



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2025 – 10:03 am BST

PDB ID : 9RXW / pdb_00009rxw
Title : Ty1 Prime Retrotransposon Capsid C-Terminal Domain, wt
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Deposited on : 2025-07-13
Resolution : 1.60 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 ⓘ 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)	:	FAILED
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

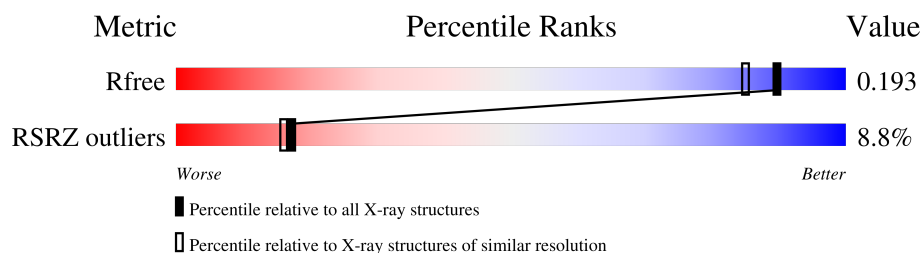
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4274 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1547 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	5	0
			735	456	125	150	4			
1	B	91	Total	C	N	O	S	0	4	0
			738	459	127	148	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	PRO	-	expression tag	UNP Q04215
A	353	LEU	-	expression tag	UNP Q04215
A	354	GLU	-	expression tag	UNP Q04215
A	355	HIS	-	expression tag	UNP Q04215
B	352	PRO	-	expression tag	UNP Q04215
B	353	LEU	-	expression tag	UNP Q04215
B	354	GLU	-	expression tag	UNP Q04215
B	355	HIS	-	expression tag	UNP Q04215

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	40	Total	O	0	0
			40	40		

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3 Data and refinement statistics

Xtriage (Phenix) 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	31.59Å 34.33Å 45.33Å 101.64° 96.35° 109.28°	Depositor
Resolution (Å)	43.58 – 1.60 43.58 – 1.60	Depositor EDS
% Data completeness (in resolution range)	82.5 (43.58-1.60) 82.5 (43.58-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0340	Depositor
R, R_{free}	0.180 , 0.202 (Not available) , 0.193	Depositor DCC
R_{free} test set	982 reflections (5.21%)	wwPDB-VP
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1547	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

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

5.1 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, 95th 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 ²)	Q<0.9
1	A	90/97 (92%)	0.39	8 (8%) 17 16	9, 21, 58, 76	5 (5%)
1	B	91/97 (93%)	0.42	8 (8%) 17 16	10, 21, 49, 75	4 (4%)
All	All	181/194 (93%)	0.41	16 (8%) 17 16	9, 21, 58, 76	9 (4%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	CYS	6.0
1	B	331	CYS	5.4
1	A	332	ILE	5.3
1	B	332	ILE	5.2
1	A	329	HIS	4.9
1	B	333	HIS	4.8
1	A	333	HIS	3.6
1	B	330	ARG	3.1
1	A	335	THR	2.4
1	A	334	MET	2.3
1	B	328	ARG	2.3
1	B	334	MET	2.2
1	A	351	GLN	2.2
1	B	262	ASP	2.1
1	A	348	GLU	2.0
1	B	324	LEU	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.