

# Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 01:47 PM EDT

PDB ID : 6NWW

Title : Crystal structure of the RRM domain of S. pombe Puf1 in the P212121 space

group

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Deposited on : 2019-02-07

Resolution : 2.06 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 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 (1)) 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:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.06 Å.

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

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Pumilio domain-containing protein C56F2.08c.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	Λ	76	Total	С	N	O	S	0	0	
1	A	70	573	364	97	109	3	U	0	
1	B	76	Total	С	N	О	S	0	1	0
1	Б	70	576	366	97	110	3	0	1	
1	С	78	Total	С	N	О	S	0	1	0
1		10	584	370	99	112	3	0	1	
1	D	76	Total	С	N	О	S	0	2	0
1	ש	10	579	368	97	111	3	U		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP O60059
A	-2	GLY	-	expression tag	UNP O60059
A	-1	GLY	-	expression tag	UNP O60059
A	0	SER	-	expression tag	UNP O60059
В	-3	SER	_	expression tag	UNP O60059
В	-2	GLY	-	expression tag	UNP O60059
В	-1	GLY	-	expression tag	UNP O60059
В	0	SER	-	expression tag	UNP O60059
С	-3	SER	-	expression tag	UNP O60059
С	-2	GLY	-	expression tag	UNP O60059
С	-1	GLY	-	expression tag	UNP O60059
С	0	SER	-	expression tag	UNP O60059
D	-3	SER	-	expression tag	UNP O60059
D	-2	GLY	-	expression tag	UNP O60059
D	-1	GLY	-	expression tag	UNP O60059
D	0	SER	_	expression tag	UNP O60059

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

#### • Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	В	54	Total O 54 54	0	0
3	С	71	Total O 71 71	0	0
3	D	39	Total O 39 39	0	0

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



### 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	54.69Å 63.90Å 79.54Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.49 - 2.06	Depositor
% Data completeness	94.6 (24.49-2.06)	Depositor
(in resolution range)	, , ,	•
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.93  (at  2.06Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
$R, R_{free}$	0.172 , $0.225$	Depositor
Wilson B-factor $(A^2)$	16.8	Xtriage
Anisotropy	0.392	Xtriage
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2539	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 28.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7375e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 4 Model quality (i)

### 4.1 Standard geometry (i)

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

#### 4.2 Too-close contacts (i)

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

### 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

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

#### 4.3.2 Protein sidechains (i)

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

#### 4.3.3 RNA (i)

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

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

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

#### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



### 5 Fit of model and data (i)

#### 5.1 Protein, DNA and RNA chains (i)

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

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

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

#### 5.3 Carbohydrates (i)

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

#### 5.4 Ligands (i)

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

#### 5.5 Other polymers (i)

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

