



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 08:57 PM UTC

PDB ID : 3ZHH / pdb_00003zhh
Title : X-ray structure of the full-length beta-lactamase from M.tuberculosis
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Deposited on : 2012-12-21
Resolution : 2.85 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)	:	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

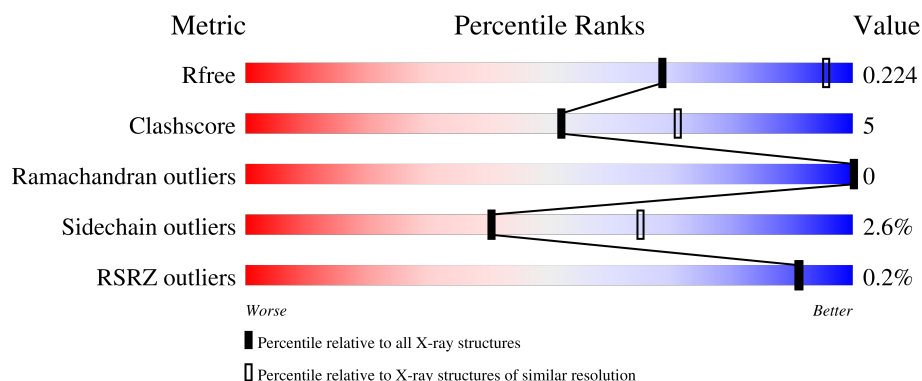
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	276	 86% 10% . .
1	B	276	 84% 11% . .
1	C	276	 84% 12% . .
1	D	276	 81% 15% . .

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	SO4	A	1295	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15935 atoms, of which 7803 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	H	N	O	S	0	0	0
			3954	1245	1962	353	388	6			
1	B	266	Total	C	H	N	O	S	0	0	0
			3937	1242	1951	350	388	6			
1	C	266	Total	C	H	N	O	S	0	0	0
			3907	1236	1932	348	385	6			
1	D	266	Total	C	H	N	O	S	0	0	0
			3950	1245	1958	353	388	6			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	30	Total	O	0	0
			30	30		
3	C	22	Total	O	0	0
			22	22		
3	D	23	Total	O	0	0
			23	23		

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.

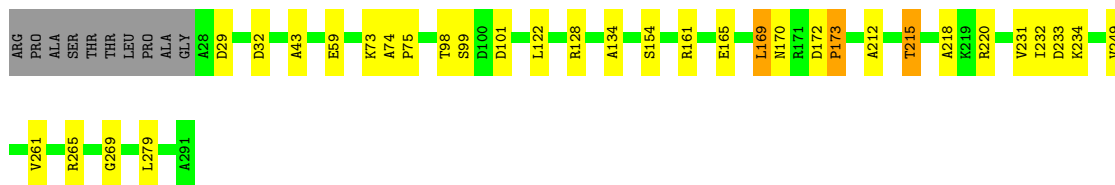
• Molecule 1: BETA-LACTAMASE

Chain A: 



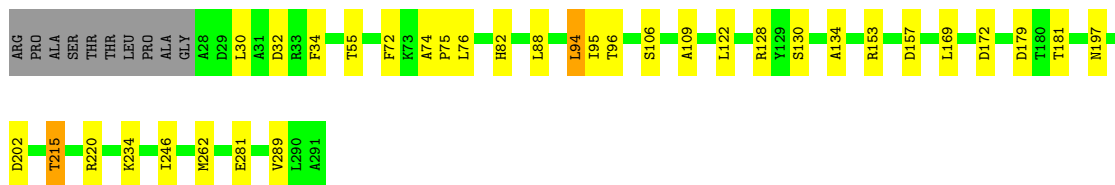
• Molecule 1: BETA-LACTAMASE

Chain B: 



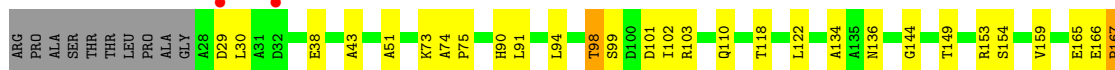
• Molecule 1: BETA-LACTAMASE

Chain C: 



• Molecule 1: BETA-LACTAMASE

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.74Å 96.44Å 111.00Å 90.00° 108.48° 90.00°	Depositor
Resolution (Å)	19.87 – 2.85 19.87 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.87-2.85) 99.3 (19.87-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.83Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.168 , 0.220 0.175 , 0.224	Depositor DCC
R_{free} test set	1788 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15935	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4

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	0.96	1/2031 (0.0%)	1.02	3/2772 (0.1%)
1	B	0.85	1/2025 (0.0%)	1.01	4/2765 (0.1%)
1	C	0.89	1/2014 (0.0%)	1.01	3/2752 (0.1%)
1	D	0.98	2/2031 (0.1%)	1.05	5/2772 (0.2%)
All	All	0.92	5/8101 (0.1%)	1.02	15/11061 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	51	ALA	CA-CB	-5.22	1.45	1.53
1	A	258	VAL	CA-CB	-5.21	1.48	1.54
1	B	218	ALA	CA-CB	-5.16	1.44	1.53
1	D	167	PRO	N-CD	5.09	1.54	1.47
1	C	220	ARG	N-CA	5.03	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	PRO	CA-C-N	8.22	128.27	119.89
1	B	173	PRO	C-N-CA	8.22	128.27	119.89
1	C	32	ASP	N-CA-C	-5.96	104.91	111.82
1	B	233	ASP	N-CA-C	5.69	116.91	108.60
1	A	144	GLY	CA-C-N	5.63	125.58	119.78

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	1962	1957	19	0
1	B	1986	1951	1946	18	0
1	C	1975	1932	1927	19	0
1	D	1992	1958	1957	24	0
2	A	25	0	0	7	0
2	B	20	0	0	0	0
2	C	15	0	0	1	0
2	D	25	0	0	0	0
3	A	27	0	0	1	0
3	B	30	0	0	1	0
3	C	22	0	0	1	0
3	D	23	0	0	0	0
All	All	8132	7803	7787	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 5.

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:170:ASN:ND2	3:B:2006:HOH:O	2.04	0.89
1:B:261:VAL:CG1	1:B:279:LEU:HD22	2.13	0.77
1:D:261:VAL:HG12	1:D:279:LEU:HD22	1.66	0.76
1:B:74:ALA:HB3	1:B:75:PRO:HD3	1.66	0.76
1:A:29:ASP:HB3	1:A:32:ASP:OD2	1.89	0.72

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	264/276 (96%)	252 (96%)	12 (4%)	0	100	100
1	B	264/276 (96%)	257 (97%)	7 (3%)	0	100	100
1	C	264/276 (96%)	256 (97%)	8 (3%)	0	100	100
1	D	264/276 (96%)	256 (97%)	8 (3%)	0	100	100
All	All	1056/1104 (96%)	1021 (97%)	35 (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	202/209 (97%)	198 (98%)	4 (2%)	48	71
1	B	201/209 (96%)	195 (97%)	6 (3%)	36	61
1	C	198/209 (95%)	193 (98%)	5 (2%)	42	66
1	D	202/209 (97%)	196 (97%)	6 (3%)	36	61
All	All	803/836 (96%)	782 (97%)	21 (3%)	40	65

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	281	GLU
1	D	98	THR
1	D	167	PRO
1	D	154	SER
1	D	94	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	HIS
1	C	191	GLN
1	D	90	HIS
1	D	112	HIS
1	D	170	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](#)

17 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	A	1292	-	4,4,4	0.25	0	6,6,6	0.55	0
2	SO4	D	1295	-	4,4,4	0.37	0	6,6,6	0.45	0
2	SO4	C	1292	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	C	1294	-	4,4,4	0.28	0	6,6,6	0.30	0
2	SO4	D	1292	-	4,4,4	0.23	0	6,6,6	0.39	0
2	SO4	B	1292	-	4,4,4	0.39	0	6,6,6	0.69	0
2	SO4	A	1295	-	4,4,4	0.22	0	6,6,6	0.09	0
2	SO4	D	1293	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	D	1294	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	B	1294	-	4,4,4	0.29	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	1295	-	4,4,4	0.46	0	6,6,6	0.43	0
2	SO4	A	1294	-	4,4,4	0.27	0	6,6,6	0.21	0
2	SO4	D	1296	-	4,4,4	0.33	0	6,6,6	0.40	0
2	SO4	C	1293	-	4,4,4	0.32	0	6,6,6	0.47	0
2	SO4	A	1296	-	4,4,4	0.29	0	6,6,6	0.62	0
2	SO4	B	1293	-	4,4,4	0.29	0	6,6,6	0.42	0
2	SO4	A	1293	-	4,4,4	0.26	0	6,6,6	0.25	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 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1292	SO4	1	0
2	C	1292	SO4	1	0
2	A	1295	SO4	6	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 [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(Å²)	Q<0.9	
1	A	266/276 (96%)	-0.90	0	100	100	1, 13, 36, 57	0
1	B	266/276 (96%)	-0.93	0	100	100	3, 14, 40, 59	0
1	C	266/276 (96%)	-0.88	0	100	100	2, 16, 37, 51	0
1	D	266/276 (96%)	-0.85	2 (0%)	82	78	2, 14, 42, 59	0
All	All	1064/1104 (96%)	-0.89	2 (0%)	91	91	1, 14, 40, 59	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	32	ASP	3.4
1	D	29	ASP	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 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($\text{\AA}^2$)	Q<0.9
2	SO4	D	1295	5/5	0.73	0.16	44,54,72,95	0
2	SO4	B	1294	5/5	0.76	0.24	101,105,114,117	0
2	SO4	B	1295	5/5	0.79	0.11	25,45,59,89	0
2	SO4	A	1296	5/5	0.85	0.11	36,42,66,84	0
2	SO4	D	1296	5/5	0.86	0.16	52,59,70,85	0
2	SO4	A	1294	5/5	0.89	0.10	30,33,59,65	0
2	SO4	C	1294	5/5	0.90	0.12	37,47,69,75	0
2	SO4	D	1293	5/5	0.91	0.09	29,37,45,52	0
2	SO4	C	1293	5/5	0.92	0.08	15,27,39,63	0
2	SO4	A	1295	5/5	0.93	0.23	189,191,196,196	0
2	SO4	D	1294	5/5	0.93	0.06	39,44,65,70	0
2	SO4	A	1293	5/5	0.94	0.09	17,22,38,43	0
2	SO4	B	1293	5/5	0.96	0.08	9,13,31,51	0
2	SO4	C	1292	5/5	0.96	0.08	2,17,48,55	0
2	SO4	B	1292	5/5	0.98	0.05	0,0,0,19	0
2	SO4	A	1292	5/5	0.99	0.04	2,8,12,17	0
2	SO4	D	1292	5/5	0.99	0.04	0,8,23,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.