WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB Geometry-Only Validation Summary Report ⓘ

May 27, 2024 – 06:29 PM EDT

PDB ID	:	5KSC
Title	:	E166A/R274N/R276N Toho-1 Beta-lactamase aztreonam acyl-enzyme intermediate
Authors	:	Vandavasi, V.G.; Langan, P.S.; Weiss, K.; Parks, J.M.; Cooper, J.B.; Ginell, S.L.; Coates, L.
Deposited on	:	2016-07-08
Resolution	:	2.10 Å(reported)

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

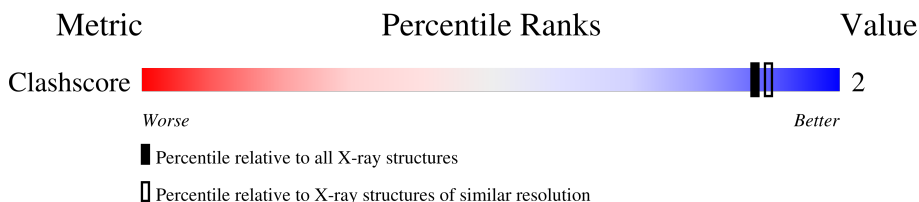|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Clashscore		2

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	261	96% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2071 atoms, of which 0 are hydrogens and 48 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.
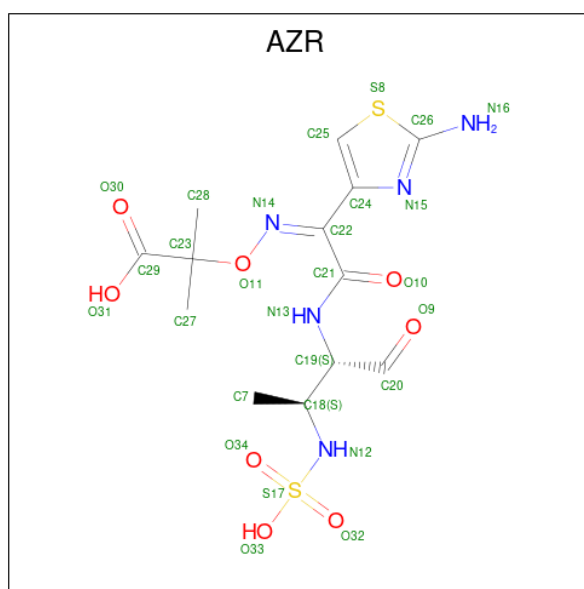
- Molecule 1 is a protein called Beta-lactamase Toho-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total 1966	C 1224	N 350	O 386	S 6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ALA	GLU	engineered mutation	UNP Q47066
A	271	ASN	ARG	engineered mutation	UNP Q47066
A	273	ASN	ARG	engineered mutation	UNP Q47066

- Molecule 2 is 2-({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-oxo-2-{[(2S,3S)-1-oxo-3-(sulfoamino) butan-2-yl]amino}ethylidene]amino}oxy)-2-methylpropanoic acid (three-letter code: AZR) (formula: $C_{13}H_{19}N_5O_8S_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 13	N 5	O 8	S 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	29	77	48	29	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. 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 Toho-1

Chain A:

96%

N27 V79 R93 S129 L137 D156 P176 T179 Q202 A280 T284 F287

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

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	0.24	0/1996	0.40	0/2710

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 ⓘ

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	1966	0	1978	8	0
2	A	28	0	17	2	0
3	A	77	0	0	2	0
All	All	2071	0	1995	8	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 2.

The worst 5 of 8 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:129:SER:OG	2:A:301:AZR:N12	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:OD2	3:A:401:DOD:O	2.23	0.52
1:A:202:GLN:OE1	1:A:202:GLN:N	2.46	0.49
1:A:79:VAL:HG21	1:A:137:LEU:HD22	1.86	0.47
1:A:280:ALA:O	1:A:284:THR:OG1	2.23	0.47

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

1 ligand is 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	AZR	A	301	1	23,28,28	4.23	13 (56%)	22,41,41	3.11	7 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AZR	A	301	1	-	13/28/35/35	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	AZR	C25-S8	-11.17	1.53	1.70
2	A	301	AZR	O32-S17	8.19	1.51	1.42
2	A	301	AZR	O34-S17	8.09	1.51	1.42
2	A	301	AZR	C24-N15	6.35	1.57	1.37
2	A	301	AZR	C18-N12	-5.94	1.42	1.47

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	AZR	N16-C26-N15	11.51	138.08	123.19
2	A	301	AZR	O11-N14-C22	4.50	118.86	111.87
2	A	301	AZR	O32-S17-O34	-3.82	111.14	120.16
2	A	301	AZR	C22-C21-N13	3.37	119.98	114.38
2	A	301	AZR	C24-C25-S8	-3.21	107.85	111.79

There are no chirality outliers.
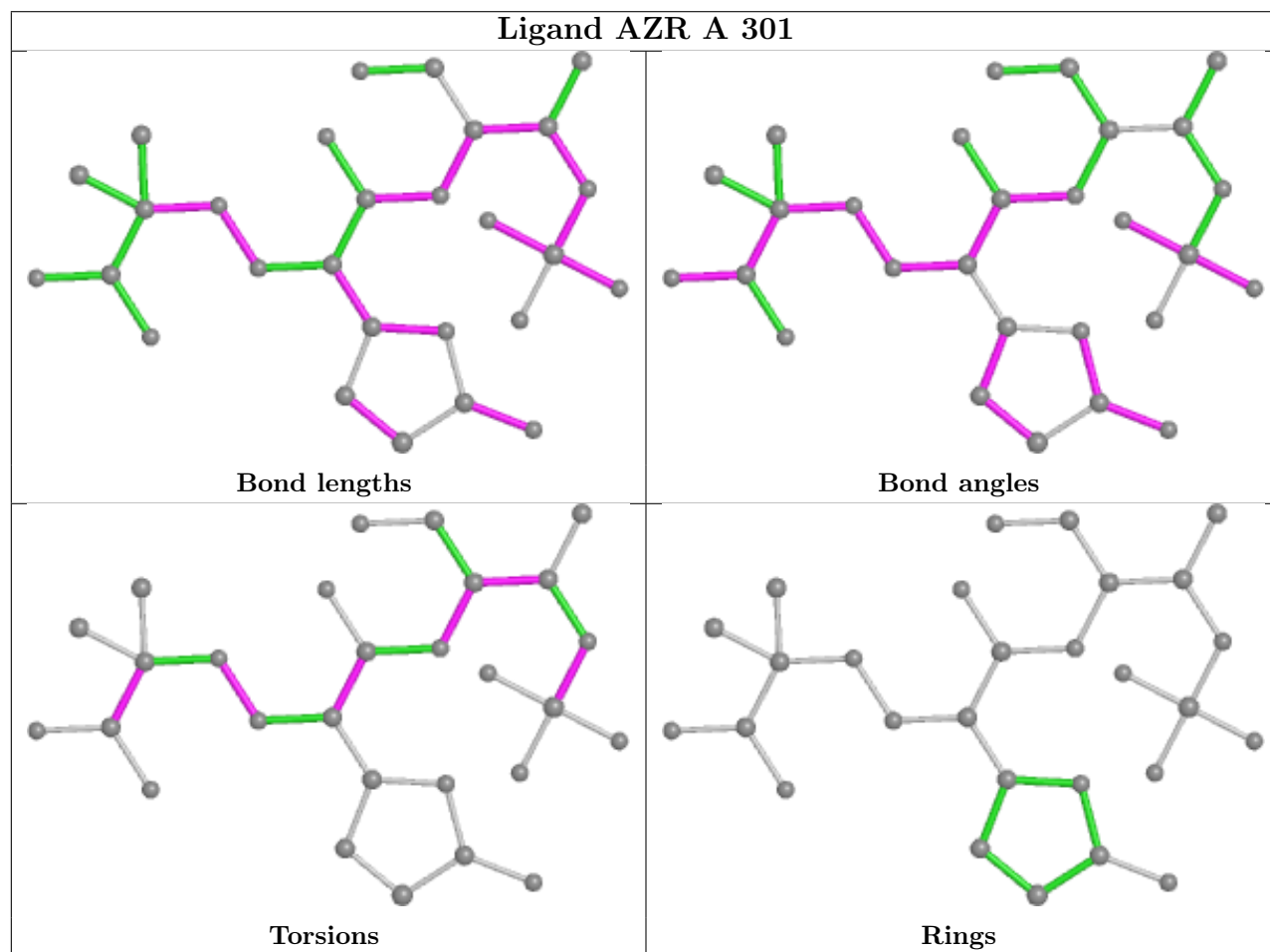
5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	AZR	C22-N14-O11-C23
2	A	301	AZR	C18-N12-S17-O34
2	A	301	AZR	C7-C18-C19-N13
2	A	301	AZR	C7-C18-C19-C20
2	A	301	AZR	N12-C18-C19-N13

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	AZR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AZR A 301

Bond lengths

Bond angles

Torsions

Rings

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.