



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 AM GMT

PDB ID : 2B4V  
Title : Structural Basis for UTP Specificity of RNA Editing TUTases From Trypanosoma Brucei  
Authors : Deng, J.; Ernst, N.L.; Turley, S.; Stuart, K.D.; Hol, W.G.  
Deposited on : 2005-09-26  
Resolution : 1.80 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

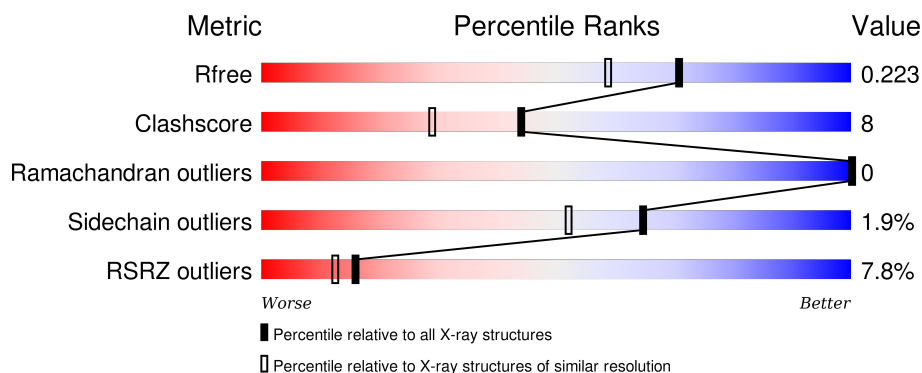
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

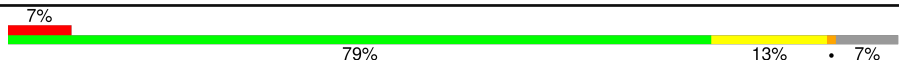
The reported resolution of this entry is 1.80 Å.

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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	468	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4072 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 RNA editing complex protein MP57.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	0	7	0
			3549	2255	631	637	11	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	56	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	86	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	92	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	94	ARG	TRP	ENGINEERED	UNP Q86MV5
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	122	ARG	TRP	ENGINEERED	UNP Q86MV5
A	198	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	207	ARG	TRP	ENGINEERED	UNP Q86MV5
A	227	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	240	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	244	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	261	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	263	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	297	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	315	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	324	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5
A	456	MSE	MET	MODIFIED RESIDUE	UNP Q86MV5

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

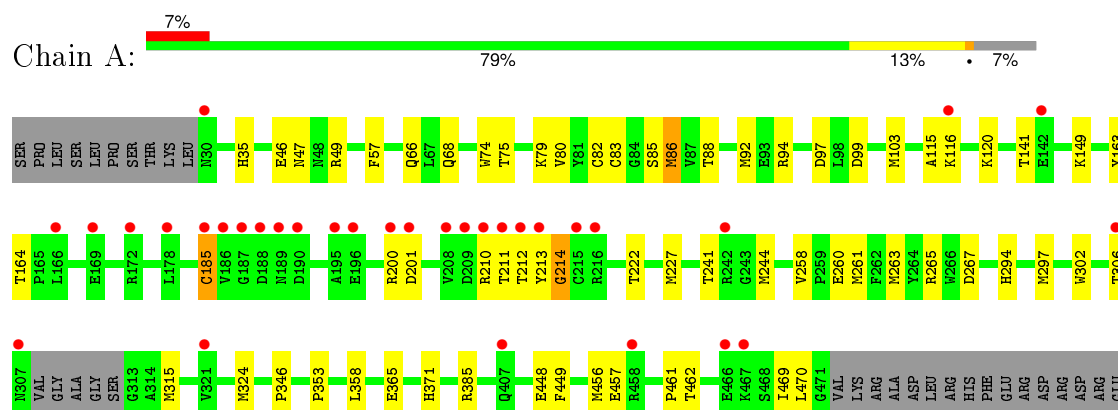
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	522	Total 522	O 522	0	2

### 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 errors 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: RNA editing complex protein MP57



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.57Å 91.57Å 163.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 36.61 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.80) 98.6 (36.61-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.196 , 0.227 0.222 , 0.223	Depositor DCC
$R_{free}$ test set	3298 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 69906 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section:  
K

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	0.49	0/3648	0.57	0/4920

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	TYR	Peptide
1	A	214	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	3549	0	3446	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	522	0	0	4	0
All	All	4072	0	3446	56	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 8.

All (56) 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:86:MSE:HE1	1:A:92:MSE:HB2	1.21	1.19
1:A:258:VAL:O	1:A:263:MSE:HE2	1.40	1.18
1:A:260:GLU:HA	1:A:263:MSE:HE3	1.39	1.00
1:A:211:THR:HG22	1:A:212:THR:H	1.27	0.99
1:A:211:THR:HB	1:A:214:GLY:HA3	1.49	0.95
1:A:211:THR:HG22	1:A:212:THR:N	1.83	0.90
1:A:94:ARG:HE	1:A:163:TYR:HE1	1.13	0.90
1:A:260:GLU:CA	1:A:263:MSE:HE3	2.01	0.89
1:A:86:MSE:CE	1:A:92:MSE:HB2	2.05	0.86
1:A:57:PHE:CD1	1:A:86:MSE:HE2	2.12	0.84
1:A:294:HIS:HA	1:A:297:MSE:CE	2.07	0.84
1:A:294:HIS:HA	1:A:297:MSE:HE3	1.61	0.81
1:A:115:ALA:HB1	1:A:141:THR:HG23	1.60	0.81
1:A:365:GLU:HG3	3:A:993:HOH:O	1.81	0.78
1:A:211:THR:CG2	1:A:212:THR:H	1.98	0.77
1:A:86:MSE:HE1	1:A:92:MSE:CB	2.12	0.74
1:A:211:THR:HB	1:A:214:GLY:CA	2.21	0.69
1:A:260:GLU:N	1:A:263:MSE:HE3	2.08	0.69
1:A:47:ASN:HD22	1:A:294:HIS:HD2	1.38	0.68
1:A:315:MSE:HE1	1:A:448:GLU:HG3	1.76	0.67
1:A:185[A]:CYS:SG	1:A:210:ARG:HG2	2.35	0.66
1:A:97[B]:ASP:OD1	1:A:265:ARG:CZ	2.45	0.65
1:A:68:GLN:HE22	1:A:80:VAL:H	1.43	0.64
1:A:35:HIS:HE1	1:A:456:MSE:O	1.80	0.63
1:A:241:THR:HG23	1:A:244:MSE:HE3	1.80	0.62
1:A:57:PHE:HD1	1:A:86:MSE:HE2	1.65	0.62
1:A:97[B]:ASP:OD1	1:A:265:ARG:NH1	2.34	0.60
1:A:83[B]:CYS:SG	1:A:99[B]:ASP:OD1	2.59	0.60
1:A:47:ASN:HD22	1:A:294:HIS:CD2	2.19	0.59
1:A:68:GLN:NE2	1:A:80:VAL:H	2.00	0.58
1:A:94:ARG:NE	1:A:163:TYR:HE1	1.94	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:CG2	1:A:244:MSE:HE3	2.36	0.55
1:A:324:MSE:HE1	1:A:449:PHE:CZ	2.42	0.54
1:A:297:MSE:HE1	1:A:358:LEU:HD11	1.89	0.54
1:A:241:THR:OG1	1:A:244:MSE:HE3	2.09	0.53
1:A:149:LYS:HG3	1:A:267[A]:ASP:OD1	2.09	0.52
1:A:371:HIS:HE1	1:A:457:GLU:OE2	1.93	0.52
1:A:294:HIS:HA	1:A:297:MSE:HE2	1.92	0.51
1:A:315:MSE:HE1	1:A:448:GLU:CG	2.43	0.47
1:A:371:HIS:HD2	3:A:587:HOH:O	1.98	0.46
1:A:82:CYS:HB3	1:A:353:PRO:HD3	1.98	0.45
1:A:66:GLN:NE2	1:A:261:MSE:H	2.14	0.45
1:A:103:MSE:HE2	1:A:346:PRO:HB3	1.99	0.45
1:A:46:GLU:OE2	1:A:49:ARG:NH1	2.50	0.45
1:A:86:MSE:CE	1:A:92:MSE:CB	2.86	0.44
1:A:116:LYS:HG3	3:A:718:HOH:O	2.17	0.44
1:A:385:ARG:HB3	1:A:385:ARG:HE	1.59	0.44
1:A:74:TRP:HZ2	1:A:120:LYS:HE3	1.83	0.44
1:A:302:TRP:O	1:A:306:THR:HG23	2.17	0.44
1:A:456:MSE:HG3	1:A:469:ILE:HD13	2.00	0.43
1:A:201:ASP:O	1:A:222:THR:HG21	2.18	0.43
1:A:85:SER:HA	1:A:88:THR:OG1	2.19	0.42
1:A:315:MSE:CE	1:A:448:GLU:HG3	2.48	0.42
1:A:79:LYS:HD2	3:A:793:HOH:O	2.19	0.41
1:A:324:MSE:HE1	1:A:449:PHE:HZ	1.86	0.41
1:A:461:PRO:HB3	1:A:470:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	440/468 (94%)	432 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	376/390 (96%)	368 (98%)	8 (2%)	61 47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	86	MSE
1	A	164	THR
1	A	185[A]	CYS
1	A	185[B]	CYS
1	A	200	ARG
1	A	227	MSE
1	A	462	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	66	GLN
1	A	68	GLN
1	A	91	GLN
1	A	277	ASN
1	A	294	HIS
1	A	334	GLN
1	A	371	HIS
1	A	391	ASN
1	A	416	ASN
1	A	438	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - 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.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	422/468 (90%)	0.52	33 (7%) 16 12	13, 22, 35, 45	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	ASP	4.7
1	A	466	GLU	4.6
1	A	242	ARG	4.0
1	A	212	THR	4.0
1	A	307	ASN	3.7
1	A	186	VAL	3.6
1	A	201	ASP	3.6
1	A	188	ASP	3.5
1	A	195	ALA	3.5
1	A	213	TYR	3.4
1	A	169	GLU	3.2
1	A	210	ARG	3.2
1	A	187	GLY	3.2
1	A	189	ASN	3.2
1	A	216	ARG	3.1
1	A	211	THR	2.9
1	A	200	ARG	2.8
1	A	306	THR	2.8
1	A	407	GLN	2.7
1	A	142	GLU	2.6
1	A	458	ARG	2.6
1	A	166	LEU	2.5
1	A	185[A]	CYS	2.5
1	A	116	LYS	2.4
1	A	208	VAL	2.3
1	A	172	ARG	2.3
1	A	190	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	321	VAL	2.2
1	A	178	LEU	2.1
1	A	30	ASN	2.1
1	A	215	CYS	2.1
1	A	467	LYS	2.1
1	A	196	GLU	2.1

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	A	1	1/1	0.99	0.06	-1.91	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.