

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 14, 2023 – 04:40 pm GMT

PDB ID : 3ZEB

Title: A complex of GlpG with isocoumarin inhibitor covalently bonded to serine 201

and histidine 150

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Deposited on : 2012-12-04

Resolution : 2.20 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 (i) 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 (1)) were used in the production of this report:

MolProbity : FAILED Xtriage (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 (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO



## 2 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	111.11Å 111.11Å 126.07Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	44.99 - 2.20	Depositor
% Data completeness	99.3 (44.99-2.20)	Depositor
(in resolution range)		
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.57  (at  2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
$R, R_{free}$	0.214 , $0.247$	Depositor
Wilson B-factor $(\mathring{A}^2)$	48.7	Xtriage
Anisotropy	0.554	Xtriage
L-test for twinning <sup>2</sup>	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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)

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

### 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 (i)

There are no chain breaks in this entry.



### 4 Fit of model and data (i)

#### 4.1 Protein, DNA and RNA chains (i)

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

#### 4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

### 4.3 Carbohydrates (i)

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

#### 4.4 Ligands (i)

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

### 4.5 Other polymers (i)

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

