Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 10:55 AM EDT

PDB ID	:	5HVI
Title	:	Crystal structure of TEM1 beta-lactamase
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Deposited on	:	2016-01-28
Resolution	:	1.64 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

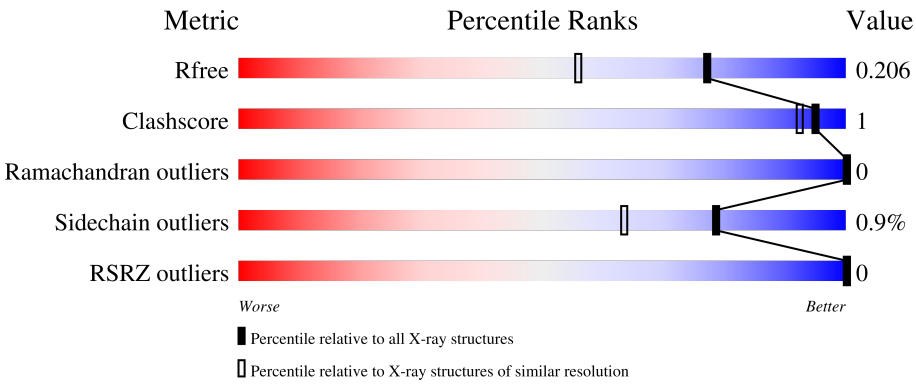
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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 <=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	95%
1	B	263	98%
1	C	263	96%
1	D	263	97%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9049 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
			Total	C	N	O	S			
1	A	263	2023	1260	358	395	10	0	3	0
1	B	263	2025	1261	359	395	10	0	2	0
1	C	263	2024	1262	358	394	10	0	2	0
1	D	263	2010	1256	356	388	10	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

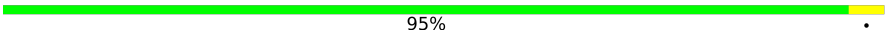
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	232	232	232	0	0
2	B	241	241	241	0	0
2	C	252	252	252	0	0
2	D	242	242	242	0	0

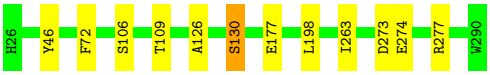
3 Residue-property plots (i)

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 TEM

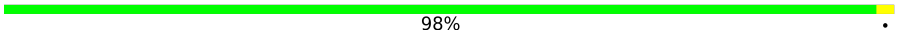
Chain A:





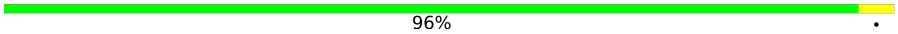
- Molecule 1: Beta-lactamase TEM

Chain B:



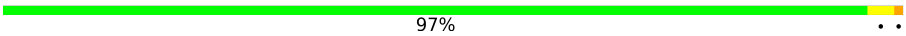
- Molecule 1: Beta-lactamase TEM

Chain C:



- Molecule 1: Beta-lactamase TEM

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.66Å 84.16Å 95.70Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	63.20 – 1.64 63.20 – 1.64	Depositor EDS
% Data completeness (in resolution range)	92.4 (63.20-1.64) 89.2 (63.20-1.64)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.64Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.167 , 0.206 0.166 , 0.206	Depositor DCC
R_{free} test set	5298 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	9.2	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.058 for h,-k,-l	Xtriage
Reported twinning fraction	0.020 for h,-k,-l	Depositor
Outliers	4 of 104957 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9049	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 48.27 % 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 8.8111e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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)

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	0.45	1/2065 (0.0%)	0.56	0/2801
1	B	0.37	0/2064	0.54	0/2798
1	C	0.36	0/2066	0.56	0/2800
1	D	0.41	0/2052	0.58	1/2782 (0.0%)
All	All	0.40	1/8247 (0.0%)	0.56	1/11181 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	GLU	CD-OE1	-7.65	1.17	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	101	ASP	N-CA-C	-6.49	93.47	111.00

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	2023	0	2006	6	0
1	B	2025	0	2015	2	0
1	C	2024	0	2020	6	0
1	D	2010	0	2004	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	232	0	0	0	0
2	B	241	0	0	0	0
2	C	252	0	0	1	1
2	D	242	0	0	2	1
All	All	9049	0	8045	20	1

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 1.

All (20) 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:274[B]:GLU:OE1	1:A:277:ARG:NH1	2.25	0.69
1:A:273:ASP:OD1	1:A:277:ARG:NH2	2.42	0.51
1:C:283:GLY:O	1:C:287:ILE:HG12	2.11	0.50
1:D:52:ASN:ND2	2:D:301:HOH:O	2.34	0.49
1:D:273:ASP:HB3	1:D:277:ARG:NH1	2.27	0.49
1:D:46:TYR:HD1	1:D:263:ILE:HG12	1.80	0.46
1:B:106:SER:HB3	1:B:109:THR:OG1	2.16	0.46
1:C:126:ALA:O	1:C:130:SER:HA	2.17	0.45
1:D:273:ASP:HB3	1:D:277:ARG:HH12	1.81	0.45
1:C:225:LEU:HD11	1:C:231:ILE:HB	2.00	0.44
1:C:206:GLN:NE2	2:C:307:HOH:O	2.43	0.43
1:D:126:ALA:O	1:D:130:SER:HA	2.19	0.43
1:A:126:ALA:O	1:A:130:SER:HA	2.18	0.43
1:A:273:ASP:OD1	1:A:277:ARG:NE	2.49	0.42
1:A:106:SER:HB3	1:A:109:THR:OG1	2.19	0.42
1:C:243[B]:SER:HB3	1:C:266:THR:HG1	1.84	0.42
1:A:46:TYR:HD1	1:A:263:ILE:HG12	1.84	0.41
1:B:46:TYR:HD1	1:B:263:ILE:HG12	1.86	0.41
1:C:273:ASP:HB3	1:C:277:ARG:HH12	1.85	0.41
1:D:111:LYS:HE2	2:D:304:HOH:O	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:449:HOH:O	2:D:404:HOH:O[2_446]	2.13	0.07

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	264/263 (100%)	259 (98%)	5 (2%)	0	100	100
1	B	263/263 (100%)	258 (98%)	5 (2%)	0	100	100
1	C	263/263 (100%)	258 (98%)	5 (2%)	0	100	100
1	D	263/263 (100%)	258 (98%)	5 (2%)	0	100	100
All	All	1053/1052 (100%)	1033 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	216/217 (100%)	213 (99%)	3 (1%)	67	45
1	B	217/217 (100%)	215 (99%)	2 (1%)	78	63
1	C	217/217 (100%)	216 (100%)	1 (0%)	88	80
1	D	213/217 (98%)	211 (99%)	2 (1%)	78	63
All	All	863/868 (99%)	855 (99%)	8 (1%)	78	63

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	PHE
1	A	130	SER

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Mol	Chain	Res	Type
1	A	198	LEU
1	B	30	LEU
1	B	130	SER
1	C	130	SER
1	D	101	ASP
1	D	130	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no ligands in this entry.

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%)	-0.58	0	100	100	5, 10, 23, 38	0
1	B	263/263 (100%)	-0.59	0	100	100	5, 9, 20, 29	0
1	C	263/263 (100%)	-0.59	0	100	100	5, 9, 19, 34	0
1	D	263/263 (100%)	-0.58	0	100	100	5, 9, 20, 44	0
All	All	1052/1052 (100%)	-0.58	0	100	100	5, 9, 20, 44	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.