



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 08:40 PM EDT

PDB ID : 7DKG / pdb_00007dkg
Title : Influenza H5N1 nucleoprotein (truncated) in complex with nucleotides
Authors : Tang, Y.S.; Xu, S.; Chen, Y.W.; Wang, J.H.; Shaw, P.C.
Deposited on : 2020-11-24
Resolution : 3.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6421 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3104	1927	576	575	26			
1	B	409	Total	C	N	O	S	0	0	0
			3205	1988	595	596	26			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q9PX50
A	-34	GLY	-	expression tag	UNP Q9PX50
A	-33	SER	-	expression tag	UNP Q9PX50
A	-32	SER	-	expression tag	UNP Q9PX50
A	-31	HIS	-	expression tag	UNP Q9PX50
A	-30	HIS	-	expression tag	UNP Q9PX50
A	-29	HIS	-	expression tag	UNP Q9PX50
A	-28	HIS	-	expression tag	UNP Q9PX50
A	-27	HIS	-	expression tag	UNP Q9PX50
A	-26	HIS	-	expression tag	UNP Q9PX50
A	-25	SER	-	expression tag	UNP Q9PX50
A	-24	SER	-	expression tag	UNP Q9PX50
A	-23	GLY	-	expression tag	UNP Q9PX50
A	-22	LEU	-	expression tag	UNP Q9PX50
A	-21	VAL	-	expression tag	UNP Q9PX50
A	-20	PRO	-	expression tag	UNP Q9PX50
A	-19	ARG	-	expression tag	UNP Q9PX50
A	-18	GLY	-	expression tag	UNP Q9PX50
A	-17	SER	-	expression tag	UNP Q9PX50
A	-16	HIS	-	expression tag	UNP Q9PX50
A	-15	MET	-	expression tag	UNP Q9PX50
A	-14	ALA	-	expression tag	UNP Q9PX50
A	-13	SER	-	expression tag	UNP Q9PX50
A	-12	MET	-	expression tag	UNP Q9PX50
A	-11	THR	-	expression tag	UNP Q9PX50

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q9PX50
A	-9	GLY	-	expression tag	UNP Q9PX50
A	-8	GLN	-	expression tag	UNP Q9PX50
A	-7	GLN	-	expression tag	UNP Q9PX50
A	-6	MET	-	expression tag	UNP Q9PX50
A	-5	GLY	-	expression tag	UNP Q9PX50
A	-4	ARG	-	expression tag	UNP Q9PX50
A	-3	GLY	-	expression tag	UNP Q9PX50
A	-2	SER	-	expression tag	UNP Q9PX50
A	-1	GLU	-	expression tag	UNP Q9PX50
A	0	PHE	-	expression tag	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
A	?	-	SER	deletion	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
A	?	-	GLY	deletion	UNP Q9PX50
A	?	-	GLN	deletion	UNP Q9PX50
A	?	-	ILE	deletion	UNP Q9PX50
A	?	-	SER	deletion	UNP Q9PX50
A	?	-	VAL	deletion	UNP Q9PX50
A	?	-	GLN	deletion	UNP Q9PX50
A	?	-	PRO	deletion	UNP Q9PX50
A	?	-	THR	deletion	UNP Q9PX50
A	?	-	PHE	deletion	UNP Q9PX50
A	?	-	SER	deletion	UNP Q9PX50
A	?	-	VAL	deletion	UNP Q9PX50
A	?	-	GLN	deletion	UNP Q9PX50
A	?	-	ARG	deletion	UNP Q9PX50
A	?	-	ASN	deletion	UNP Q9PX50
A	?	-	LEU	deletion	UNP Q9PX50
A	?	-	PRO	deletion	UNP Q9PX50
A	?	-	PHE	deletion	UNP Q9PX50
A	?	-	GLU	deletion	UNP Q9PX50
A	?	-	ARG	deletion	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
A	?	-	THR	deletion	UNP Q9PX50
A	?	-	ILE	deletion	UNP Q9PX50
A	?	-	MET	deletion	UNP Q9PX50
A	?	-	ALA	deletion	UNP Q9PX50
B	-35	MET	-	initiating methionine	UNP Q9PX50
B	-34	GLY	-	expression tag	UNP Q9PX50
B	-33	SER	-	expression tag	UNP Q9PX50
B	-32	SER	-	expression tag	UNP Q9PX50

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-31	HIS	-	expression tag	UNP Q9PX50
B	-30	HIS	-	expression tag	UNP Q9PX50
B	-29	HIS	-	expression tag	UNP Q9PX50
B	-28	HIS	-	expression tag	UNP Q9PX50
B	-27	HIS	-	expression tag	UNP Q9PX50
B	-26	HIS	-	expression tag	UNP Q9PX50
B	-25	SER	-	expression tag	UNP Q9PX50
B	-24	SER	-	expression tag	UNP Q9PX50
B	-23	GLY	-	expression tag	UNP Q9PX50
B	-22	LEU	-	expression tag	UNP Q9PX50
B	-21	VAL	-	expression tag	UNP Q9PX50
B	-20	PRO	-	expression tag	UNP Q9PX50
B	-19	ARG	-	expression tag	UNP Q9PX50
B	-18	GLY	-	expression tag	UNP Q9PX50
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B	-6	MET	-	expression tag	UNP Q9PX50
B	-5	GLY	-	expression tag	UNP Q9PX50
B	-4	ARG	-	expression tag	UNP Q9PX50
B	-3	GLY	-	expression tag	UNP Q9PX50
B	-2	SER	-	expression tag	UNP Q9PX50
B	-1	GLU	-	expression tag	UNP Q9PX50
B	0	PHE	-	expression tag	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50
B	?	-	SER	deletion	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50
B	?	-	GLY	deletion	UNP Q9PX50
B	?	-	GLN	deletion	UNP Q9PX50
B	?	-	ILE	deletion	UNP Q9PX50
B	?	-	SER	deletion	UNP Q9PX50
B	?	-	VAL	deletion	UNP Q9PX50
B	?	-	GLN	deletion	UNP Q9PX50
B	?	-	PRO	deletion	UNP Q9PX50

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q9PX50
B	?	-	PHE	deletion	UNP Q9PX50
B	?	-	SER	deletion	UNP Q9PX50
B	?	-	VAL	deletion	UNP Q9PX50
B	?	-	GLN	deletion	UNP Q9PX50
B	?	-	ARG	deletion	UNP Q9PX50
B	?	-	ASN	deletion	UNP Q9PX50
B	?	-	LEU	deletion	UNP Q9PX50
B	?	-	PRO	deletion	UNP Q9PX50
B	?	-	PHE	deletion	UNP Q9PX50
B	?	-	GLU	deletion	UNP Q9PX50
B	?	-	ARG	deletion	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50
B	?	-	THR	deletion	UNP Q9PX50
B	?	-	ILE	deletion	UNP Q9PX50
B	?	-	MET	deletion	UNP Q9PX50
B	?	-	ALA	deletion	UNP Q9PX50

- Molecule 2 is a DNA chain called RNA (5'-R(P*(OMU)P*(OMU)P*(OMU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	P	0	0	0
			63	30	6	24	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	30	Total	O	0	0
			30	30		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.81Å 60.12Å 81.37Å 107.31° 106.68° 96.11°	Depositor
Resolution (Å)	36.61 – 3.00	Depositor
% Data completeness (in resolution range)	86.1 (36.61-3.00)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.289 , 0.332	Depositor
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.211	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,h+k+l	Xtriage
Total number of atoms	6421	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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](#)

Of 3 non-standard protein/DNA/RNA residues modelled in this entry, 3 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - 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.

4.5 Carbohydrates [i](#)

There are no oligosaccharides 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.