



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:59 PM UTC

PDB ID : 4AXE / pdb\_00004axe  
Title : Inositol 1,3,4,5,6-pentakisphosphate 2-kinase in complex with ADP  
Authors : I Banos-Sanz, J.; Sanz-Aparicio, J.; Gonzalez, B.  
Deposited on : 2012-06-12  
Resolution : 2.50 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](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**  
Mogul : **FAILED**  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : **FAILED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

PERCENTILES INFOmissingINFO

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

GLOBAL-STATISTICS INFOmissingINFO

## 1 Model quality [i](#)

### 1.1 Standard geometry [i](#)

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

### 1.2 Too-close contacts [i](#)

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

### 1.3 Torsion angles [i](#)

#### 1.3.1 Protein backbone [i](#)

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

#### 1.3.2 Protein sidechains [i](#)

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

#### 1.3.3 RNA [i](#)

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

### 1.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 1.5 Carbohydrates [i](#)

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

### 1.6 Ligand geometry [i](#)

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

### 1.7 Other polymers [i](#)

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

## 1.8 Polymer linkage issues

There are no chain breaks in this entry.

## 2 Fit of model and data [i](#)

### 2.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	212/456 (46%)	0.39	12 (5%) <span style="border: 1px solid red; padding: 2px;">29</span> <span style="border: 1px solid red; padding: 2px;">26</span>	22, 38, 67, 80	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	157	THR	4.2
1	1-A	1	MET	4.0
1	1-A	47	ASN	3.3
1	1-A	58	VAL	2.8
1	1-A	46	ARG	2.8
1	1-A	156	ILE	2.5
1	1-A	153	SER	2.5
1	1-A	60	VAL	2.4
1	1-A	3	MET	2.3
1	1-A	45	ARG	2.2
1	1-A	56	GLY	2.1
1	1-A	2	GLU	2.1

### 2.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 2.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

## 2.4 Other polymers [i](#)

There are no such residues in this entry.