

wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 08:18 AM EDT

PDB ID : 6NHU

Title : Crystal Structure of the Beta Lactamase Class D YbxI from Agrobacterium

fabrum

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tural Genomics of Infectious Diseases (CSGID)

Deposited on : 2018-12-23

Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (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 (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 5 unique types of molecules in this entry. The entry contains 7750 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	Λ	243	Total	С	N	О	S	0	0	0
1	A	243	1895	1199	345	347	4	0		
1	В	243	Total	С	N	О	S	0	1	0
1	Б		1906	1205	349	348	4	U	1	
1	С	244	Total	С	N	О	S	0	0	0
1		244	1902	1204	346	348	4	0	U	
1	D	244	Total	С	N	О	S	0	0	0
1			1902	1204	346	348	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	SER	-	expression tag	UNP Q7D0B8
A	24	ASN	-	expression tag	UNP Q7D0B8
A	25	ALA	-	expression tag	UNP Q7D0B8
В	23	SER	-	expression tag	UNP Q7D0B8
В	24	ASN	_	expression tag	UNP Q7D0B8
В	25	ALA	-	expression tag	UNP Q7D0B8
С	23	SER	_	expression tag	UNP Q7D0B8
С	24	ASN	-	expression tag	UNP Q7D0B8
С	25	ALA	-	expression tag	UNP Q7D0B8
D	23	SER	-	expression tag	UNP Q7D0B8
D	24	ASN	-	expression tag	UNP Q7D0B8
D	25	ALA	_	expression tag	UNP Q7D0B8

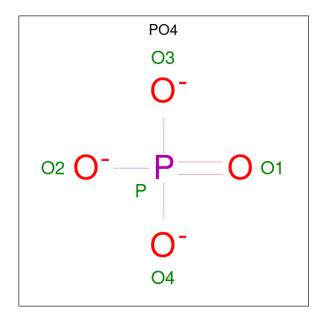
• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





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

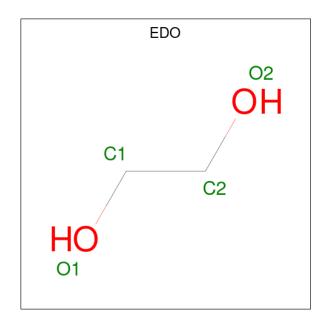
 \bullet Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total O P 5 4 1	0	0
3	С	1	Total O P 5 4 1	0	0

 \bullet Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	34	Total O 34 34	0	0
5	В	23	Total O 23 23	0	0
5	С	25	Total O 25 25	0	0
5	D	31	Total O 31 31	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	49.88Å 165.96Å 75.43Å	Depositor
a, b, c, α , β , γ	90.00° 90.02° 90.00°	Depositor
Resolution (Å)	44.61 - 2.30	Depositor
% Data completeness	96.8 (44.61-2.30)	Depositor
(in resolution range)	,	1
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.90 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.187 , 0.223	Depositor
Wilson B-factor (\mathring{A}^2)	39.3	Xtriage
Anisotropy	0.193	Xtriage
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
Total number of atoms	7750	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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)

7 ligands 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	Tuno	Chain	Res	Link	В	ond leng	$_{ m gths}$	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	EDO	D	301	-	3,3,3	0.45	0	2,2,2	0.41	0
4	EDO	В	302	-	3,3,3	0.46	0	2,2,2	0.34	0
3	PO4	С	300	-	4,4,4	0.96	0	6,6,6	0.43	0
4	EDO	С	301	-	3,3,3	0.46	0	2,2,2	0.27	0
3	PO4	В	300	-	4,4,4	0.98	0	6,6,6	0.43	0
2	GOL	A	301	-	5,5,5	0.93	0	5,5,5	1.05	0
4	EDO	В	301	-	3,3,3	0.46	0	2,2,2	0.34	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	EDO	D	301	-	-	0/1/1/1	-
4	EDO	В	302	-	-	0/1/1/1	-
4	EDO	С	301	-	-	1/1/1/1	-
2	GOL	A	301	-	-	3/4/4/4	-
4	EDO	В	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GOL	C1-C2-C3-O3
2	A	301	GOL	O2-C2-C3-O3
2	A	301	GOL	O1-C1-C2-C3
4	С	301	EDO	O1-C1-C2-O2
4	В	301	EDO	O1-C1-C2-O2

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

