



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2025 – 10:04 am BST

PDB ID : 9RXX / pdb_00009rxx
Title : Ty1 Prime Retrotransposon Capsid C-Terminal Domain, F323S
Authors : Cottee, M.A.; Taylor, I.A.
Deposited on : 2025-07-13
Resolution : 1.62 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

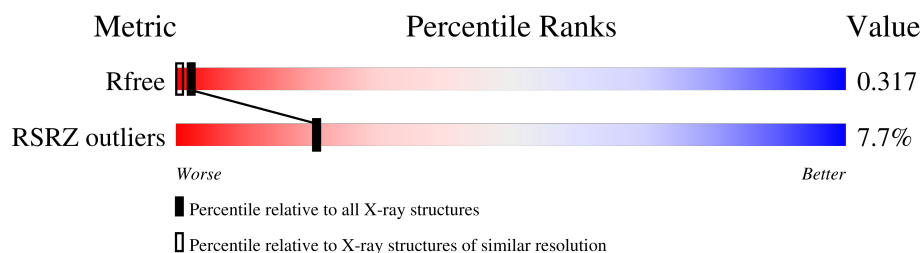
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	6077 (1.64-1.60)
RSRZ outliers	164620	6075 (1.64-1.60)

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 1431 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	92	Total	C	N	O	S	0	1	1
			694	429	124	135	6			
1	B	91	Total	C	N	O	S	0	2	0
			705	434	126	139	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	SER	PHE	engineered mutation	UNP Q04215
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	323	SER	PHE	engineered mutation	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	16	Total	O	0	0
			16	16		
2	B	16	Total	O	0	0
			16	16		

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

3 Data and refinement statistics

Xtriage (Phenix) 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	36.23Å 52.75Å 45.96Å 90.00° 108.54° 90.00°	Depositor
Resolution (Å)	43.58 – 1.62 43.57 – 1.62	Depositor EDS
% Data completeness (in resolution range)	71.4 (43.58-1.62) 71.4 (43.57-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.8.0340	Depositor
R, R_{free}	0.222 , 0.268 (Not available) , 0.317	Depositor DCC
R_{free} test set	759 reflections (4.80%)	wwPDB-VP
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1431	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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](#)

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

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	92/97 (94%)	0.79	4 (4%) 40 41	14, 39, 68, 81	1 (1%)
1	B	91/97 (93%)	0.86	10 (10%) 12 11	14, 36, 70, 78	2 (2%)
All	All	183/194 (94%)	0.82	14 (7%) 21 21	14, 38, 69, 81	3 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	TYR	4.9
1	A	326	TYR	3.4
1	B	327	ALA	3.3
1	B	262	ASP	3.3
1	B	329	HIS	3.0
1	B	332	ILE	2.7
1	A	332	ILE	2.6
1	B	298	ASN	2.5
1	B	333	HIS	2.3
1	B	352	PRO	2.2
1	A	351	GLN	2.1
1	B	295	ASP	2.1
1	A	302	ILE	2.1
1	B	299	ASN	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

There are no ligands in this entry.

5.5 Other polymers

There are no such residues in this entry.