



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2023 – 05:12 am GMT

PDB ID : 4D03  
Title : Structure of the Cys65Asp mutant of phenylacetone monooxygenase: oxidised state  
Authors : Brondani, P.B.; Dudek, H.M.; Martinoli, C.; Mattevi, A.; Fraaije, M.W.  
Deposited on : 2014-04-24  
Resolution : 1.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
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 1.81 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	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.74Å 107.74Å 106.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.30 – 1.81	Depositor
% Data completeness (in resolution range)	99.8 (93.30-1.81)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 1.82Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.193 , 0.230	Depositor
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtrriage
Anisotropy	0.037	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtrriage
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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

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.