



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:48 pm BST

PDB ID : 5ODZ
Title : CRYSTAL STRUCTURE OF THE BETA-LACTAMASE OXA-163
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Deposited on : 2017-07-07
Resolution : 2.07 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

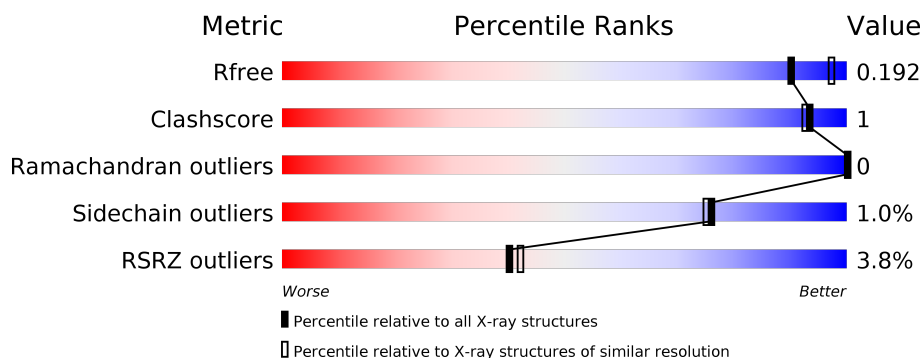
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	B	252	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
1	D	252	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8102 atoms, of which 3791 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	238	Total	C	H	N	O	S	0	6	0
			3832	1245	1880	340	359	8			
1	D	239	Total	C	H	N	O	S	0	8	0
			3871	1256	1897	349	361	8			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP F6KZJ2
B	11	HIS	-	expression tag	UNP F6KZJ2
B	12	HIS	-	expression tag	UNP F6KZJ2
B	13	HIS	-	expression tag	UNP F6KZJ2
B	14	HIS	-	expression tag	UNP F6KZJ2
B	15	HIS	-	expression tag	UNP F6KZJ2
B	16	GLU	-	expression tag	UNP F6KZJ2
B	17	ASN	-	expression tag	UNP F6KZJ2
B	18	LEU	-	expression tag	UNP F6KZJ2
B	19	TYR	-	expression tag	UNP F6KZJ2
B	20	PHE	-	expression tag	UNP F6KZJ2
B	21	GLN	-	expression tag	UNP F6KZJ2
B	22	GLY	-	expression tag	UNP F6KZJ2
D	10	HIS	-	expression tag	UNP F6KZJ2
D	11	HIS	-	expression tag	UNP F6KZJ2
D	12	HIS	-	expression tag	UNP F6KZJ2
D	13	HIS	-	expression tag	UNP F6KZJ2
D	14	HIS	-	expression tag	UNP F6KZJ2
D	15	HIS	-	expression tag	UNP F6KZJ2
D	16	GLU	-	expression tag	UNP F6KZJ2
D	17	ASN	-	expression tag	UNP F6KZJ2
D	18	LEU	-	expression tag	UNP F6KZJ2
D	19	TYR	-	expression tag	UNP F6KZJ2
D	20	PHE	-	expression tag	UNP F6KZJ2
D	21	GLN	-	expression tag	UNP F6KZJ2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	GLY	-	expression tag	UNP F6KZJ2

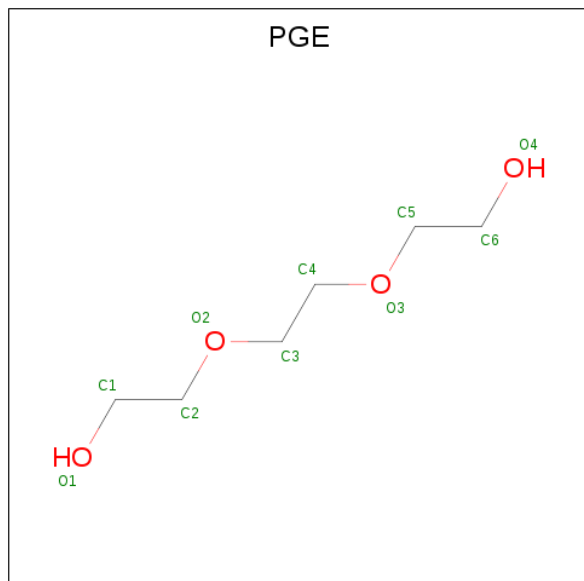
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	D	2	Total Cl 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Mg 2 2	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



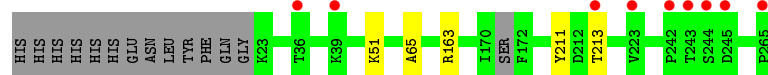
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C H O 24 6 14 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	195	Total 195	O 195	0	0
5	D	173	Total 173	O 173	0	0

i

- Molecule 1: Beta-lactamase



HIS	HIS	HIS	HIS	HIS	HIS	GLU	ASN	LEU	TYR	PHE	GLN	GLY	K23	W31	N32	A33	T36	N57	D82	Q98	K137	I162	T213	K218	I219	P242	T243	S244	D245	G246	P265
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4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.92Å 121.92Å 160.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.49 – 2.07 24.49 – 2.07	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.49-2.07) 100.0 (24.49-2.07)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.145 , 0.187 0.152 , 0.192	Depositor DCC
R_{free} test set	2186 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8102	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, KCX, CL

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	B	0.52	0/2010	0.60	0/2717
1	D	0.55	0/2048	0.60	0/2769
All	All	0.54	0/4058	0.60	0/5486

There are no bond length outliers.

There are no bond angle outliers.

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	B	1952	1880	1841	3	0
1	D	1974	1897	1863	6	0
2	B	2	0	0	0	0
2	D	2	0	0	2	0
3	B	2	0	0	0	0
3	D	1	0	0	0	0
4	D	10	14	14	4	0
5	B	195	0	0	1	1
5	D	173	0	0	3	1
All	All	4311	3791	3718	11	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 1.

All (11) 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)
2:D:303:CL:CL	5:D:566:HOH:O	2.09	1.07
2:D:302:CL:CL	5:D:511:HOH:O	2.46	0.71
1:B:211:TYR:CZ	1:B:213:THR:HA	2.48	0.49
1:D:98:GLN:OE1	5:D:401:HOH:O	2.20	0.48
1:B:65:ALA:HB1	1:B:163:ARG:HB3	1.95	0.48
1:D:137:LYS:HD3	4:D:301:PGE:H6	1.99	0.45
1:D:137:LYS:HE2	4:D:301:PGE:H22	2.01	0.43
1:B:51:LYS:HE3	5:B:519:HOH:O	2.17	0.43
1:D:31:TRP:HB2	1:D:57:ASN:HB3	2.01	0.42
1:D:137:LYS:HE2	4:D:301:PGE:C2	2.50	0.41
1:D:137:LYS:CE	4:D:301:PGE:H22	2.51	0.40

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)
5:B:590:HOH:O	5:D:477:HOH:O[11_454]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	B	239/252 (95%)	233 (98%)	6 (2%)	0	100	100
1	D	244/252 (97%)	235 (96%)	9 (4%)	0	100	100
All	All	483/504 (96%)	468 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	B	204/219 (93%)	204 (100%)	0	100	100
1	D	210/219 (96%)	206 (98%)	4 (2%)	57	53
All	All	414/438 (94%)	410 (99%)	4 (1%)	76	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	82	ASP
1	D	162	ILE
1	D	213	THR
1	D	219	ILE

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

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	KCX	D	73	1	7,11,12	0.99	0	4,12,14	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	73	1	7,11,12	0.88	0	4,12,14	0.64	0

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	KCX	D	73	1	-	0/7/10/12	-
1	KCX	B	73	1	-	0/7/10/12	-

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.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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
4	PGE	D	301	-	9,9,9	0.44	0	8,8,8	0.71	0

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
4	PGE	D	301	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	301	PGE	O3-C5-C6-O4
4	D	301	PGE	O2-C3-C4-O3
4	D	301	PGE	C6-C5-O3-C4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	PGE	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	B	237/252 (94%)	-0.13	9 (3%)	40	42	16, 27, 59, 82	5 (2%)
1	D	238/252 (94%)	-0.01	9 (3%)	40	42	16, 27, 67, 82	4 (1%)
All	All	475/504 (94%)	-0.07	18 (3%)	40	42	16, 27, 63, 82	9 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	THR	6.0
1	B	243	THR	5.0
1	B	265	PRO	4.5
1	B	245	ASP	4.5
1	B	242	PRO	4.4
1	D	265	PRO	4.2
1	D	244	SER	4.0
1	D	245	ASP	3.9
1	D	242	PRO	3.8
1	D	246	GLY	3.4
1	D	213	THR	2.7
1	B	36	THR	2.7
1	D	33	ALA	2.6
1	D	36	THR	2.5
1	B	39	LYS	2.3
1	B	244	SER	2.3
1	B	213	THR	2.2
1	B	223	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. 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	B-factors(\AA^2)	Q<0.9
1	KCX	D	73	12/13	0.98	0.17	15,19,22,24	0
1	KCX	B	73	12/13	0.98	0.15	12,19,28,28	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. 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	B-factors(\AA^2)	Q<0.9
3	MG	D	304	1/1	0.84	0.39	61,61,61,61	0
4	PGE	D	301	10/10	0.86	0.20	48,58,68,70	0
3	MG	B	303	1/1	0.94	0.17	39,39,39,39	0
3	MG	B	304	1/1	0.96	0.06	50,50,50,50	0
2	CL	D	303	1/1	0.97	0.12	59,59,59,59	0
2	CL	B	302	1/1	0.97	0.34	60,60,60,60	0
2	CL	D	302	1/1	0.97	0.15	47,47,47,47	0
2	CL	B	301	1/1	0.99	0.14	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.