2760 (0.1%)
1	C	0.38	0/2041	0.74	2/2767 (0.1%)
1	D	0.33	0/2042	0.70	0/2769
All	All	0.41	5/8148 (0.1%)	0.73	6/11053 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLU	C-O	-9.75	1.11	1.24
1	A	282[A]	ILE	CA-C	8.49	1.63	1.52
1	A	282[B]	ILE	CA-C	8.49	1.63	1.52
1	A	104	GLU	N-CA	-7.08	1.37	1.46
1	A	104	GLU	C-O	-6.73	1.15	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	282[A]	ILE	CA-C-O	8.28	129.66	120.64
1	A	282[B]	ILE	CA-C-O	8.28	129.66	120.64
1	C	167	PRO	CA-N-CD	-5.42	103.91	111.50
1	C	166	GLU	C-N-CD	5.39	132.46	120.60
1	B	144	GLY	CA-C-N	5.12	125.16	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1992	0	1977	29	0
1	B	1999	0	1971	18	0
1	C	2002	0	1990	20	0
1	D	2005	0	1994	23	0
2	A	2	0	0	2	0
2	B	2	0	0	3	0
2	C	2	0	0	2	0
2	D	2	0	0	4	0
3	A	149	0	0	0	0
3	B	162	0	0	2	0
3	C	144	0	0	0	0
3	D	153	0	0	4	0
All	All	8614	0	7932	90	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 90 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:D:221:LEU:HD21	2:D:302:XE:XE	1.95	1.43
1:C:221:LEU:HD21	2:C:302:XE:XE	2.04	1.35
1:D:221:LEU:CD2	2:D:302:XE:XE	2.77	1.10
1:C:221:LEU:CD2	2:C:302:XE:XE	2.97	0.90
1:A:46:TYR:CE1	1:A:282[B]:ILE:HD11	2.09	0.88

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	263/263 (100%)	252 (96%)	11 (4%)	0	100	100
1	B	261/263 (99%)	256 (98%)	5 (2%)	0	100	100
1	C	262/263 (100%)	252 (96%)	10 (4%)	0	100	100
1	D	262/263 (100%)	257 (98%)	5 (2%)	0	100	100
All	All	1048/1052 (100%)	1017 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	206/217 (95%)	206 (100%)	0	100	100
1	B	210/217 (97%)	209 (100%)	1 (0%)	81	82
1	C	211/217 (97%)	206 (98%)	5 (2%)	43	36
1	D	211/217 (97%)	207 (98%)	4 (2%)	50	45
All	All	838/868 (96%)	828 (99%)	10 (1%)	63	61

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	55	LYS
1	D	101	ASP
1	D	221	LEU
1	C	201	LEU
1	C	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	175	ASN
1	B	205	GLN
1	D	205	GLN
1	C	88	GLN
1	C	263	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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

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 [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, 95th 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 ²)	Q<0.9
1	A	263/263 (100%)	-1.13	0 100 100	5, 12, 21, 29	2 (0%)
1	B	263/263 (100%)	-1.15	0 100 100	5, 12, 23, 35	0
1	C	263/263 (100%)	-1.18	0 100 100	4, 10, 20, 26	1 (0%)
1	D	263/263 (100%)	-1.14	0 100 100	4, 11, 21, 28	1 (0%)
All	All	1052/1052 (100%)	-1.15	0 100 100	4, 11, 21, 35	4 (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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	XE	B	301	1/1	0.95	0.05	13,13,13,13	1
2	XE	A	301	1/1	0.96	0.10	29,29,29,29	1
2	XE	C	302	1/1	0.96	0.06	22,22,22,22	1
2	XE	B	302	1/1	0.97	0.05	14,14,14,14	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XE	C	301	1/1	0.97	0.07	29,29,29,29	1
2	XE	A	302	1/1	0.97	0.05	11,11,11,11	1
2	XE	D	301	1/1	0.97	0.06	20,20,20,20	1
2	XE	D	302	1/1	0.97	0.07	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.