



# Full wwPDB Geometry-Only Validation Report ⓘ

May 27, 2024 – 06:07 PM EDT

PDB ID : 5AI2  
Title : Anomalous Neutron phased crystal structure of  $^{113}\text{Cd}$ -substituted Perdeuterated *Pyrococcus furiosus* rubredoxin to 1.75Å 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 Full wwPDB Geometry-Only Validation 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**  
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

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

There are no chain breaks in this entry.