



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2025 – 10:04 am BST

PDB ID : 9RXY / pdb_00009rxy
Title : Drt2, an Endogenised Ty1 Gag CA-CTD Restriction Factor, F323S Y329S
Authors : Cottee, M.A.; Taylor, I.A.
Deposited on : 2025-07-13
Resolution : 3.18 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 ⓘ 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

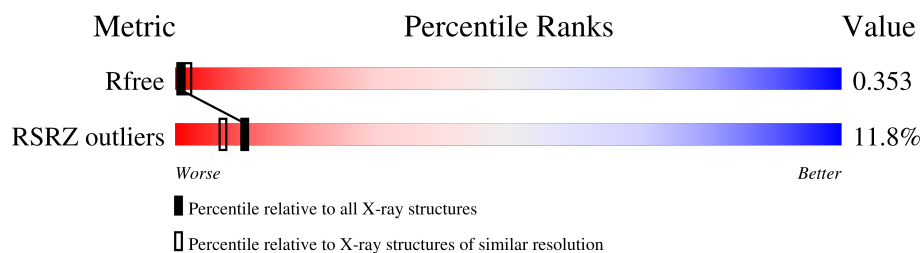
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1851 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

MolProbity 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 2313 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 Domesticated Restriction of Ty1-Prime Relic 2 (Drt2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			661	416	112	129	4			
1	B	89	Total	C	N	O	S	0	0	0
			642	405	106	128	3			
1	C	76	Total	C	N	O	S	0	0	0
			463	282	82	97	2			
1	D	84	Total	C	N	O	S	0	0	0
			547	340	93	113	1			

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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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	91.76Å 38.83Å 111.21Å 90.00° 96.65° 90.00°	Depositor
Resolution (Å)	45.57 – 3.18 45.57 – 3.18	Depositor EDS
% Data completeness (in resolution range)	59.0 (45.57-3.18) 59.1 (45.57-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.300 , 0.339 (Not available) , 0.353	Depositor DCC
R_{free} test set	191 reflections (4.74%)	wwPDB-VP
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 105.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	2313	wwPDB-VP
Average B, all atoms (Å ²)	62.0	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](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

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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	90/101 (89%)	0.75	9 (10%) 14 9	26, 44, 83, 103	0
1	B	89/101 (88%)	0.64	8 (8%) 17 11	22, 47, 89, 109	0
1	C	76/101 (75%)	0.82	11 (14%) 7 4	57, 78, 109, 146	0
1	D	84/101 (83%)	0.74	12 (14%) 7 5	59, 76, 98, 114	0
All	All	339/404 (83%)	0.73	40 (11%) 10 7	22, 63, 102, 146	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	ILE	3.6
1	A	317	LEU	3.5
1	A	329	SER	3.5
1	C	286	PHE	3.5
1	C	285	ALA	3.2

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.