wwPDB Geometry-Only Validation Summary Report (i)

May 27, 2024 – 06:07 PM EDT

PDB ID	:	5AI2
Title	:	Anomalous Neutron phased crystal structure of 113Cd-substituted Perdeuterated Pyrococcus furiosus rubredoxin to 1.75A resolution at 295K
Authors	:	Cuypers, M.G.; Mossou, E.; Mason, S.A.
Deposited on	:	2015-02-11
Resolution	:	1.75 Å(reported)

This is a wwPDB Geometry-Only 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
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Model quality (i)

2.1 Standard geometry (i)

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

2.2 Too-close contacts (i)

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

2.3 Torsion angles (i)

2.3.1 Protein backbone (i)

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

2.3.2 Protein sidechains (i)

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

2.3.3 RNA (i)

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

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

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

2.5 Carbohydrates (i)

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

2.6 Ligand geometry (i)

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

2.7 Other polymers (i)

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

2.8 Polymer linkage issues (i)

There are no chain breaks in this entry.