



wwPDB X-ray Structure Validation Summary Report

Dec 16, 2023 – 07:13 PM EST

PDB ID : 3NNL
Title : Halogenase domain from CurA module (crystal form III)
Authors : Khare, D.; Smith, J.L.
Deposited on : 2010-06-23
Resolution : 2.88 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  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) : 2.36

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 2.88 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	Total	C	N	O	S	0	0	0
			2524	1622	424	471	7			
1	B	291	Total	C	N	O	S	0	0	0
			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
B	-23	MET	-	expression tag	UNP Q6DNF2

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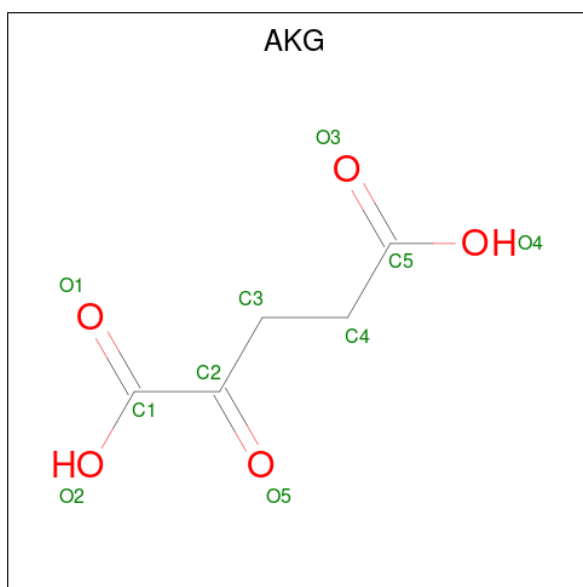
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP Q6DNF2
B	-21	HIS	-	expression tag	UNP Q6DNF2
B	-20	HIS	-	expression tag	UNP Q6DNF2
B	-19	HIS	-	expression tag	UNP Q6DNF2
B	-18	HIS	-	expression tag	UNP Q6DNF2
B	-17	HIS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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 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	B	4	Total O 4 4	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	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.04Å 79.45Å 85.17Å 90.00° 103.02° 90.00°	Depositor
Resolution (Å)	40.39 – 2.88	Depositor
% Data completeness (in resolution range)	98.8 (40.39-2.88)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.258 , 0.287	Depositor
Wilson B-factor (Å ²)	85.0	Xtrriage
Anisotropy	0.259	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4948	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage'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.*

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 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					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	Observed(Å)	Ideal(Å)
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	Z	Observed(°)	Ideal(°)
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.