



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 09:08 PM EDT

PDB ID : 6UUT
Title : Crystal structure of a high molecular weight 3-oxoacyl-ACP reductase (FabG) from *Acinetobacter baumannii* crystal form 2
Authors : Cross, E.M.; Forwood, J.K.
Deposited on : 2019-10-31
Resolution : 1.65 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**
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 1.65 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 2 unique types of molecules in this entry. The entry contains 7013 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 3-ketoacyl-ACP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	460	Total 3363	C 2122	N 593	O 641	S 7	0	1	0
1	B	432	Total 3147	C 1979	N 559	O 603	S 6	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A219C8F5
A	-22	HIS	-	expression tag	UNP A0A219C8F5
A	-21	HIS	-	expression tag	UNP A0A219C8F5
A	-20	HIS	-	expression tag	UNP A0A219C8F5
A	-19	HIS	-	expression tag	UNP A0A219C8F5
A	-18	HIS	-	expression tag	UNP A0A219C8F5
A	-17	HIS	-	expression tag	UNP A0A219C8F5
A	-16	SER	-	expression tag	UNP A0A219C8F5
A	-15	SER	-	expression tag	UNP A0A219C8F5
A	-14	GLY	-	expression tag	UNP A0A219C8F5
A	-13	VAL	-	expression tag	UNP A0A219C8F5
A	-12	ASP	-	expression tag	UNP A0A219C8F5
A	-11	LEU	-	expression tag	UNP A0A219C8F5
A	-10	GLY	-	expression tag	UNP A0A219C8F5
A	-9	THR	-	expression tag	UNP A0A219C8F5
A	-8	GLU	-	expression tag	UNP A0A219C8F5
A	-7	ASN	-	expression tag	UNP A0A219C8F5
A	-6	LEU	-	expression tag	UNP A0A219C8F5
A	-5	TYR	-	expression tag	UNP A0A219C8F5
A	-4	PHE	-	expression tag	UNP A0A219C8F5
A	-3	GLN	-	expression tag	UNP A0A219C8F5
A	-2	SER	-	expression tag	UNP A0A219C8F5
A	-1	ASN	-	expression tag	UNP A0A219C8F5
A	0	ALA	-	expression tag	UNP A0A219C8F5
B	-23	MET	-	initiating methionine	UNP A0A219C8F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP A0A219C8F5
B	-21	HIS	-	expression tag	UNP A0A219C8F5
B	-20	HIS	-	expression tag	UNP A0A219C8F5
B	-19	HIS	-	expression tag	UNP A0A219C8F5
B	-18	HIS	-	expression tag	UNP A0A219C8F5
B	-17	HIS	-	expression tag	UNP A0A219C8F5
B	-16	SER	-	expression tag	UNP A0A219C8F5
B	-15	SER	-	expression tag	UNP A0A219C8F5
B	-14	GLY	-	expression tag	UNP A0A219C8F5
B	-13	VAL	-	expression tag	UNP A0A219C8F5
B	-12	ASP	-	expression tag	UNP A0A219C8F5
B	-11	LEU	-	expression tag	UNP A0A219C8F5
B	-10	GLY	-	expression tag	UNP A0A219C8F5
B	-9	THR	-	expression tag	UNP A0A219C8F5
B	-8	GLU	-	expression tag	UNP A0A219C8F5
B	-7	ASN	-	expression tag	UNP A0A219C8F5
B	-6	LEU	-	expression tag	UNP A0A219C8F5
B	-5	TYR	-	expression tag	UNP A0A219C8F5
B	-4	PHE	-	expression tag	UNP A0A219C8F5
B	-3	GLN	-	expression tag	UNP A0A219C8F5
B	-2	SER	-	expression tag	UNP A0A219C8F5
B	-1	ASN	-	expression tag	UNP A0A219C8F5
B	0	ALA	-	expression tag	UNP A0A219C8F5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	279	Total O 279 279	0	0
2	B	224	Total O 224 224	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	64.60Å 80.32Å 76.58Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	80.32 – 1.65	Depositor
% Data completeness (in resolution range)	99.7 (80.32-1.65)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 1.65Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.202 , 0.235	Depositor
Wilson B-factor (Å ²)	15.2	Xtrriage
Anisotropy	0.056	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7013	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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 60.69 % 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 1.4643e-05. 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](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

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.