



Full wwPDB EM Validation Report ⓘ

Apr 27, 2026 – 06:36 PM EDT

PDB ID : 2H8A / pdb_00002h8a
Title : Structure of Microsomal Glutathione Transferase 1 in Complex with Glutathione
Authors : Hebert, H.
Deposited on : 2006-06-07
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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)
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:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.20 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 6	Depositor
Cell constants a, b, c, α , β , γ	81.80Å 81.80Å 100.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	79.2 (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.97Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.339 , 0.376	Depositor
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.629	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.27$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.377 for h,-h-k,-l	Xtriage
Total number of atoms	984	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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](#)

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3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

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3.3.2 Protein sidechains [i](#)

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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](#)

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3.5 Carbohydrates [i](#)

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

3.6 Ligand geometry [i](#)

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

3.7 Other polymers [i](#)

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

3.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.