



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 AM GMT

PDB ID : 2B56  
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 : 2005-09-27  
Resolution : 1.97 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

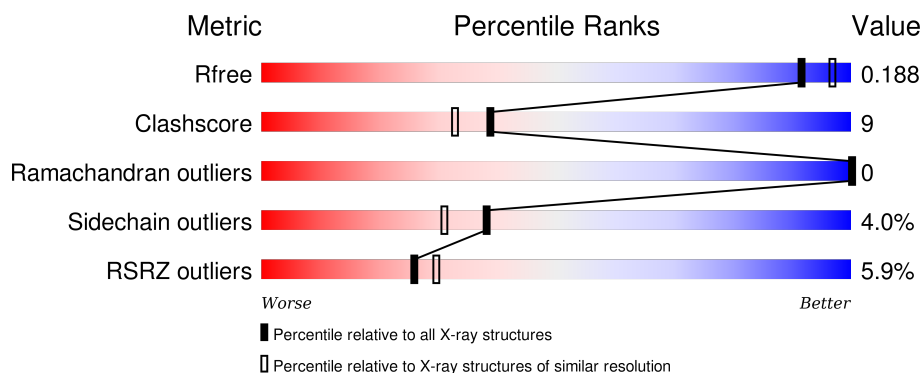
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	U5P	A	601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	U5P	A	602	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3917 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	444	Total	C	N	O	S	0	0	0
			3565	2265	636	640	24			

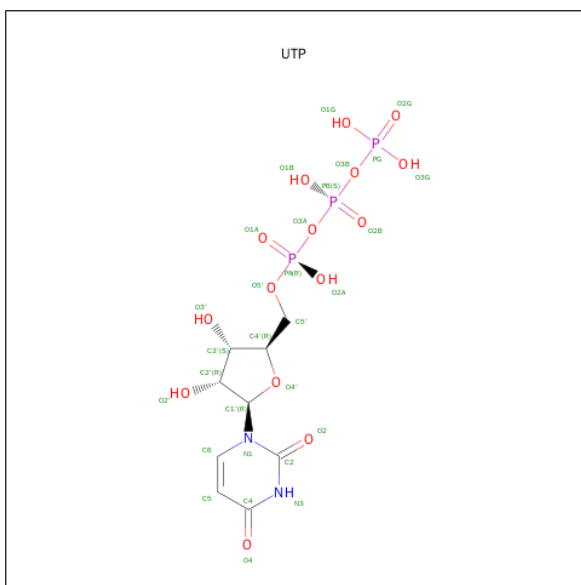
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ARG	TRP	ENGINEERED	UNP Q86MV5
A	122	ARG	TRP	ENGINEERED	UNP Q86MV5
A	207	ARG	TRP	ENGINEERED	UNP Q86MV5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

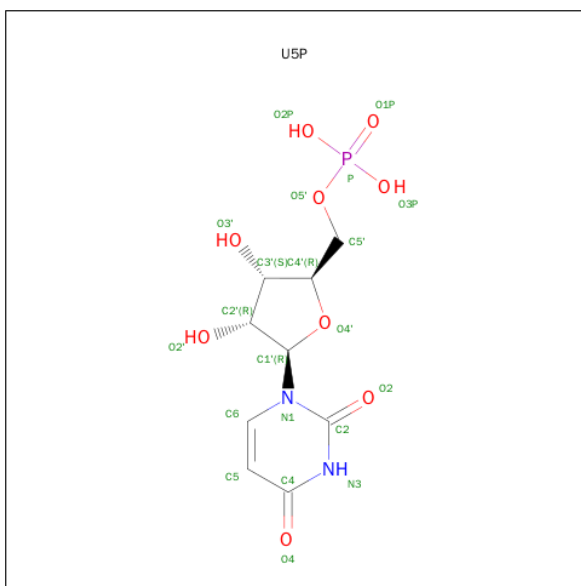
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>2</sub>O<sub>15</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 4 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula:  $\text{C}_9\text{H}_{13}\text{N}_2\text{O}_9\text{P}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 21	C 9	N 2	O 9	P 1	0	0
4	A	1	Total 21	C 9	N 2	O 9	P 1	0	0

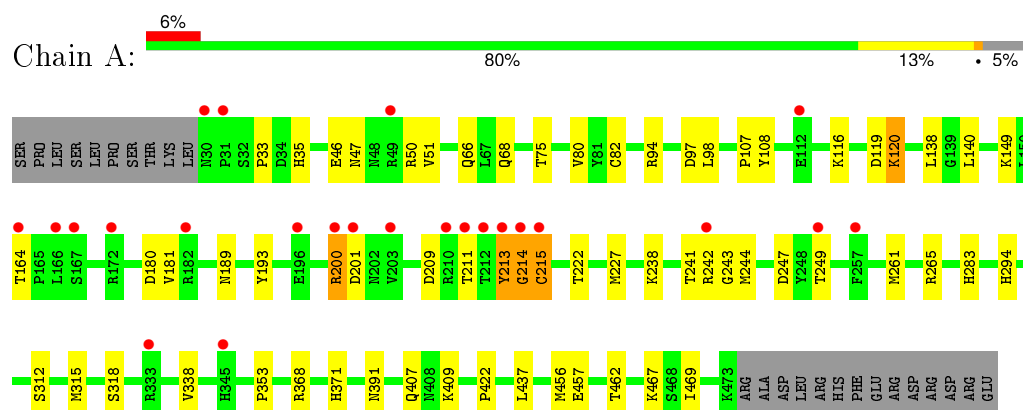
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	280	Total 280	O 280	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 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, $\alpha$ , $\beta$ , $\gamma$	91.44Å 91.44Å 162.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.97 46.61 – 1.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.97) 100.0 (46.61-1.97)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.193 , 0.221 0.194 , 0.188	Depositor DCC
$R_{free}$ test set	2467 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49306 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: MG, UTP, U5P

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	0.54	0/3660	0.59	1/4961 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ASP	CB-CG-OD2	5.22	123.00	118.30

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	3565	0	3456	60	0
2	A	1	0	0	0	0
3	A	29	0	11	0	0
4	A	42	0	22	4	0
5	A	280	0	0	9	0
All	All	3917	0	3489	64	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 9.

All (64) 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:200:ARG:NH2	1:A:201:ASP:HB2	1.48	1.27
1:A:200:ARG:HH21	1:A:201:ASP:CB	1.52	1.20
1:A:200:ARG:NE	1:A:201:ASP:H	1.48	1.11
1:A:200:ARG:HE	1:A:201:ASP:N	1.46	1.11
1:A:200:ARG:HD3	1:A:200:ARG:H	1.05	1.10
1:A:241:THR:H	1:A:244:MET:HE3	1.16	1.08
1:A:200:ARG:CD	1:A:200:ARG:H	1.76	0.98
1:A:241:THR:N	1:A:244:MET:HE3	1.79	0.95
1:A:200:ARG:N	1:A:200:ARG:HD3	1.81	0.95
1:A:200:ARG:CD	1:A:200:ARG:N	2.30	0.91
1:A:200:ARG:HH21	1:A:201:ASP:HB2	0.73	0.89
1:A:409:LYS:HD2	5:A:706:HOH:O	1.75	0.86
4:A:602:U5P:H5'1	5:A:768:HOH:O	1.74	0.86
1:A:211:THR:OG1	1:A:214:GLY:HA2	1.79	0.82
4:A:602:U5P:C5'	5:A:768:HOH:O	2.31	0.76
1:A:211:THR:OG1	1:A:214:GLY:CA	2.35	0.75
1:A:47:ASN:HD22	1:A:294:HIS:HD2	1.35	0.74
1:A:181:VAL:HB	1:A:215:CYS:SG	2.33	0.69
1:A:51:VAL:O	1:A:94:ARG:NH1	2.23	0.69
1:A:200:ARG:NE	1:A:200:ARG:N	2.41	0.68
1:A:391:ASN:HD21	1:A:422:PRO:HA	1.60	0.64
1:A:200:ARG:NH2	1:A:201:ASP:CB	2.30	0.64
1:A:68:GLN:HE22	1:A:80:VAL:H	1.46	0.62
1:A:35:HIS:HE1	1:A:456:MET:O	1.82	0.61
1:A:47:ASN:HD22	1:A:294:HIS:CD2	2.18	0.61
1:A:201:ASP:O	1:A:222:THR:HG21	2.03	0.58
1:A:68:GLN:NE2	1:A:80:VAL:H	2.02	0.56
1:A:371:HIS:HE1	1:A:457:GLU:OE2	1.89	0.55
1:A:200:ARG:HE	1:A:201:ASP:H	0.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:O	1:A:120:LYS:HD3	2.09	0.52
1:A:33:PRO:HG3	1:A:368:ARG:HH22	1.73	0.52
1:A:200:ARG:CZ	1:A:201:ASP:H	2.20	0.51
1:A:241:THR:HG22	1:A:242:ARG:N	2.26	0.51
1:A:98:LEU:HD11	5:A:671:HOH:O	2.10	0.51
1:A:138:LEU:HD11	1:A:151:ARG:HD3	1.93	0.50
1:A:193:TYR:OH	1:A:238:LYS:HD3	2.12	0.50
1:A:306:THR:OG1	1:A:308:VAL:HG13	2.12	0.49
1:A:371:HIS:CE1	1:A:457:GLU:OE2	2.66	0.49
1:A:213:TYR:N	1:A:214:GLY:CA	2.75	0.49
1:A:467:LYS:HD3	5:A:797:HOH:O	2.12	0.49
4:A:601:U5P:O5'	4:A:601:U5P:H6	2.13	0.48
1:A:97:ASP:HB3	1:A:265:ARG:NH1	2.28	0.48
1:A:283:HIS:HE1	5:A:692:HOH:O	1.96	0.48
1:A:241:THR:HG22	1:A:243:GLY:H	1.78	0.48
1:A:300:LYS:HD2	1:A:318:SER:HB3	1.94	0.47
1:A:66:GLN:NE2	1:A:261:MET:H	2.12	0.47
1:A:180:ASP:HB3	1:A:249:THR:HB	1.96	0.47
4:A:602:U5P:H5'2	5:A:768:HOH:O	2.10	0.46
1:A:407:GLN:O	1:A:409:LYS:HG2	2.16	0.45
1:A:107:PRO:HG2	1:A:108:TYR:CE2	2.51	0.45
1:A:82:CYS:HB3	1:A:353:PRO:HD3	1.99	0.45
1:A:200:ARG:NH2	1:A:201:ASP:CG	2.70	0.45
1:A:409:LYS:HE2	5:A:670:HOH:O	2.16	0.44
1:A:193:TYR:OH	1:A:238:LYS:CD	2.66	0.44
1:A:35:HIS:CE1	1:A:456:MET:O	2.67	0.43
1:A:456:MET:HG3	1:A:469:ILE:HD13	2.00	0.42
1:A:467:LYS:HB2	1:A:467:LYS:HE3	1.82	0.41
1:A:244:MET:O	1:A:247:ASP:HB2	2.20	0.41
1:A:241:THR:CG2	1:A:242:ARG:N	2.83	0.41
1:A:97:ASP:HB3	1:A:265:ARG:HH12	1.85	0.41
1:A:213:TYR:H	1:A:214:GLY:CA	2.33	0.40
1:A:46:GLU:HG3	1:A:50:ARG:NH2	2.36	0.40
1:A:391:ASN:ND2	5:A:610:HOH:O	2.53	0.40
1:A:140:LEU:HD11	1:A:149:LYS:HE3	2.04	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	442/468 (94%)	432 (98%)	10 (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	374/405 (92%)	359 (96%)	15 (4%)	38	31

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	THR
1	A	119	ASP
1	A	120	LYS
1	A	156	GLU
1	A	164	THR
1	A	189	ASN
1	A	200	ARG
1	A	215	CYS
1	A	227	MET
1	A	308	VAL
1	A	312	SER
1	A	315	MET
1	A	338	VAL

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Mol	Chain	Res	Type
1	A	437	LEU
1	A	462	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	184	GLN
1	A	189	ASN
1	A	283	HIS
1	A	294	HIS
1	A	334	GLN
1	A	348	HIS
1	A	371	HIS
1	A	380	HIS
1	A	391	ASN

### 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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	UTP	A	501	2	20,30,30	1.35	1 (5%)	30,47,47	1.69	4 (13%)
4	U5P	A	601	-	16,22,22	1.53	3 (18%)	21,33,33	1.82	3 (14%)
4	U5P	A	602	-	16,22,22	1.44	1 (6%)	21,33,33	1.52	2 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UTP	A	501	2	-	0/18/38/38	0/2/2/2
4	U5P	A	601	-	-	0/6/26/26	0/2/2/2
4	U5P	A	602	-	-	0/6/26/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	U5P	P-O3P	2.16	1.62	1.54
4	A	601	U5P	O4'-C1'	2.36	1.44	1.41
4	A	601	U5P	O4-C4	4.63	1.35	1.24
4	A	602	U5P	O4-C4	4.68	1.35	1.24
3	A	501	UTP	O4-C4	4.94	1.36	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	UTP	O3'-C3'-C2'	-2.28	104.42	111.83
3	A	501	UTP	O2'-C2'-C3'	-2.09	105.04	111.83
4	A	601	U5P	O4'-C1'-N1	2.11	112.53	108.08
4	A	601	U5P	O2P-P-O1P	2.59	118.92	110.58
3	A	501	UTP	O3G-PG-O1G	2.64	117.44	107.38
4	A	602	U5P	O2P-P-O1P	3.09	120.53	110.58
4	A	602	U5P	C4-N3-C2	5.71	119.80	114.14
3	A	501	UTP	C4-N3-C2	6.47	120.55	114.14
4	A	601	U5P	C4-N3-C2	6.61	120.69	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	U5P	1	0
4	A	602	U5P	3	0

## 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	444/468 (94%)	0.69	26 (5%)	26 30	16, 28, 40, 50	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	ARG	6.1
1	A	201	ASP	4.9
1	A	242	ARG	4.4
1	A	213	TYR	4.1
1	A	215	CYS	3.9
1	A	196	GLU	3.9
1	A	163	TYR	3.6
1	A	210	ARG	3.5
1	A	172	ARG	3.0
1	A	182	ARG	2.8
1	A	31	PRO	2.8
1	A	333	ARG	2.8
1	A	166	LEU	2.7
1	A	211	THR	2.7
1	A	156	GLU	2.6
1	A	203	VAL	2.6
1	A	112	GLU	2.4
1	A	214	GLY	2.4
1	A	345	HIS	2.4
1	A	257	PHE	2.4
1	A	164	THR	2.3
1	A	30	ASN	2.3
1	A	167	SER	2.3
1	A	212	THR	2.2
1	A	249	THR	2.2
1	A	49	ARG	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(Å <sup>2</sup> )	Q<0.9
4	U5P	A	602	21/21	0.82	0.20	5.16	31,36,38,40	4
4	U5P	A	601	21/21	0.88	0.20	2.66	32,43,59,59	0
3	UTP	A	501	29/29	0.95	0.10	-3.90	19,24,34,39	0
2	MG	A	488	1/1	0.94	0.09	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.