



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:09 pm BST

PDB ID : 4N92
Title : Crystal structure of beta-lactamase PenP_E166S
Authors : Pan, X.; Wong, W.; Zhao, Y.
Deposited on : 2013-10-19
Resolution : 1.93 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

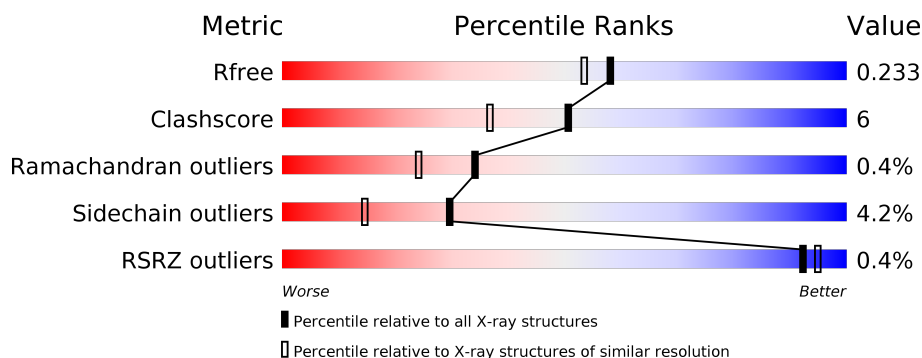
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 $\leq 5\%$. 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	268	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	268	<div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4529 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	256	Total	C	N	O	S	0	10	0
			2052	1296	350	403	3			
1	A	256	Total	C	N	O	S	0	10	0
			2052	1296	350	403	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	GLY	-	EXPRESSION TAG	UNP P00808
B	24	PRO	-	EXPRESSION TAG	UNP P00808
B	25	MET	-	EXPRESSION TAG	UNP P00808
B	166	SER	GLU	ENGINEERED MUTATION	UNP P00808
A	23	GLY	-	EXPRESSION TAG	UNP P00808
A	24	PRO	-	EXPRESSION TAG	UNP P00808
A	25	MET	-	EXPRESSION TAG	UNP P00808
A	166	SER	GLU	ENGINEERED MUTATION	UNP P00808

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	277	Total	O	0	0
			277	277		
2	A	148	Total	O	0	0
			148	148		

- Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.31Å 46.19Å 66.28Å 78.43° 75.71° 69.36°	Depositor
Resolution (Å)	42.88 – 1.93 42.88 – 1.93	Depositor EDS
% Data completeness (in resolution range)	92.8 (42.88-1.93) 92.8 (42.88-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.61 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.230 0.183 , 0.233	Depositor DCC
R_{free} test set	1648 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.22% 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

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	0.95	5/2112 (0.2%)	1.03	8/2859 (0.3%)
1	B	0.99	5/2112 (0.2%)	1.02	6/2859 (0.2%)
All	All	0.97	10/4224 (0.2%)	1.03	14/5718 (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	2
1	B	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	ALA	C-N	14.26	1.66	1.34
1	B	252	PRO	C-N	12.55	1.58	1.34
1	B	238	ALA	C-N	11.75	1.61	1.34
1	A	252	PRO	C-N	10.76	1.54	1.34
1	A	57	VAL	C-N	6.46	1.48	1.34
1	B	83[A]	GLN	C-N	5.93	1.47	1.34
1	B	83[B]	GLN	C-N	5.93	1.47	1.34
1	A	109	THR	CB-OG1	-5.61	1.32	1.43
1	B	57	VAL	C-N	5.53	1.46	1.34
1	A	268	ASP	CB-CG	5.29	1.62	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	204	ARG	NE-CZ-NH2	-9.42	115.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83[A]	GLN	O-C-N	-8.40	109.26	122.70
1	A	83[B]	GLN	O-C-N	-8.40	109.26	122.70
1	B	83[A]	GLN	O-C-N	-7.92	110.03	122.70
1	B	83[B]	GLN	O-C-N	-7.92	110.03	122.70
1	A	267	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	128	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	204	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	204	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	179	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	213	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	157	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	128	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83[A]	GLN	Mainchain
1	A	83[B]	GLN	Mainchain
1	B	57	VAL	Mainchain

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	2052	0	2105	30	1
1	B	2052	0	2105	21	0
2	A	148	0	0	5	0
2	B	277	0	0	5	1
All	All	4529	0	4210	47	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 6.

All (47) 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:227:ASP:O	1:A:111:LYS:HE3	1.36	1.24
1:B:77[B]:VAL:HG21	1:B:127:LEU:HD11	1.45	0.98
1:B:227:ASP:O	1:A:111:LYS:CE	2.22	0.88
1:A:77[B]:VAL:HG21	1:A:127:LEU:HD11	1.59	0.84
1:B:228:GLY:HA3	1:A:111:LYS:HD2	1.64	0.80
1:A:51:THR:HG22	1:A:257:ASP:HB3	1.66	0.78
1:B:51:THR:HB	1:B:258:PRO:O	1.91	0.69
1:A:254:PRO:HG2	1:A:255:LYS:NZ	2.13	0.63
1:A:268:ASP:CB	2:A:343:HOH:O	2.47	0.63
1:A:51:THR:HB	1:A:258:PRO:O	1.99	0.62
1:A:268:ASP:HB3	2:A:343:HOH:O	2.02	0.60
1:B:228:GLY:HA3	1:A:111:LYS:CD	2.30	0.59
1:B:33:PHE:CE1	1:B:46[A]:ILE:HD13	2.37	0.59
1:A:163:GLU:OE2	1:A:178[A]:GLN:HB2	2.04	0.57
1:A:33:PHE:CD1	1:A:46[A]:ILE:HD13	2.40	0.57
1:A:33:PHE:CE1	1:A:46[A]:ILE:HD13	2.41	0.56
1:B:112:HIS:HD2	2:B:538:HOH:O	1.89	0.55
1:B:53:THR:HG21	1:B:55:ARG:HH12	1.72	0.55
1:B:51:THR:HG21	2:B:421:HOH:O	2.07	0.53
1:A:73:LYS:HE3	1:A:135:GLN:HB2	1.90	0.52
1:B:103:VAL:HB	2:B:414:HOH:O	2.09	0.52
1:A:124:ASP:OD2	2:A:364:HOH:O	2.19	0.50
1:A:119:LEU:HD21	1:A:141[A]:GLN:HG3	1.93	0.50
1:A:207:LEU:O	1:A:211:MET:HG3	2.12	0.50
1:A:254:PRO:HG2	1:A:255:LYS:HZ1	1.75	0.49
1:A:51:THR:CG2	1:A:257:ASP:HB3	2.37	0.49
1:B:51:THR:CG2	2:B:421:HOH:O	2.61	0.48
1:A:107:PRO:O	1:A:111:LYS:HE2	2.13	0.48
1:A:255:LYS:H	1:A:255:LYS:HE2	1.80	0.46
1:A:252:PRO:HB2	1:A:255:LYS:O	2.17	0.45
1:A:59:ALA:HB1	1:A:62:PRO:HG3	1.99	0.44
1:A:243:THR:HA	1:A:265:SER:O	2.18	0.44
1:B:83[B]:GLN:OE1	2:B:475:HOH:O	2.21	0.44
1:A:139[B]:LEU:HD11	2:A:431:HOH:O	2.17	0.44
1:B:77[B]:VAL:HG23	1:B:207:LEU:HD13	2.00	0.43
1:A:35:LYS:HB2	1:A:35:LYS:NZ	2.34	0.43
1:A:48:ALA:O	1:A:56:THR:HA	2.19	0.43
1:A:74:ALA:HA	1:A:127:LEU:HD21	2.01	0.43
1:B:48:ALA:HB2	1:B:261:LEU:HD13	2.01	0.42
1:A:202[A]:GLU:HB2	2:A:425:HOH:O	2.19	0.42
1:B:51:THR:HG22	1:B:257:ASP:HB3	2.01	0.42
1:B:225:VAL:CG1	1:B:229:TRP:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77[B]:VAL:HG23	1:A:207:LEU:HD13	2.02	0.42
1:B:152:LEU:O	1:B:155:ILE:HG13	2.20	0.42
1:B:225:VAL:HG12	1:B:229:TRP:HB2	2.03	0.41
1:B:149:LYS:HB2	1:B:162:PRO:HD2	2.03	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)
1:A:99:ARG:NH1	2:B:375:HOH:O[1_645]	2.17	0.03

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	264/268 (98%)	257 (97%)	6 (2%)	1 (0%)	34	24
1	B	264/268 (98%)	258 (98%)	5 (2%)	1 (0%)	34	24
All	All	528/536 (98%)	515 (98%)	11 (2%)	2 (0%)	34	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	VAL
1	B	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	226/226 (100%)	214 (95%)	12 (5%)	22	9
1	B	226/226 (100%)	218 (96%)	8 (4%)	36	21
All	All	452/452 (100%)	432 (96%)	20 (4%)	30	13

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	THR
1	B	163	GLU
1	B	167	PRO
1	B	202[A]	GLU
1	B	202[B]	GLU
1	B	233	ASP
1	B	255	LYS
1	B	268	ASP
1	A	31	ASP
1	A	51	THR
1	A	55	ARG
1	A	56	THR
1	A	130	SER
1	A	150	LYS
1	A	163	GLU
1	A	202[A]	GLU
1	A	202[B]	GLU
1	A	233	ASP
1	A	255	LYS
1	A	268	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	GLN
1	B	93	GLN
1	B	112	HIS
1	B	170	ASN
1	A	112	HIS
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 carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	238:ALA	C	240:SER	N	1.66
1	B	238:ALA	C	240:SER	N	1.61

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	256/268 (95%)	-0.36	2 (0%) 86 89	7, 14, 28, 58	0
1	B	256/268 (95%)	-0.39	0 100 100	8, 14, 28, 45	0
All	All	512/536 (95%)	-0.37	2 (0%) 92 95	7, 14, 28, 58	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	LYS	2.7
1	A	254	PRO	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 carbohydrates 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.