

# Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 07:13 PM EST

PDB ID : 3NNL

Title: Halogenase domain from CurA module (crystal form III)

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Deposited on : 2010-06-23

Resolution : 2.88 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) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.88 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 4948 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 CurA.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	306	Total		11	0	S	0	0	0
			2524	1622	424	471	7		Ů	
1	B	291	Total	$^{\mathrm{C}}$	N	O	$\mathbf{S}$	0	0	0
1	Ъ	291	2406	1554	403	442	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q6DNF2
A	-22	HIS	-	expression tag	UNP Q6DNF2
A	-21	HIS	-	expression tag	UNP Q6DNF2
A	-20	HIS	_	expression tag	UNP Q6DNF2
A	-19	HIS	-	expression tag	UNP Q6DNF2
A	-18	HIS	-	expression tag	UNP Q6DNF2
A	-17	HIS	-	expression tag	UNP Q6DNF2
A	-16	SER	-	expression tag	UNP Q6DNF2
A	-15	SER	-	expression tag	UNP Q6DNF2
A	-14	GLY	-	expression tag	UNP Q6DNF2
A	-13	VAL	-	expression tag	UNP Q6DNF2
A	-12	ASP	-	expression tag	UNP Q6DNF2
A	-11	LEU	-	expression tag	UNP Q6DNF2
A	-10	GLY	-	expression tag	UNP Q6DNF2
A	-9	THR	-	expression tag	UNP Q6DNF2
A	-8	GLU	-	expression tag	UNP Q6DNF2
A	-7	ASN	-	expression tag	UNP Q6DNF2
A	-6	LEU	-	expression tag	UNP Q6DNF2
A	-5	TYR	-	expression tag	UNP Q6DNF2
A	-4	PHE	-	expression tag	UNP Q6DNF2
A	-3	GLN	-	expression tag	UNP Q6DNF2
A	-2	SER	-	expression tag	UNP Q6DNF2
A	-1	ASN	-	expression tag	UNP Q6DNF2
A	0	ALA	-	expression tag	UNP Q6DNF2
В	-23	MET	-	expression tag	UNP Q6DNF2

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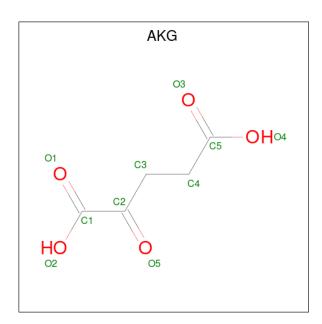
Chain	Residue	Modelled	Actual	Comment	Reference
В	-22	HIS	-	expression tag	UNP Q6DNF2
В	-21	HIS	-	expression tag	UNP Q6DNF2
В	-20	HIS	-	expression tag	UNP Q6DNF2
В	-19	HIS	-	expression tag	UNP Q6DNF2
В	-18	HIS	-	expression tag	UNP Q6DNF2
В	-17	HIS	-	expression tag	UNP Q6DNF2
В	-16	SER	-	expression tag	UNP Q6DNF2
В	-15	SER	-	expression tag	UNP Q6DNF2
В	-14	GLY	-	expression tag	UNP Q6DNF2
В	-13	VAL	-	expression tag	UNP Q6DNF2
В	-12	ASP	-	expression tag	UNP Q6DNF2
В	-11	LEU	-	expression tag	UNP Q6DNF2
В	-10	GLY	-	expression tag	UNP Q6DNF2
В	-9	THR	-	expression tag	UNP Q6DNF2
В	-8	GLU	-	expression tag	UNP Q6DNF2
В	-7	ASN	-	expression tag	UNP Q6DNF2
В	-6	LEU	-	expression tag	UNP Q6DNF2
В	-5	TYR	-	expression tag	UNP Q6DNF2
В	-4	PHE	-	expression tag	UNP Q6DNF2
В	-3	GLN	-	expression tag	UNP Q6DNF2
В	-2	SER	-	expression tag	UNP Q6DNF2
В	-1	ASN	-	expression tag	UNP Q6DNF2
В	0	ALA	-	expression tag	UNP Q6DNF2

• Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0

• Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	1	Total 10	C 5	O 5	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	В	4	Total O 4 4	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	50.04Å 79.45Å 85.17Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 103.02° 90.00°	Depositor
Resolution (Å)	40.39 - 2.88	Depositor
% Data completeness	98.8 (40.39-2.88)	Depositor
(in resolution range)	,	-
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.85  (at  2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
$R, R_{free}$	0.258 , $0.287$	Depositor
Wilson B-factor $(\mathring{A}^2)$	85.0	Xtriage
Anisotropy	0.259	Xtriage
L-test for twinning <sup>2</sup>	$  <  L  > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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)

Of 4 ligands modelled in this entry, 3 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).

$\mathbf{M}$		Type	Chain	Res	Link	B	ond leng	$\operatorname{gths}$	В	ond ang	cles
101	.01					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
	3	AKG	A	500	2	9,9,9	1.37	1 (11%)	11,11,11	1.77	1 (9%)

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
3	AKG	A	500	2	-	0/9/9/9	-

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(A)
3	A	500	AKG	C4-C5	2.54	1.56	1.50

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	500	AKG	O1-C1-C2	-4.86	115.22	121.72

There are no chirality outliers.

There are no torsion outliers.

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.

