



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:52 PM EDT

PDB ID : 6NLW
Title : The crystal structure of class D carbapenem-hydrolyzing beta-lactamase BlaA from *Shewanella oneidensis* MR-1
Authors : Tan, K.; Tesar, C.; Endres, M.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-01-09
Resolution : 1.85 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 1.85 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8674 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
			Total	C	N	O	S			
1	A	243	1997	1274	351	365	7	0	2	0
1	B	242	1978	1262	348	361	7	0	0	0
1	C	243	1975	1259	347	362	7	0	0	0
1	D	242	1982	1265	348	362	7	0	2	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	-	expression tag	UNP Q6RFZ0
A	21	ASN	-	expression tag	UNP Q6RFZ0
A	22	ALA	-	expression tag	UNP Q6RFZ0
B	20	SER	-	expression tag	UNP Q6RFZ0
B	21	ASN	-	expression tag	UNP Q6RFZ0
B	22	ALA	-	expression tag	UNP Q6RFZ0
C	20	SER	-	expression tag	UNP Q6RFZ0
C	21	ASN	-	expression tag	UNP Q6RFZ0
C	22	ALA	-	expression tag	UNP Q6RFZ0
D	20	SER	-	expression tag	UNP Q6RFZ0
D	21	ASN	-	expression tag	UNP Q6RFZ0
D	22	ALA	-	expression tag	UNP Q6RFZ0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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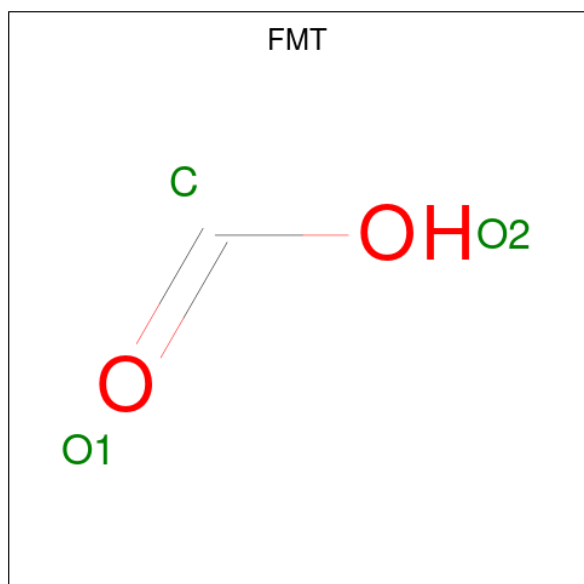
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	2	Total	Cl	0	0
			2	2		
4	C	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		

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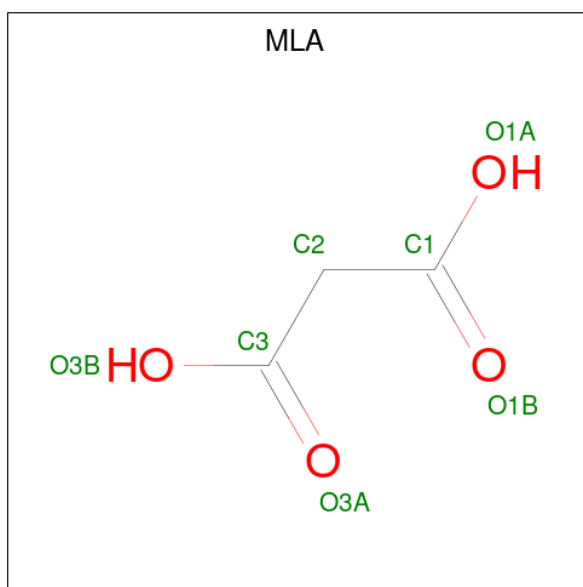
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	A	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	C	1	Total	C	O	0	0
			3	1	2		
5	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 7 3 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	157	Total O 158 158	0	1
8	B	112	Total O 112 112	0	0
8	C	126	Total O 126 126	0	0
8	D	139	Total O 139 139	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.33Å 61.39Å 122.80Å 90.00° 119.53° 90.00°	Depositor
Resolution (Å)	39.03 – 1.85	Depositor
% Data completeness (in resolution range)	99.9 (39.03-1.85)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.84Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.183 , 0.225	Depositor
Wilson B-factor (Å ²)	22.8	Xtrriage
Anisotropy	0.434	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8674	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2446e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 6 are monoatomic - leaving 42 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
3	SO4	A	308	-	4,4,4	0.14	0	6,6,6	0.10	0
2	GOL	A	301	-	5,5,5	1.04	0	5,5,5	0.75	0
3	SO4	B	307	-	4,4,4	0.13	0	6,6,6	0.13	0
5	FMT	B	311	-	2,2,2	0.65	0	1,1,1	0.18	0
2	GOL	C	301	-	5,5,5	1.32	1 (20%)	5,5,5	0.71	0
5	FMT	D	311	-	2,2,2	0.61	0	1,1,1	0.11	0
3	SO4	D	306	-	4,4,4	0.16	0	6,6,6	0.08	0
3	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	304	-	4,4,4	0.16	0	6,6,6	0.11	0
5	FMT	B	312	-	2,2,2	0.67	0	1,1,1	0.23	0
3	SO4	C	303	-	4,4,4	0.16	0	6,6,6	0.16	0
5	FMT	A	311	-	2,2,2	0.70	0	1,1,1	0.22	0
3	SO4	B	306	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	D	305	-	4,4,4	0.14	0	6,6,6	0.10	0
3	SO4	B	308	-	4,4,4	0.12	0	6,6,6	0.10	0
3	SO4	B	303	-	4,4,4	0.15	0	6,6,6	0.29	0
2	GOL	B	301	-	5,5,5	0.80	0	5,5,5	1.18	0
5	FMT	A	312	-	2,2,2	0.67	0	1,1,1	0.21	0
3	SO4	A	305	-	4,4,4	0.16	0	6,6,6	0.10	0
2	GOL	D	301	-	5,5,5	0.99	0	5,5,5	1.04	0
3	SO4	D	302	-	4,4,4	0.22	0	6,6,6	0.42	0
5	FMT	A	314	-	2,2,2	0.73	0	1,1,1	0.28	0
3	SO4	A	306	-	4,4,4	0.13	0	6,6,6	0.25	0
3	SO4	D	307	-	4,4,4	0.14	0	6,6,6	0.07	0
2	GOL	A	302	-	5,5,5	0.76	0	5,5,5	0.94	0
7	MLA	D	312	-	6,6,6	1.29	0	7,7,7	1.29	0
3	SO4	C	305	-	4,4,4	0.18	0	6,6,6	0.13	0
5	FMT	C	308	-	2,2,2	0.65	0	1,1,1	0.16	0
3	SO4	A	309	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	D	309	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	A	307	-	4,4,4	0.15	0	6,6,6	0.07	0
3	SO4	D	308	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	D	304	-	4,4,4	0.13	0	6,6,6	0.10	0
3	SO4	A	303	-	4,4,4	0.08	0	6,6,6	0.43	0
5	FMT	A	313	-	2,2,2	0.64	0	1,1,1	0.11	0
5	FMT	C	309	-	2,2,2	0.70	0	1,1,1	0.17	0
6	PEG	B	313	-	6,6,6	0.48	0	5,5,5	0.29	0
3	SO4	A	304	-	4,4,4	0.12	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	303	-	4,4,4	0.44	0	6,6,6	1.20	1 (16%)
3	SO4	C	302	-	4,4,4	0.13	0	6,6,6	0.29	0
3	SO4	B	305	-	4,4,4	0.74	0	6,6,6	1.19	1 (16%)

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	GOL	A	301	-	-	0/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	A	302	-	-	1/4/4/4	-
7	MLA	D	312	-	-	0/4/4/4	-
6	PEG	B	313	-	-	1/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	D	301	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	GOL	O2-C2	-2.13	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	SO4	O3-S-O1	-2.38	96.87	109.31
3	D	303	SO4	O3-S-O1	-2.28	97.39	109.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	C1-C2-C3-O3
2	D	301	GOL	C1-C2-C3-O3
2	D	301	GOL	O1-C1-C2-O2
2	D	301	GOL	O1-C1-C2-C3
2	D	301	GOL	O2-C2-C3-O3
2	B	301	GOL	O2-C2-C3-O3
2	C	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	313	PEG	C1-C2-O2-C3
2	A	302	GOL	O2-C2-C3-O3
2	C	301	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.