Full wwPDB X-ray Structure Validation Report (i)

Feb 7, 2017 – 01:38 PM EST

PDB ID	:	5GLA
Title	:	Crystal strucutre of the class A beta-lactamase PenL-tTR10 containing 10 residues insertion in omega-loop
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Deposited on	:	2016-07-10
Resolution	:	1.50 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
http://wwpdb.org/validation/2016/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:

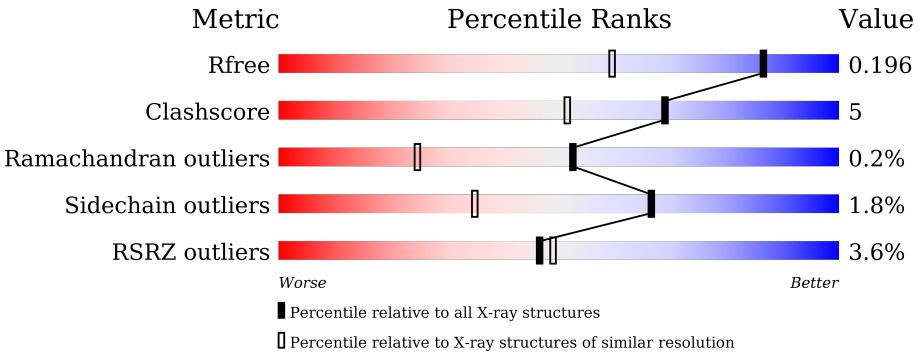
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.50 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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. 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	278	4% 88% 7% ·
1	B	278	3% 86% 9% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4598 atoms, of which 23 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	A	267	Total	C	H	N	O	S	0	0	0
			2007	1238	3	380	378	8			
1	B	266	Total	C	H	N	O	S	0	0	0
			2019	1235	20	379	377	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP A0A096YVR7
A	23	SER	-	expression tag	UNP A0A096YVR7
A	24	HIS	-	expression tag	UNP A0A096YVR7
A	25	MET	-	expression tag	UNP A0A096YVR7
A	173	ILE	-	insertion	UNP A0A096YVR7
A	174	PRO	-	insertion	UNP A0A096YVR7
A	175	GLY	-	insertion	UNP A0A096YVR7
A	176	ASP	-	insertion	UNP A0A096YVR7
A	177	GLU	-	insertion	UNP A0A096YVR7
A	178	ARG	-	insertion	UNP A0A096YVR7
A	179	ASP	-	insertion	UNP A0A096YVR7
A	180	THR	-	insertion	UNP A0A096YVR7
A	181	THR	-	insertion	UNP A0A096YVR7
A	182	THR	-	insertion	UNP A0A096YVR7
B	22	GLY	-	expression tag	UNP A0A096YVR7
B	23	SER	-	expression tag	UNP A0A096YVR7
B	24	HIS	-	expression tag	UNP A0A096YVR7
B	25	MET	-	expression tag	UNP A0A096YVR7
B	173	ILE	-	insertion	UNP A0A096YVR7
B	174	PRO	-	insertion	UNP A0A096YVR7
B	175	GLY	-	insertion	UNP A0A096YVR7
B	176	ASP	-	insertion	UNP A0A096YVR7
B	177	GLU	-	insertion	UNP A0A096YVR7
B	178	ARG	-	insertion	UNP A0A096YVR7
B	179	ASP	-	insertion	UNP A0A096YVR7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	THR	-	insertion	UNP A0A096YVR7
B	181	THR	-	insertion	UNP A0A096YVR7
B	182	THR	-	insertion	UNP A0A096YVR7

- Molecule 2 is water.

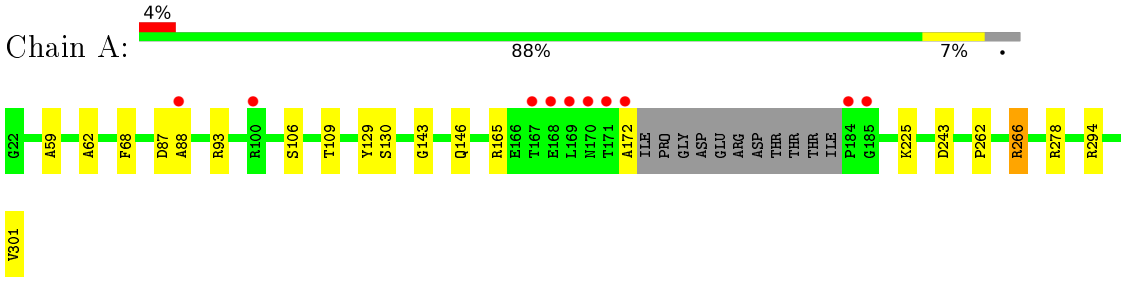
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	297	Total O 297 297	0	0
2	B	275	Total O 275 275	0	0

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 errors 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.

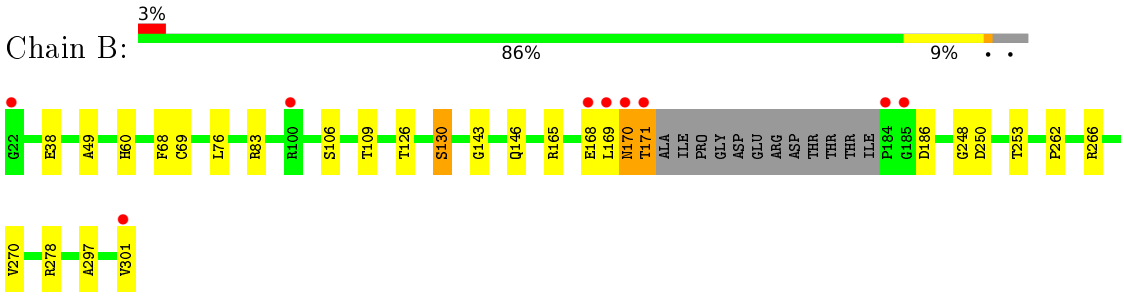
- Molecule 1: Beta-lactamase

Chain A:



- Molecule 1: Beta-lactamase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	35.03Å 92.55Å 68.87Å 90.00° 92.61° 90.00°	Depositor
Resolution (Å)	32.24 – 1.50 32.24 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.24-1.50) 99.8 (32.24-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.11 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.169 , 0.196 0.170 , 0.196	Depositor DCC
R_{free} test set	3534 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4598	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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

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	0.48	1/2034 (0.0%)	0.63	2/2757 (0.1%)
1	B	0.43	0/2029	0.68	4/2750 (0.1%)
All	All	0.46	1/4063 (0.0%)	0.65	6/5507 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	TYR	CG-CD2	-5.05	1.32	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	ARG	NE-CZ-NH2	10.69	125.64	120.30
1	A	278	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	B	278	ARG	NE-CZ-NH1	-9.11	115.75	120.30
1	A	278	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	171	THR	N-CA-CB	6.07	121.83	110.30
1	B	186	ASP	CB-CG-OD2	-5.07	113.74	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2004	3	2003	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1999	20	1998	23	0
2	A	297	0	0	7	0
2	B	275	0	0	6	0
All	All	4575	23	4001	37	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 5.

All (37) 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:143:GLY:O	1:A:146:GLN:NE2	1.73	1.20
1:B:69:CYS:SG	1:B:171:THR:OG1	2.10	1.07
1:A:87:ASP:OD2	1:A:88:ALA:N	2.01	0.93
1:B:171:THR:HA	1:B:250:ASP:OD1	1.77	0.84
1:B:171:THR:OG1	1:B:248:GLY:HA3	1.77	0.83
1:B:171:THR:HG21	1:B:253:THR:OG1	1.83	0.77
1:B:171:THR:HB	1:B:250:ASP:N	1.99	0.77
1:B:170:ASN:HB2	2:B:463:HOH:O	1.90	0.70
1:B:262:PRO:HB2	1:B:266:ARG:HB2	1.82	0.61
1:B:83:ARG:HD2	2:B:502:HOH:O	2.01	0.59
1:B:169:LEU:O	1:B:170:ASN:O	2.20	0.59
1:A:225:LYS:HE3	2:A:422:HOH:O	2.05	0.57
1:B:266:ARG:NH2	2:B:409:HOH:O	2.38	0.56
1:A:172:ALA:HB1	2:A:406:HOH:O	2.10	0.51
1:A:106:SER:HB3	1:A:109:THR:OG1	2.11	0.51
1:A:165:ARG:NH1	2:A:412:HOH:O	2.44	0.50
1:B:143:GLY:O	1:B:146:GLN:NE2	2.33	0.49
1:A:59:ALA:HB1	1:A:62:ALA:HB2	1.95	0.48
1:B:38:GLU:OE2	1:B:60:HIS:HE1	1.97	0.48
1:A:262:PRO:HB2	1:A:266:ARG:HG3	1.97	0.47
1:B:170:ASN:O	1:B:171:THR:C	2.51	0.47
1:A:225:LYS:CE	2:A:422:HOH:O	2.62	0.47
1:B:165:ARG:NH2	2:B:414:HOH:O	2.47	0.47
1:A:294:ARG:NH1	2:A:413:HOH:O	2.44	0.47
1:B:266:ARG:CZ	2:B:409:HOH:O	2.63	0.47
1:B:171:THR:HG21	1:B:253:THR:HG1	1.80	0.46
1:B:266:ARG:NE	2:B:409:HOH:O	2.47	0.46
1:A:301:VAL:HG13	1:A:301:VAL:O	2.16	0.45
1:A:87:ASP:OD2	1:A:87:ASP:C	2.54	0.45
1:B:126:THR:O	1:B:130:SER:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:NH2	2:A:410:HOH:O	2.43	0.43
1:B:49:ALA:HA	1:B:270:VAL:O	2.17	0.43
1:A:93:ARG:NE	2:A:410:HOH:O	2.49	0.42
1:B:168:GLU:OE1	1:B:168:GLU:N	2.50	0.41
1:B:171:THR:CB	1:B:248:GLY:HA3	2.49	0.40
1:B:297:ALA:O	1:B:301:VAL:HG13	2.22	0.40
1:B:106:SER:HB3	1:B:109:THR:OG1	2.22	0.40

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	263/278 (95%)	254 (97%)	9 (3%)	0	100 100
1	B	262/278 (94%)	255 (97%)	6 (2%)	1 (0%)	39 14
All	All	525/556 (94%)	509 (97%)	15 (3%)	1 (0%)	52 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ASN

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	197/207 (95%)	193 (98%)	4 (2%)	63 29
1	B	197/207 (95%)	194 (98%)	3 (2%)	72 44
All	All	394/414 (95%)	387 (98%)	7 (2%)	66 35

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	PHE
1	A	130	SER
1	A	243	ASP
1	A	266	ARG
1	B	68	PHE
1	B	76	LEU
1	B	130	SER

Some 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 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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	267/278 (96%)	-0.01	10 (3%) 45 48	6, 11, 26, 42	0
1	B	266/278 (95%)	-0.01	9 (3%) 49 51	6, 12, 24, 40	1 (0%)
All	All	533/556 (95%)	-0.01	19 (3%) 46 49	6, 11, 26, 42	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	ALA	10.0
1	A	171	THR	7.9
1	A	185	GLY	7.1
1	B	170	ASN	6.4
1	B	171	THR	6.2
1	A	172	ALA	6.0
1	B	185	GLY	5.0
1	B	169	LEU	4.6
1	B	184	PRO	4.4
1	A	170	ASN	3.6
1	A	167	THR	3.5
1	A	184	PRO	3.3
1	B	301	VAL	3.2
1	B	168	GLU	3.1
1	A	169	LEU	2.8
1	A	168	GLU	2.8
1	A	100	ARG	2.5
1	B	22	GLY	2.3
1	B	100	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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.