



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:45 pm BST

PDB ID : 3TVV  
Title : Structure of the tandem PH domains of Rtt106 (residues 68-315)  
Authors : Su, D.; Thompson, J.R.; Mer, G.  
Deposited on : 2011-09-20  
Resolution : 2.59 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

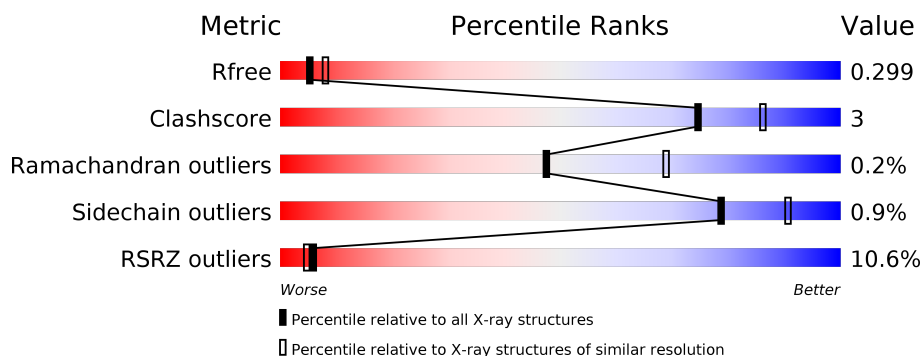
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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))
$R_{free}$	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	251	 12% 87% 6% 7%
1	B	251	 7% 80% 13% 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7974 atoms, of which 3955 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 Histone chaperone RTT106.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	233	Total	C	H	N	O	S	Se		0	7	0
			3891	1242	1970	305	364	3	7				
1	B	235	Total	C	H	N	O	S	Se		0	7	0
			3935	1262	1985	307	371	3	7				

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P40161
A	-1	HIS	-	EXPRESSION TAG	UNP P40161
A	0	MSE	-	EXPRESSION TAG	UNP P40161
A	171	LYS	ASN	SEE REMARK 999	UNP P40161
B	-2	GLY	-	EXPRESSION TAG	UNP P40161
B	-1	HIS	-	EXPRESSION TAG	UNP P40161
B	0	MSE	-	EXPRESSION TAG	UNP P40161
B	171	LYS	ASN	SEE REMARK 999	UNP P40161

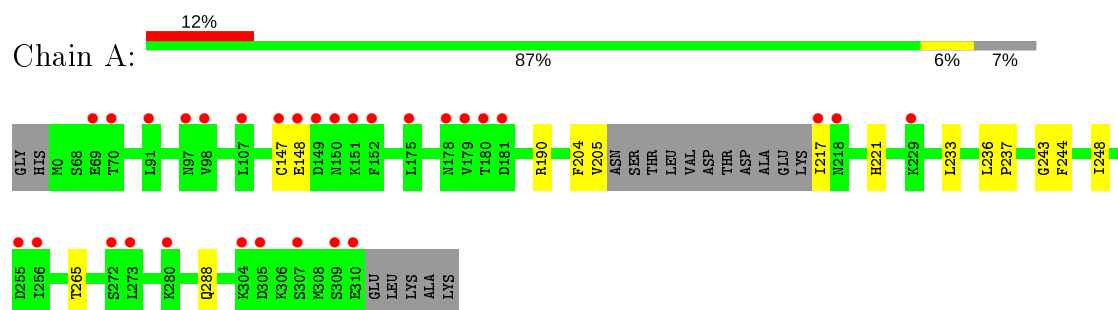
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O		
			79	79	0	1
2	B	69	Total	O		
			69	69	0	0

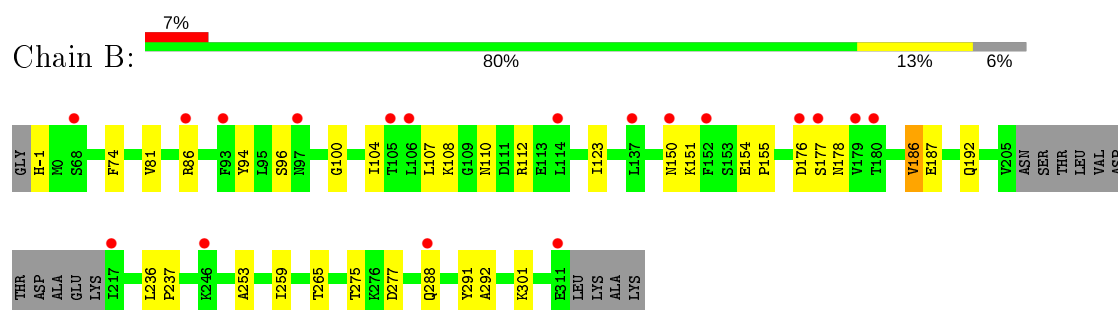
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Histone chaperone RTT106



- Molecule 1: Histone chaperone RTT106



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.66Å 60.64Å 77.17Å 90.00° 102.49° 90.00°	Depositor
Resolution (Å)	31.31 – 2.59 34.30 – 2.56	Depositor EDS
% Data completeness (in resolution range)	83.6 (31.31-2.59) 92.6 (34.30-2.56)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.57Å)	Xtriage
Refinement program	PHENIX dev_886, REFMAC 5.5.0070	Depositor
R, $R_{free}$	0.238 , 0.294 0.247 , 0.299	Depositor DCC
$R_{free}$ test set	973 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/1972	0.40	0/2644
1	B	0.23	0/2005	0.40	0/2690
All	All	0.23	0/3977	0.40	0/5334

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	GLY	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1921	1970	1970	8	0
1	B	1950	1985	1984	17	0
2	A	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	69	0	0	1	0
All	All	4019	3955	3954	25	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:THR:O	1:A:288:GLN:NE2	2.20	0.74
1:B:94:TYR:OH	1:B:112:ARG:NH2	2.33	0.61
1:B:275:THR:OG1	1:B:277:ASP:OD1	2.20	0.57
1:B:81:VAL:O	1:B:86:ARG:HA	2.05	0.56
1:A:236:LEU:HB3	1:A:237:PRO:HD2	1.88	0.56
1:A:244:PHE:HA	1:A:248:ILE:HG12	1.92	0.52
1:B:176[B]:ASP:OD1	1:B:177:SER:N	2.45	0.50
1:A:221:HIS:HA	1:A:233:LEU:O	2.12	0.49
1:A:190:ARG:NH1	2:A:25:HOH:O	2.45	0.49
1:B:265:THR:O	1:B:288:GLN:NE2	2.45	0.49
1:B:150:ASN:O	1:B:151:LYS:HB2	2.13	0.49
1:B:253:ALA:HB1	1:B:301:LYS:HG2	1.95	0.48
1:B:186:VAL:O	1:B:187:GLU:C	2.54	0.46
1:B:178:ASN:ND2	2:B:36:HOH:O	2.47	0.46
1:A:147:CYS:SG	1:A:148:GLU:N	2.87	0.46
1:A:204:PHE:O	1:A:205:VAL:HB	2.15	0.46
1:B:74:PHE:HB2	1:B:192:GLN:HG2	1.96	0.46
1:B:236:LEU:HB3	1:B:237:PRO:HD2	1.98	0.45
1:B:236:LEU:HB3	1:B:237:PRO:CD	2.46	0.45
1:B:259:ILE:HG23	1:B:259:ILE:O	2.19	0.42
1:B:96:SER:O	1:B:100:GLY:N	2.51	0.42
1:A:217:ILE:HD12	1:A:217:ILE:N	2.34	0.42
1:B:291:TYR:O	1:B:292:ALA:C	2.59	0.41
1:B:104:ILE:HD12	1:B:123[A]:ILE:HD11	2.04	0.40
1:B:154[A]:GLU:HA	1:B:155:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	236/251 (94%)	220 (93%)	16 (7%)	0	100	100
1	B	239/251 (95%)	220 (92%)	18 (8%)	1 (0%)	34	55
All	All	475/502 (95%)	440 (93%)	34 (7%)	1 (0%)	47	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	226/227 (100%)	226 (100%)	0	100	100
1	B	229/227 (101%)	225 (98%)	4 (2%)	60	79
All	All	455/454 (100%)	451 (99%)	4 (1%)	78	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	-1	HIS
1	B	107	LEU
1	B	108	LYS
1	B	110	ASN



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/251 (90%)	0.95	30 (13%) <b>3</b> <b>2</b>	40, 63, 107, 146	0
1	B	228/251 (90%)	0.63	18 (7%) <b>12</b> <b>10</b>	37, 68, 111, 132	0
All	All	454/502 (90%)	0.79	48 (10%) <b>6</b> <b>5</b>	37, 66, 111, 146	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	CYS	9.5
1	A	149	ASP	7.3
1	A	273	LEU	5.2
1	A	180	THR	5.0
1	A	69	GLU	5.0
1	A	148	GLU	4.9
1	A	307	SER	4.9
1	A	152	PHE	4.7
1	B	152[A]	PHE	4.6
1	A	178	ASN	4.6
1	A	217	ILE	4.4
1	A	150	ASN	4.3
1	B	176[A]	ASP	3.9
1	A	309	SER	3.8
1	A	304	LYS	3.8
1	A	179	VAL	3.8
1	B	288	GLN	3.5
1	B	311	GLU	3.5
1	B	150	ASN	3.3
1	A	97[A]	ASN	3.2
1	A	175	LEU	3.2
1	B	97[A]	ASN	3.2
1	A	305	ASP	3.2
1	B	217	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	310	GLU	3.0
1	A	107	LEU	3.0
1	A	256	ILE	2.8
1	B	105	THR	2.8
1	A	70	THR	2.7
1	A	255[A]	ASP	2.5
1	B	86	ARG	2.5
1	B	114	LEU	2.5
1	B	68	SER	2.4
1	A	151	LYS	2.4
1	B	106	LEU	2.4
1	B	179	VAL	2.4
1	B	246	LYS	2.3
1	A	218[A]	ASN	2.3
1	B	180	THR	2.3
1	B	93	PHE	2.2
1	B	177	SER	2.2
1	B	137	LEU	2.2
1	A	181	ASP	2.2
1	A	272	SER	2.2
1	A	280	LYS	2.1
1	A	229[A]	LYS	2.1
1	A	91	LEU	2.1
1	A	98	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.