



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:09 PM EDT

PDB ID : 4PTH / pdb_00004pth
Title : Ensemble model for Escherichia coli dihydrofolate reductase at 100K
Authors : Keedy, D.A.; van den Bedem, H.; Sivak, D.A.; Petsko, G.A.; Ringe, D.; Wilson, M.A.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 0.85 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
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 0.85 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	33.96Å 44.82Å 98.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 0.85	Depositor
% Data completeness (in resolution range)	98.0 (49.00-0.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 0.85Å)	Xtriage
Refinement program	PHENIX 1.8.4-1496	Depositor
R, R_{free}	0.126 , 0.144	Depositor
Wilson B-factor (Å ²)	7.7	Xtriage
Anisotropy	0.182	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	699880	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.86% 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.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

Of 250 non-standard protein/DNA/RNA residues modelled in this entry, 250 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 1000 ligands modelled in this entry, 1000 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

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

4.2 Non-standard residues in protein, DNA, RNA chains

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

4.3 Carbohydrates

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

4.4 Ligands

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

4.5 Other polymers

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