



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:00 PM GMT

PDB ID : 5ACQ
Title : W228A-Investigation of the impact from residues W228 and Y233 in the met
allo-beta-lactamase GIM-1
Authors : Skagseth, S.; Carlsen, T.J.; Bjerga, G.E.K.; Spencer, J.; Samuelsen, O.; Leiros,
H.-K.S.
Deposited on : 2015-08-17
Resolution : 1.70 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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-20026982

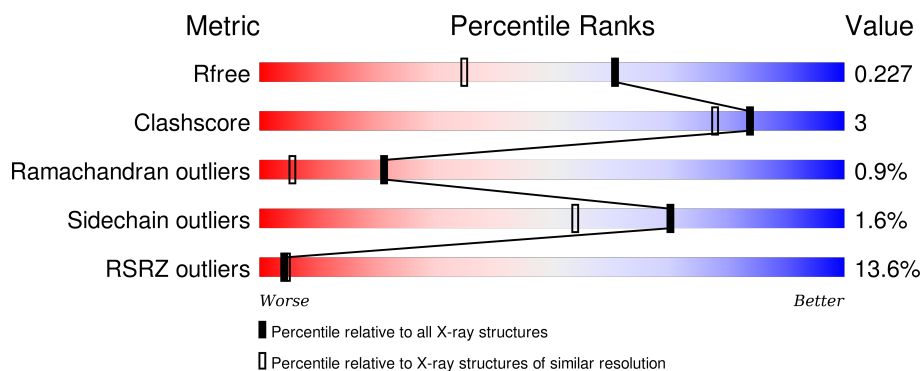
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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))
R_{free}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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	250	<div> <div>6%</div> <div>80%</div> <div>8%</div> <div>13%</div> </div>
1	B	250	<div> <div>18%</div> <div>80%</div> <div>6%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	B	1296	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7013 atoms, of which 3346 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	218	Total	C	H	N	O	S	4	2	0
			3381	1081	1682	280	334	4			
1	B	217	Total	C	H	N	O	S	5	1	0
			3348	1072	1664	276	333	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ALA	TRP	ENGINEERED MUTATION	UNP Q704V1
B	228	ALA	TRP	ENGINEERED MUTATION	UNP Q704V1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	196	Total	O	0	0
			196	196		
3	B	85	Total	O	0	0
			85	85		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.55Å 131.80Å 40.58Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70 25.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.8 (25.00-1.70) 95.7 (25.00-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.188 , 0.227 0.188 , 0.227	Depositor DCC
R_{free} test set	2135 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.6	EDS
Estimated twinning fraction	0.039 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 42278 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.64	0/1731	0.74	0/2350
1	B	0.48	0/1715	0.61	1/2328 (0.0%)
All	All	0.57	0/3446	0.68	1/4678 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	182	LEU	CA-CB-CG	5.39	127.69	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	123	ALA	Peptide

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	1699	1682	1670	12	1
1	B	1684	1664	1656	9	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	A	196	0	0	2	1
3	B	85	0	0	3	1
All	All	3667	3346	3326	20	2

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 3.

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:B:263:HIS:NE2	3:B:2010:HOH:O	2.05	0.90
1:B:173:LYS:NZ	3:B:2046:HOH:O	2.19	0.73
1:A:258[A]:MET:SD	1:A:277:VAL:HG11	2.31	0.71
1:A:257:GLN:NE2	3:A:2010:HOH:O	2.23	0.67
1:B:89:GLU:OE1	3:B:2015:HOH:O	2.13	0.67
1:B:68:ASP:O	1:B:263:HIS:ND1	2.29	0.65
1:A:221:OCS:OD3	1:A:263:HIS:CD2	2.54	0.61
1:A:179:GLU:OE2	1:A:252:LYS:NZ	2.34	0.60
1:A:40:LYS:HD3	1:A:66:LEU:HD21	1.89	0.54
1:A:181[B]:THR:HG21	1:A:185:GLY:HA2	1.88	0.54
1:B:59:LYS:HG2	1:B:87:TRP:CE2	2.42	0.53
1:A:258[A]:MET:HG3	1:A:277:VAL:CG1	2.44	0.47
1:A:196:HIS:CD2	1:A:221:OCS:HB3	2.51	0.46
1:A:64:TYR:CE1	1:B:67:VAL:HB	2.50	0.46
1:A:258[A]:MET:CG	1:A:277:VAL:CG1	2.94	0.46
1:B:123:ALA:HA	1:B:126:LYS:H	1.80	0.46
1:B:258:MET:HE3	1:B:277:VAL:HG21	1.97	0.44
1:A:252:LYS:O	3:A:2176:HOH:O	2.21	0.44
1:A:197:THR:H	1:A:200:ASN:ND2	2.15	0.44
1:B:59:LYS:HB2	1:B:67:VAL:CG2	2.49	0.42

All (2) 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:229:GLU:OE2	3:A:2107:HOH:O[1_554]	2.04	0.16
3:B:2015:HOH:O	3:B:2081:HOH:O[1_556]	2.11	0.09

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	217/250 (87%)	210 (97%)	5 (2%)	2 (1%)	21	5
1	B	215/250 (86%)	205 (95%)	8 (4%)	2 (1%)	21	5
All	All	432/500 (86%)	415 (96%)	13 (3%)	4 (1%)	21	5

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	ASP
1	A	84	ASP
1	B	63	GLY
1	A	195	GLY

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	186/211 (88%)	185 (100%)	1 (0%)	92	88
1	B	184/211 (87%)	179 (97%)	5 (3%)	52	31
All	All	370/422 (88%)	364 (98%)	6 (2%)	70	54

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	B	87	TRP
1	B	89	GLU
1	B	121	ARG
1	B	226	HIS
1	B	257	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	B	200	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	OCS	A	221	1,2	6,8,9	2.20	1 (16%)	7,11,13	2.01	3 (42%)
1	OCS	B	221	1	6,8,9	1.29	1 (16%)	7,11,13	3.03	3 (42%)

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
1	OCS	A	221	1,2	-	0/4/7/9	0/0/0/0
1	OCS	B	221	1	-	0/4/7/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	221	OCS	CB-SG	-4.51	1.72	1.77
1	B	221	OCS	CB-SG	2.34	1.80	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	OCS	OD3-SG-CB	-4.98	103.41	106.92
1	A	221	OCS	OD3-SG-CB	-2.99	104.82	106.92
1	A	221	OCS	O-C-CA	-2.71	118.46	125.72
1	B	221	OCS	OD2-SG-CB	2.34	109.84	104.99
1	A	221	OCS	OD3-SG-OD1	2.72	121.64	113.96
1	B	221	OCS	OD1-SG-CB	5.44	110.75	106.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	221	OCS	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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	217/250 (86%)	0.28	15 (6%)	20 22	20, 33, 50, 72	11 (5%)
1	B	216/250 (86%)	1.15	44 (20%)	1 1	31, 54, 73, 90	15 (6%)
All	All	433/500 (86%)	0.72	59 (13%)	4 5	20, 42, 72, 90	26 (6%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	TRP	18.9
1	B	64	TYR	7.7
1	B	121	ARG	6.9
1	B	294	SER	6.2
1	A	64	TYR	5.1
1	B	293	ALA	5.0
1	B	123	ALA	4.8
1	B	218	PHE	4.2
1	B	220	GLY	4.1
1	A	294	SER	4.0
1	A	66	LEU	3.9
1	A	218	PHE	3.7
1	A	115	THR	3.5
1	B	287	ILE	3.4
1	B	219	GLY	3.4
1	B	113	ILE	3.3
1	B	61	ILE	3.2
1	A	61	ILE	3.1
1	B	291	GLU	3.1
1	A	220	GLY	3.0
1	A	121	ARG	3.0
1	B	184	ASN	3.0
1	B	66	LEU	3.0
1	B	148	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	83	ILE	2.8
1	B	295	ASN	2.8
1	B	90	GLU	2.7
1	B	234	VAL	2.7
1	B	247	LYS	2.7
1	B	223	VAL	2.7
1	B	263	HIS	2.6
1	B	41	PRO	2.6
1	B	120	ASP	2.5
1	B	222	LEU	2.5
1	B	62	GLU	2.5
1	B	122	THR	2.5
1	B	173	LYS	2.5
1	A	253	LYS	2.4
1	B	63	GLY	2.4
1	B	185	GLY	2.4
1	A	251	SER	2.3
1	B	59	LYS	2.3
1	B	67	VAL	2.3
1	B	149	GLU	2.3
1	A	222	LEU	2.3
1	B	201	ILE	2.3
1	B	292	SER	2.2
1	B	85	THR	2.2
1	B	78	ASN	2.2
1	B	72	LEU	2.1
1	B	202	VAL	2.1
1	B	289	LEU	2.1
1	A	83	ILE	2.1
1	A	150	GLY	2.1
1	A	219	GLY	2.1
1	B	58	PHE	2.0
1	B	260	VAL	2.0
1	B	115	THR	2.0
1	A	67	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	OCS	A	221	9/10	0.82	0.25	-	24,32,47,54	2
1	OCS	B	221	9/10	0.94	0.17	-	39,44,51,51	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	B	1296	1/1	0.95	0.24	5.43	43,43,43,43	1
2	ZN	A	1297	1/1	0.99	0.23	0.92	17,17,17,17	1
2	ZN	A	1296	1/1	0.82	0.10	-1.28	35,35,35,35	1

6.5 Other polymers [i](#)

There are no such residues in this entry.