

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 05:37 AM EDT

PDB ID : 6N6T

Title : OXA-23 mutant F110A/M221A low pH form

Authors: Smith, C.A.; Vakulenko, S.B.

Deposited on : 2018-11-27

Resolution : 1.25 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 (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 1.25 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 3 unique types of molecules in this entry. The entry contains 2156 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.

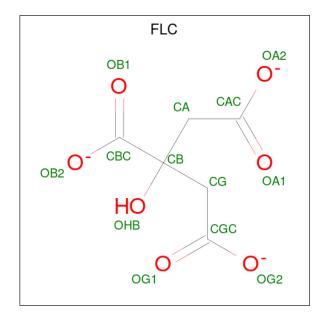
• Molecule 1 is a protein called Beta-lactamase oxa23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	232	Total	С	N	О	S	0	7	0
1	Λ	232	1881	1210	318	344	9	0	'	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	PHE	engineered mutation	UNP Q9L4P2
A	221	ALA	MET	engineered mutation	UNP Q9L4P2

• Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 13	C 6	O 7	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	260	Total O 262 262	0	2

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 21 21 2	Depositor	
Cell constants	136.58Å 43.99Å 46.55Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	38.47 - 1.25	Depositor	
% Data completeness	98.8 (38.47-1.25)	Depositor	
(in resolution range)	,	Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.36 (at 1.20Å)	Xtriage	
Refinement program	PHENIX 1.14_3260	Depositor	
R, R_{free}	0.154 , 0.180	Depositor	
Wilson B-factor (\mathring{A}^2)	14.5	Xtriage	
Anisotropy	0.279	Xtriage	
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	2156	wwPDB-VP	
Average B, all atoms (Å ²)	23.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.81% 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)

1 ligand is 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	Pog	Link	Во	nd leng	$ ag{ths}$	В	ond ang	les
WIOI	туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FLC	A	301	-	12,12,12	0.96	0	17,17,17	5.08	8 (47%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	A	301	-	-	6/16/16/16	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	301	FLC	OHB-CB-CBC	-12.36	91.51	108.86
2	A	301	FLC	OHB-CB-CG	-10.26	85.40	109.40
2	A	301	FLC	OHB-CB-CA	-10.11	85.74	109.40
2	A	301	FLC	CG-CB-CA	6.01	124.83	109.16
2	A	301	FLC	CG-CB-CBC	4.22	119.18	110.11
2	A	301	FLC	CA-CB-CBC	2.46	115.39	110.11
2	A	301	FLC	OG2-CGC-CG	2.39	122.03	114.35
2	A	301	FLC	OG1-CGC-CG	-2.20	116.51	122.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FLC	CAC-CA-CB-CG
2	A	301	FLC	CA-CB-CG-CGC
2	A	301	FLC	CA-CB-CBC-OB1
2	A	301	FLC	CA-CB-CBC-OB2
2	A	301	FLC	CBC-CB-CG-CGC
2	A	301	FLC	CG-CB-CBC-OB2

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.

