wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 07:09 PM EDT

PDB ID	:	6PNO
Title	:	Human GSTO1-1 complexed with 2-chloro-N-(4-chloro-3-(N-isopropylsulfamoyl)phenyl)acetamide
Authors	:	Oakley, A.J.
Deposited on	:	2019-07-02
Resolution	:	1.82 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*
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 (i)) 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)	:	2.35.1

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 1.82 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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	57.26Å 57.26Å 139.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.50 – 1.82	Depositor
% Data completeness (in resolution range)	99.8 (40.50-1.82)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.00 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.238	Depositor
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.031	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
Total number of atoms	2325	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

3 Model quality

3.1 Standard geometry

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

3.2 Too-close contacts

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

3.3 Torsion angles

3.3.1 Protein backbone

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

3.3.2 Protein sidechains

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

3.3.3 RNA

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

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

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

3.5 Carbohydrates

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

3.6 Ligand geometry

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

3.7 Other polymers

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

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.