



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 04:37 pm GMT

PDB ID : 4AEY
Title : Crystal structure of FolX from Pseudomonas aeruginosa
Authors : Gabrielsen, M.; Beckham, K.S.H.; Roe, A.J.
Deposited on : 2012-01-13
Resolution : 3.00 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 : 4.02b-467
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

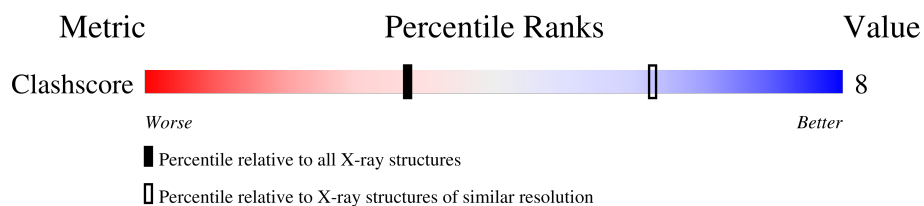
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 762 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 D-ERYTHRO-7,8-DIHYDRONEOPTERIN TRIPHOSPHATE EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	107	754	476	129	146	3	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	MET	-	expression tag	UNP Q9HYG7
A	-31	HIS	-	expression tag	UNP Q9HYG7
A	-30	HIS	-	expression tag	UNP Q9HYG7
A	-29	HIS	-	expression tag	UNP Q9HYG7
A	-28	HIS	-	expression tag	UNP Q9HYG7
A	-27	HIS	-	expression tag	UNP Q9HYG7
A	-26	HIS	-	expression tag	UNP Q9HYG7
A	-25	GLY	-	expression tag	UNP Q9HYG7
A	-24	LYS	-	expression tag	UNP Q9HYG7
A	-23	PRO	-	expression tag	UNP Q9HYG7
A	-22	ILE	-	expression tag	UNP Q9HYG7
A	-21	PRO	-	expression tag	UNP Q9HYG7
A	-20	ASN	-	expression tag	UNP Q9HYG7
A	-19	PRO	-	expression tag	UNP Q9HYG7
A	-18	LEU	-	expression tag	UNP Q9HYG7
A	-17	LEU	-	expression tag	UNP Q9HYG7
A	-16	GLY	-	expression tag	UNP Q9HYG7
A	-15	LEU	-	expression tag	UNP Q9HYG7
A	-14	ASP	-	expression tag	UNP Q9HYG7
A	-13	SER	-	expression tag	UNP Q9HYG7
A	-12	THR	-	expression tag	UNP Q9HYG7
A	-11	GLU	-	expression tag	UNP Q9HYG7
A	-10	ASN	-	expression tag	UNP Q9HYG7
A	-9	LEU	-	expression tag	UNP Q9HYG7
A	-8	TYR	-	expression tag	UNP Q9HYG7
A	-7	PHE	-	expression tag	UNP Q9HYG7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLN	-	expression tag	UNP Q9HYG7
A	-5	GLY	-	expression tag	UNP Q9HYG7
A	-4	ILE	-	expression tag	UNP Q9HYG7
A	-3	ASP	-	expression tag	UNP Q9HYG7
A	-2	PRO	-	expression tag	UNP Q9HYG7
A	-1	PHE	-	expression tag	UNP Q9HYG7
A	0	THR	-	expression tag	UNP Q9HYG7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	133.98Å 133.98Å 133.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.99 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (66.99-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.283 , 0.311	Depositor
Wilson B-factor (Å ²)	120.2	Xtrriage
Anisotropy	0.000	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	762	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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](#)

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/765	0.77	0/1039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	682	11	0
2	A	8	0	0	2	0
All	All	762	0	682	11	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:HA	2:A:2004:HOH:O	1.83	0.78
1:A:8:MET:HB3	2:A:2002:HOH:O	1.97	0.63
1:A:20:THR:HG22	1:A:21:PHE:H	1.66	0.60
1:A:87:LEU:O	1:A:90:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HG22	1:A:21:PHE:N	2.20	0.57
1:A:109:LEU:HG	1:A:115:VAL:HG21	1.91	0.53
1:A:18:LEU:HD12	1:A:37:ILE:HD12	1.95	0.49
1:A:109:LEU:HG	1:A:115:VAL:CG2	2.44	0.48
1:A:18:LEU:HD21	1:A:68:ILE:HG23	1.97	0.47
1:A:83:THR:HG23	1:A:101:VAL:HG12	1.98	0.46
1:A:35:VAL:HG22	1:A:103:VAL:HG12	2.00	0.43

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 [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](#)

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5.5 Other polymers [i](#)

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