



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 12:01 PM EDT

PDB ID : 4JX8 / pdb_00004jx8
Title : Crystal Structure of E.coli Enoyl Reductase in Complex with NAD and AEA16
Authors : Subramanya, H.; Rao, K.N.; Anirudha, L.
Deposited on : 2013-03-28
Resolution : 3.20 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 ⓘ 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.20 Å.

There are no overall percentile quality scores available for this entry.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3896 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 Enoyl-[acyl-carrier-protein] reductase [NADH] FabI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1894	1191	326	364	13			
1	B	244	Total	C	N	O	S	0	0	0
			1802	1135	307	348	12			

There are 40 discrepancies between the modelled and reference sequences:

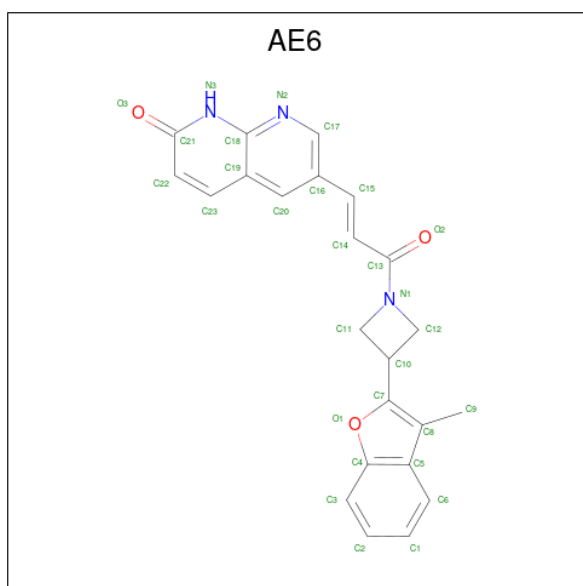
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0AEK4
A	-18	GLY	-	expression tag	UNP P0AEK4
A	-17	SER	-	expression tag	UNP P0AEK4
A	-16	SER	-	expression tag	UNP P0AEK4
A	-15	HIS	-	expression tag	UNP P0AEK4
A	-14	HIS	-	expression tag	UNP P0AEK4
A	-13	HIS	-	expression tag	UNP P0AEK4
A	-12	HIS	-	expression tag	UNP P0AEK4
A	-11	HIS	-	expression tag	UNP P0AEK4
A	-10	HIS	-	expression tag	UNP P0AEK4
A	-9	SER	-	expression tag	UNP P0AEK4
A	-8	SER	-	expression tag	UNP P0AEK4
A	-7	GLY	-	expression tag	UNP P0AEK4
A	-6	LEU	-	expression tag	UNP P0AEK4
A	-5	VAL	-	expression tag	UNP P0AEK4
A	-4	PRO	-	expression tag	UNP P0AEK4
A	-3	ARG	-	expression tag	UNP P0AEK4
A	-2	GLY	-	expression tag	UNP P0AEK4
A	-1	SER	-	expression tag	UNP P0AEK4
A	0	HIS	-	expression tag	UNP P0AEK4
B	-19	MET	-	expression tag	UNP P0AEK4
B	-18	GLY	-	expression tag	UNP P0AEK4
B	-17	SER	-	expression tag	UNP P0AEK4
B	-16	SER	-	expression tag	UNP P0AEK4
B	-15	HIS	-	expression tag	UNP P0AEK4

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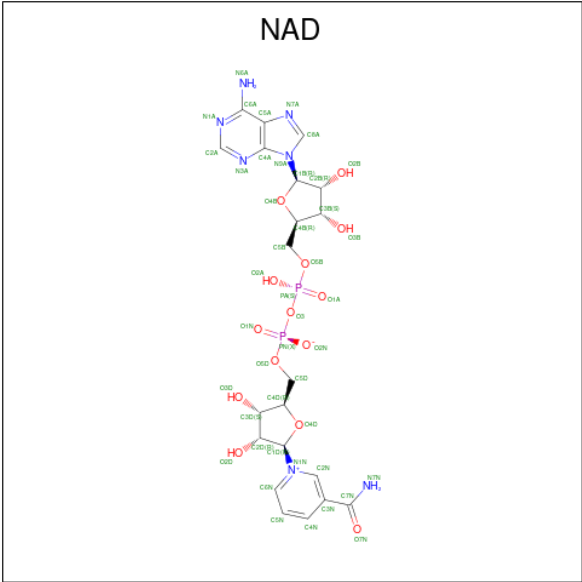
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P0AEK4
B	-13	HIS	-	expression tag	UNP P0AEK4
B	-12	HIS	-	expression tag	UNP P0AEK4
B	-11	HIS	-	expression tag	UNP P0AEK4
B	-10	HIS	-	expression tag	UNP P0AEK4
B	-9	SER	-	expression tag	UNP P0AEK4
B	-8	SER	-	expression tag	UNP P0AEK4
B	-7	GLY	-	expression tag	UNP P0AEK4
B	-6	LEU	-	expression tag	UNP P0AEK4
B	-5	VAL	-	expression tag	UNP P0AEK4
B	-4	PRO	-	expression tag	UNP P0AEK4
B	-3	ARG	-	expression tag	UNP P0AEK4
B	-2	GLY	-	expression tag	UNP P0AEK4
B	-1	SER	-	expression tag	UNP P0AEK4
B	0	HIS	-	expression tag	UNP P0AEK4

- Molecule 2 is 6-((1E)-3-[3-(3-methyl-1-benzofuran-2-yl)azetidin-1-yl]-3-oxoprop-1-en-1-yl)-1,8-naphthyridin-2(1H)-one (CCD ID: AE6) (formula: C₂₃H₁₉N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	23	3	3		
2	B	1	Total	C	N	O	0	0
			29	23	3	3		

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	28	Total	O	0	0
			28	28		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.63Å 79.63Å 323.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.24 – 3.20	Depositor
% Data completeness (in resolution range)	77.0 (29.24-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.87 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.326	Depositor
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.227	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3896	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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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](#)

validation-pack failed to run properly - this section is therefore empty.

4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

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 ⓘ

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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.