Full wwPDB Geometry-Only Validation Report (i)

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PDB ID	:	5A90
Title	:	100K Neutron Ligand Free: Exploring the Mechanism of beta-Lactam Ring Protonation in the Class A beta-lactamase Acylation Mechanism Using Neutron and X-ray Crystallography
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Deposited on	:	2015-07-17
Resolution	:	1.70 Å(reported)

This is a Full wwPDB Geometry-Only 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 (1)) were used in the production of this report:

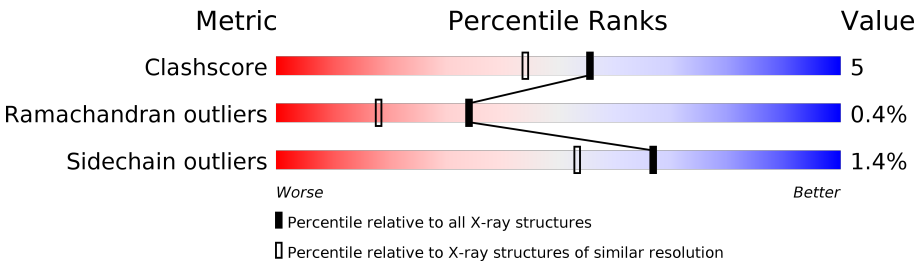
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

The reported resolution of this entry is 1.70 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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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 on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	262	91% 8% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4255 atoms, of which 0 are hydrogens and 1977 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 CTX-M-97.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	D	N	O	S			
1	A	260	3938	1221	1977	349	385	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	ALA	GLU	engineered mutation	UNP E1ANH6
A	274	ASN	SER	conflict	UNP E1ANH6
A	276	ASN	ARG	conflict	UNP E1ANH6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	317	317	317	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 CTX-M-97

Chain A:

4 Model quality (i)

4.1 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	0.41	0/1991	0.59	0/2703

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3938	0	1977	20	0
2	A	317	0	0	18	3
All	All	4255	0	1977	20	3

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.

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:99:LYS:NZ	2:A:2127:HOH:O	2.00	0.94
1:A:186:MET:SD	2:A:2077:HOH:O	2.28	0.92
1:A:203:GLN:NE2	2:A:2093:HOH:O	2.08	0.85
1:A:85:GLU:N	2:A:2093:HOH:O	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:NZ	2:A:2015:HOH:O	2.16	0.79
1:A:107:PRO:O	2:A:2141:HOH:O	2.10	0.69
1:A:50:ASN:OD1	2:A:2033:HOH:O	2.13	0.65
1:A:202:THR:O	2:A:2234:HOH:O	2.17	0.62
1:A:290:PHE:N	2:A:2309:HOH:O	2.40	0.55
1:A:227:LYS:O	2:A:2272:HOH:O	2.22	0.54
1:A:288:HIS:O	1:A:290:PHE:N	2.40	0.54
1:A:28:SER:N	1:A:31:GLN:HE21	2.01	0.53
1:A:31:GLN:NE2	2:A:2005:HOH:O	2.40	0.49
1:A:85:GLU:CA	2:A:2093:HOH:O	2.59	0.46
1:A:281:ALA:O	2:A:2305:HOH:O	2.25	0.45
1:A:272:ALA:O	2:A:2284:HOH:O	2.26	0.43
1:A:55:SER:OG	2:A:2045:HOH:O	2.18	0.43
1:A:84:SER:OG	2:A:2093:HOH:O	2.25	0.42
1:A:121:GLU:O	2:A:2158:HOH:O	2.26	0.41
1:A:110:GLU:O	2:A:2145:HOH:O	2.26	0.40

All (3) 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:A:2095:HOH:O	2:A:2262:HOH:O[3_455]	1.99	0.21
2:A:2061:HOH:O	2:A:2123:HOH:O[5_555]	2.18	0.02
2:A:2315:HOH:O	2:A:2315:HOH:O[5_555]	2.19	0.01

4.3 Torsion angles (i)

4.3.1 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	258/262 (98%)	252 (98%)	5 (2%)	1 (0%)	34 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	GLY

4.3.2 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	208/209 (100%)	205 (99%)	3 (1%)	67 53

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	233	ASP
1	A	288	HIS

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

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no carbohydrates in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.