Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 04:53 AM EDT

PDB ID	:	6N3H
Title	:	Crystal structure of Kelch domain of the human NS1 binding protein
Authors	:	Zhang, K.; Shang, G.; Padavannil, A.; Fontoura, B.M.A.; Chook, Y.M.
Deposited on	:	2018-11-15
Resolution	:	2.60 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 (i)) 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 2.60 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 2 unique types of molecules in this entry. The entry contains 8855 atoms, of which 4264 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 Influenza virus NS1A-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	304	4577	1474	2227	417	436	23	0	0	0
1	B	276	4159	1329	2037	372	398	23	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	MET	-	initiating methionine	UNP Q9Y6Y0
A	643	LEU	-	expression tag	UNP Q9Y6Y0
A	644	GLU	-	expression tag	UNP Q9Y6Y0
A	645	HIS	-	expression tag	UNP Q9Y6Y0
A	646	HIS	-	expression tag	UNP Q9Y6Y0
A	647	HIS	-	expression tag	UNP Q9Y6Y0
A	648	HIS	-	expression tag	UNP Q9Y6Y0
A	649	HIS	-	expression tag	UNP Q9Y6Y0
A	650	HIS	-	expression tag	UNP Q9Y6Y0
B	320	MET	-	initiating methionine	UNP Q9Y6Y0
B	643	LEU	-	expression tag	UNP Q9Y6Y0
B	644	GLU	-	expression tag	UNP Q9Y6Y0
B	645	HIS	-	expression tag	UNP Q9Y6Y0
B	646	HIS	-	expression tag	UNP Q9Y6Y0
B	647	HIS	-	expression tag	UNP Q9Y6Y0
B	648	HIS	-	expression tag	UNP Q9Y6Y0
B	649	HIS	-	expression tag	UNP Q9Y6Y0
B	650	HIS	-	expression tag	UNP Q9Y6Y0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	66	66	66	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	53	53	53	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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.20Å 61.88Å 87.34Å 90.00° 95.18° 90.00°	Depositor
Resolution (Å)	43.49 – 2.60	Depositor
% Data completeness (in resolution range)	95.3 (43.49-2.60)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.20 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.211 , 0.234	Depositor
Wilson B-factor (Å^2)	40.9	Xtriage
Anisotropy	0.134	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8855	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

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.