Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 02:33 PM EDT

PDB ID	:	1BZA
Title	:	BETA-LACTAMASE TOHO-1 FROM ESCHERICHIA COLI TUH12191
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Deposited on	:	1998-10-28
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

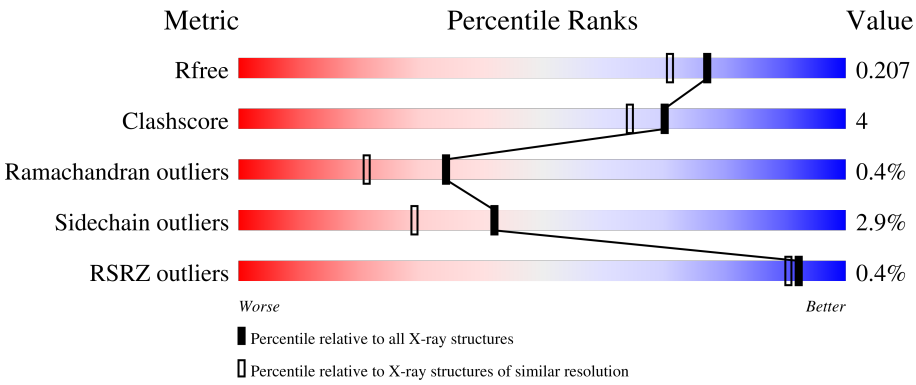
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 <=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	262	84% 13% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2814 atoms, of which 732 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
			Total	C	H	N	O	S			
1	A	257	2399	1205	462	347	379	6	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLN	LYS	conflict	UNP Q47066
A	34	GLU	ALA	conflict	UNP Q47066
A	35	ALA	GLU	conflict	UNP Q47066
A	38	LYS	ARG	conflict	UNP Q47066
A	39	SER	GLN	conflict	UNP Q47066
A	77	ALA	VAL	conflict	UNP Q47066
A	83	GLN	LYS	conflict	UNP Q47066
A	87	ASP	GLU	conflict	UNP Q47066
A	88	LYS	PRO	conflict	UNP Q47066
A	89	HIS	ASN	conflict	UNP Q47066
A	114	ASN	ASP	conflict	UNP Q47066
A	118	THR	SER	conflict	UNP Q47066
A	123	GLY	SER	conflict	UNP Q47066
A	133	THR	VAL	conflict	UNP Q47066
A	140	ALA	SER	conflict	UNP Q47066
A	142	LEU	VAL	conflict	UNP Q47066
A	146	ASP	ALA	conflict	UNP Q47066
A	147	LYS	SER	conflict	UNP Q47066
A	154	SER	GLN	conflict	UNP Q47066
A	166	ALA	GLU	engineered mutation	UNP Q47066
A	182	THR	SER	conflict	UNP Q47066
A	184	LEU	ARG	conflict	UNP Q47066
A	191	LYS	ARG	conflict	UNP Q47066
A	200	ALA	GLY	conflict	UNP Q47066
A	201	GLU	ASP	conflict	UNP Q47066
A	202	THR	SER	conflict	UNP Q47066
A	211	LEU	MET	conflict	UNP Q47066

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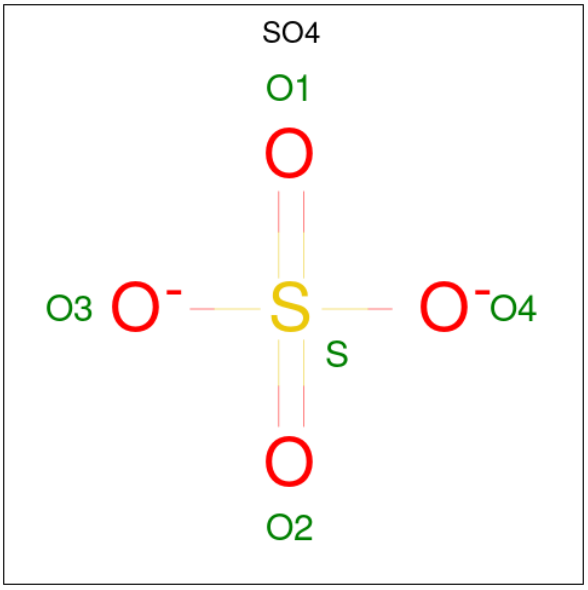
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	ALA	conflict	UNP Q47066
A	222	ARG	GLN	conflict	UNP Q47066
A	227	LYS	ALA	conflict	UNP Q47066
A	254	GLU	LYS	conflict	UNP Q47066
A	255	ASN	ASP	conflict	UNP Q47066
A	256	HIS	ARG	conflict	UNP Q47066
A	260	VAL	ILE	conflict	UNP Q47066
A	269	GLU	GLN	conflict	UNP Q47066
A	270	GLN	PRO	conflict	UNP Q47066
A	274	ARG	SER	conflict	UNP Q47066
A	278	ILE	VAL	conflict	UNP Q47066
A	281	ALA	SER	conflict	UNP Q47066
A	288	HIS	ASN	conflict	UNP Q47066

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

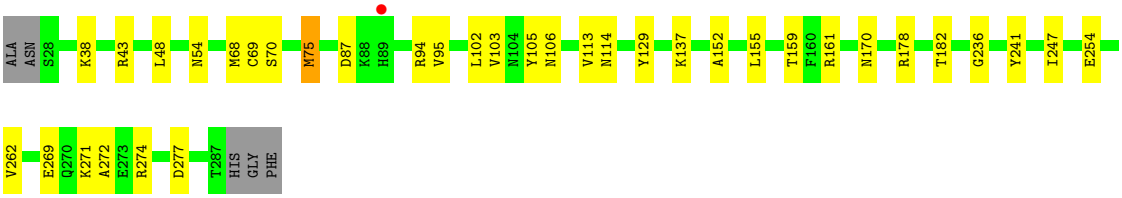
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	135	405	270	135	0	0

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: BETA-LACTAMASE

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	73.31Å 73.31Å 99.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 1.80 39.13 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (6.00-1.80) 98.6 (39.13-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 1.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.182 , 0.217 0.177 , 0.207	Depositor DCC
R_{free} test set	1460 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	18.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2814	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.81	0/1965	1.21	5/2669 (0.2%)

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	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	MET	CG-SD-CE	5.85	109.55	100.20
1	A	68	MET	CG-SD-CE	5.26	108.62	100.20
1	A	43	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	87	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	277	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ARG	Sidechain
1	A	178	ARG	Sidechain
1	A	94	ARG	Sidechain

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	1937	462	1961	14	0
2	A	10	0	0	0	0
3	A	135	270	0	0	0
All	All	2082	732	1961	14	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 4.

All (14) 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:A:75:MET:HE3	1:A:152:ALA:HA	1.79	0.64
1:A:102:LEU:HD11	1:A:113:VAL:CG2	2.36	0.56
1:A:159:THR:HG21	1:A:182:THR:HG23	1.90	0.55
1:A:75:MET:HE1	1:A:155:LEU:HD12	1.91	0.52
1:A:247:ILE:HG22	1:A:262:VAL:HG13	1.92	0.51
1:A:69:CYS:HA	1:A:170:ASN:HD22	1.77	0.50
1:A:113:VAL:O	1:A:114:ASN:HB2	2.11	0.49
1:A:75:MET:CE	1:A:152:ALA:HA	2.42	0.49
1:A:95:VAL:HG11	1:A:137:LYS:HD3	1.95	0.47
1:A:269:GLU:HG2	1:A:272:ALA:HB2	1.99	0.45
1:A:241:TYR:HA	1:A:269:GLU:O	2.18	0.44
1:A:70:SER:HB2	1:A:236:GLY:HA2	1.99	0.43
1:A:38:LYS:HE3	1:A:38:LYS:HB2	1.83	0.43
1:A:105:TYR:HE2	1:A:129:TYR:O	2.02	0.42

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	255/262 (97%)	249 (98%)	5 (2%)	1 (0%)	34 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	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	205/209 (98%)	199 (97%)	6 (3%)	42 29

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	54	ASN
1	A	106	ASN
1	A	254	GLU
1	A	271	LYS
1	A	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	112	HIS
1	A	128	GLN
1	A	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	423	-	4,4,4	0.93	0	6,6,6	0.49	0
2	SO4	A	424	-	4,4,4	0.13	0	6,6,6	0.74	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.

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	257/262 (98%)	-0.54	1 (0%)	92	90	8, 15, 34, 40	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	HIS	2.5

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 monosaccharides 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	SO4	A	424	5/5	0.96	0.09	27,29,30,30	0
2	SO4	A	423	5/5	0.99	0.12	24,30,32,33	0

6.5 Other polymers (i)

There are no such residues in this entry.