

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

Oct 1, 2023 – 10:25 PM EDT

PDB ID : 6MN6

Title: Crystal structure of the cytosolic domain of human CNNM3

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Deposited on : 2018-10-01

Resolution : 3.36 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 (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-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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 is only 1 type of molecule in this entry. The entry contains 8950 atoms, of which 4399 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 Metal transporter CNNM3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	A	293	Total 4433	C 1458	H 2174	N 362	O 433	S 6	0	0	0
							455	U			
1	R	297	Total	$\mathbf{C}$	Η	Ν	O	$\mathbf{S}$	0	0	0
	Ъ		4517	1472	2225	377	436	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLY	-	expression tag	UNP Q8NE01
A	295	PRO	-	expression tag	UNP Q8NE01
A	296	LEU	-	expression tag	UNP Q8NE01
A	297	GLY	-	expression tag	UNP Q8NE01
A	298	SER	-	expression tag	UNP Q8NE01
В	294	GLY	-	expression tag	UNP Q8NE01
В	295	PRO	-	expression tag	UNP Q8NE01
В	296	LEU	-	expression tag	UNP Q8NE01
В	297	GLY	-	expression tag	UNP Q8NE01
В	298	SER	-	expression tag	UNP Q8NE01

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 32 2 1	Depositor	
Cell constants	128.06Å 128.06Å 111.32Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$		
Resolution (Å)	49.75 - 3.36	Depositor	
% Data completeness	65.7 (49.75-3.36)	Depositor	
(in resolution range)	,	-	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	0.15	Depositor	
$< I/\sigma(I) > 1$	1.52 (at 3.48Å)	Xtriage	
Refinement program	PHENIX 1.12-2829	Depositor	
$R, R_{free}$	0.217 , $0.263$	Depositor	
Wilson B-factor $(\mathring{A}^2)$	42.4	Xtriage	
Anisotropy	0.300	Xtriage	
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage	
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage	
Total number of atoms	8950	wwPDB-VP	
Average B, all atoms $(\mathring{A}^2)$	61.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.

<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)

There are no ligands in this entry.

### 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.

