



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:45 AM GMT

PDB ID : 2IKF  
Title : Terminal uridylyl transferase 4 from Trypanosoma brucei with bound UTP  
Authors : Luecke, H.; Stagno, J.  
Deposited on : 2006-10-02  
Resolution : 2.00 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

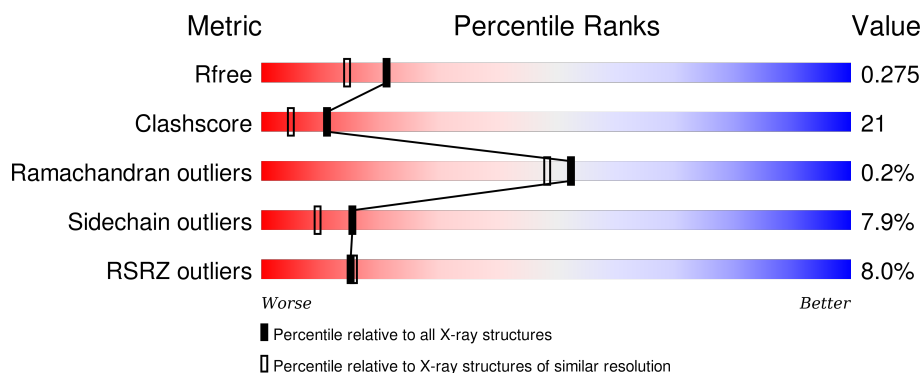
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

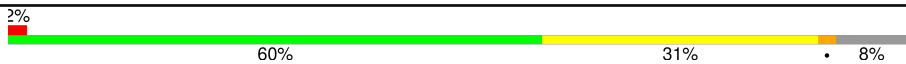

The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	353	
1	B	353	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5333 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 uridylyl transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2601	1653	465	476	7			
1	B	310	Total	C	N	O	S	0	0	0
			2486	1587	441	451	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q381M1
A	-18	GLY	-	CLONING ARTIFACT	UNP Q381M1
A	-17	SER	-	CLONING ARTIFACT	UNP Q381M1
A	-16	SER	-	CLONING ARTIFACT	UNP Q381M1
A	-15	HIS	-	EXPRESSION TAG	UNP Q381M1
A	-14	HIS	-	EXPRESSION TAG	UNP Q381M1
A	-13	HIS	-	EXPRESSION TAG	UNP Q381M1
A	-12	HIS	-	EXPRESSION TAG	UNP Q381M1
A	-11	HIS	-	EXPRESSION TAG	UNP Q381M1
A	-10	HIS	-	EXPRESSION TAG	UNP Q381M1
A	-9	SER	-	CLONING ARTIFACT	UNP Q381M1
A	-8	SER	-	CLONING ARTIFACT	UNP Q381M1
A	-7	GLY	-	CLONING ARTIFACT	UNP Q381M1
A	-6	LEU	-	CLONING ARTIFACT	UNP Q381M1
A	-5	VAL	-	CLONING ARTIFACT	UNP Q381M1
A	-4	PRO	-	CLONING ARTIFACT	UNP Q381M1
A	-3	ARG	-	CLONING ARTIFACT	UNP Q381M1
A	-2	GLY	-	CLONING ARTIFACT	UNP Q381M1
A	-1	SER	-	CLONING ARTIFACT	UNP Q381M1
A	0	HIS	-	CLONING ARTIFACT	UNP Q381M1
B	-19	MET	-	CLONING ARTIFACT	UNP Q381M1
B	-18	GLY	-	CLONING ARTIFACT	UNP Q381M1
B	-17	SER	-	CLONING ARTIFACT	UNP Q381M1
B	-16	SER	-	CLONING ARTIFACT	UNP Q381M1
B	-15	HIS	-	EXPRESSION TAG	UNP Q381M1

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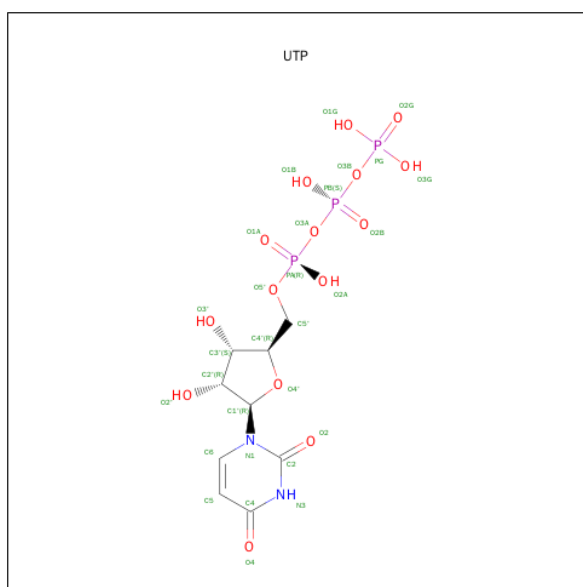
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-13	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-12	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-11	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-10	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-9	SER	-	CLONING ARTIFACT	UNP Q381M1
B	-8	SER	-	CLONING ARTIFACT	UNP Q381M1
B	-7	GLY	-	CLONING ARTIFACT	UNP Q381M1
B	-6	LEU	-	CLONING ARTIFACT	UNP Q381M1
B	-5	VAL	-	CLONING ARTIFACT	UNP Q381M1
B	-4	PRO	-	CLONING ARTIFACT	UNP Q381M1
B	-3	ARG	-	CLONING ARTIFACT	UNP Q381M1
B	-2	GLY	-	CLONING ARTIFACT	UNP Q381M1
B	-1	SER	-	CLONING ARTIFACT	UNP Q381M1
B	0	HIS	-	CLONING ARTIFACT	UNP Q381M1

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

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

- 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	B	60	Total	O	0	0
			60	60		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.77Å 41.52Å 103.79Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	51.71 – 2.00 51.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (51.71-2.00) 94.3 (51.70-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.228 , 0.275 0.227 , 0.275	Depositor DCC
$R_{free}$ test set	2222 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.9	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	0 of 43270 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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: UTP, MG

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	0.77	0/2658	0.89	0/3605
1	B	0.60	0/2541	0.80	1/3444 (0.0%)
All	All	0.69	0/5199	0.85	1/7049 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ILE	N-CA-C	-5.04	97.39	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2601	0	2604	79	0
1	B	2486	0	2489	136	0
2	A	1	0	0	0	0
3	A	29	0	11	1	0
4	A	156	0	0	5	0
4	B	60	0	0	2	0
All	All	5333	0	5104	213	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 21.

All (213) 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:B:126:ARG:HB2	1:B:126:ARG:NH1	1.70	1.06
1:B:126:ARG:HB2	1:B:126:ARG:HH11	0.88	1.04
1:A:185:SER:HB3	1:A:313:LYS:HD3	1.39	1.01
1:B:106:ARG:HG2	1:B:114:VAL:HG11	1.49	0.92
1:B:126:ARG:CB	1:B:126:ARG:HH11	1.81	0.89
1:B:142:ARG:O	1:B:145:VAL:HG22	1.73	0.89
1:B:124:VAL:HG21	1:B:136:ASP:HB3	1.59	0.83
1:B:319:ARG:HH12	1:B:323:LYS:HD3	1.44	0.82
1:B:102:ALA:O	1:B:106:ARG:HG3	1.82	0.79
1:B:7:VAL:HG22	1:B:10:ARG:NH2	2.01	0.75
1:B:146:ARG:NH1	1:B:213:ILE:O	2.19	0.75
1:B:163:TRP:CZ2	1:B:227:LEU:HD11	2.21	0.75
1:A:191:PHE:HA	1:A:194:MET:HE3	1.67	0.75
1:A:63:LYS:HE2	1:A:64:GLY:N	2.01	0.75
1:A:318:ARG:O	1:A:322:GLU:HG3	1.88	0.73
1:B:43:VAL:O	1:B:44:ASP:HB2	1.88	0.73
1:B:116:GLU:HG2	1:B:125:VAL:HG22	1.71	0.72
1:B:105:ILE:HD11	1:B:114:VAL:CG2	2.20	0.72
1:A:135:PHE:HE1	1:A:137:ILE:HD11	1.55	0.71
1:A:332:ILE:HG23	1:A:332:ILE:O	1.91	0.71
1:B:91:LYS:C	1:B:91:LYS:HD2	2.12	0.70
1:B:7:VAL:HG22	1:B:10:ARG:HH22	1.58	0.69
1:B:50:TYR:CD2	1:B:220:PRO:HA	2.27	0.68
1:B:105:ILE:HD11	1:B:114:VAL:HB	1.76	0.68
1:A:39:CYS:SG	1:A:105:ILE:HD13	2.34	0.68
1:A:47:MET:HG2	1:A:71:VAL:HG13	1.75	0.68
1:A:10:ARG:HG2	1:A:233:GLU:HG3	1.76	0.67
1:A:131:GLY:C	1:A:133:VAL:H	1.99	0.66
1:B:158:ASN:HD22	1:B:160:PRO:HD2	1.60	0.66
1:B:30:ASP:HA	1:B:221:LEU:HD21	1.76	0.66
1:B:100:LYS:O	1:B:104:VAL:HG23	1.95	0.65
1:B:42:ALA:HB3	1:B:104:VAL:HG11	1.79	0.65
1:B:108:LYS:HG3	1:B:109:HIS:CE1	2.33	0.64
1:A:163:TRP:CZ2	1:A:227:LEU:HD13	2.34	0.63
1:B:32:THR:OG1	1:B:133:VAL:HG22	1.98	0.63
1:A:283:ARG:HG3	1:A:287:GLU:O	1.99	0.63
1:B:98:LEU:HB3	1:B:125:VAL:HG23	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:VAL:HG23	1:B:138:THR:HG23	1.80	0.62
1:B:194:MET:HG2	1:B:259:ILE:HD13	1.81	0.62
1:B:25:HIS:ND1	1:B:27:ARG:HG3	2.14	0.61
1:A:174:GLN:HB2	1:A:330:LEU:HD12	1.81	0.61
1:B:105:ILE:HG13	1:B:106:ARG:N	2.14	0.61
1:B:24:LEU:HB3	1:B:60:VAL:HB	1.81	0.61
1:A:327:THR:C	1:A:332:ILE:HG22	2.21	0.60
1:B:39:CYS:O	1:B:42:ALA:HB3	2.01	0.60
1:A:169:LYS:HG3	4:A:655:HOH:O	2.02	0.60
1:A:324:ALA:HB1	1:A:329:LEU:HD23	1.84	0.59
1:A:3:PRO:HD3	1:A:326:ASP:HA	1.83	0.59
1:B:114:VAL:O	1:B:114:VAL:HG22	2.01	0.59
1:B:105:ILE:HD11	1:B:114:VAL:CB	2.32	0.59
1:A:135:PHE:CE1	1:A:137:ILE:HD11	2.37	0.58
1:B:185:SER:HB3	1:B:313:LYS:HD3	1.86	0.58
1:B:124:VAL:HG23	1:B:137:ILE:C	2.24	0.58
1:B:98:LEU:HB3	1:B:125:VAL:CG2	2.33	0.58
1:B:322:GLU:HA	1:B:325:ARG:HH11	1.69	0.58
1:B:42:ALA:O	1:B:43:VAL:HG13	2.04	0.58
1:B:202:ARG:NH2	1:B:251:GLU:OE1	2.32	0.58
1:A:295:ILE:HB	1:A:305:VAL:HB	1.86	0.58
1:B:16:PHE:O	1:B:20:VAL:HG23	2.04	0.57
1:A:198:TYR:OH	1:A:243:ASP:HB3	2.04	0.57
1:B:232:ASP:O	1:B:233:GLU:HG3	2.04	0.57
1:B:113:ASN:HB2	1:B:128:LYS:HB2	1.86	0.57
1:B:29:VAL:HG22	1:B:67:VAL:HG21	1.86	0.57
1:A:185:SER:HB3	1:A:313:LYS:CD	2.26	0.57
1:B:33:TYR:CD2	1:B:221:LEU:HD22	2.40	0.57
1:B:241:VAL:HG11	1:B:329:LEU:HD22	1.86	0.57
1:B:315:ASP:HB3	1:B:318:ARG:NH2	2.19	0.57
1:B:93:LEU:HD23	1:B:93:LEU:O	2.04	0.57
1:B:93:LEU:HD22	1:B:140:TYR:HE2	1.69	0.56
1:B:292:GLN:HB3	1:B:314:ARG:HD3	1.88	0.56
1:A:283:ARG:NH1	1:A:287:GLU:HA	2.20	0.56
1:B:197:TYR:O	1:B:201:GLN:HG2	2.05	0.56
1:B:124:VAL:HG23	1:B:137:ILE:O	2.04	0.56
1:B:47:MET:HE2	1:B:73:ASN:HB2	1.86	0.56
1:B:47:MET:HG2	1:B:73:ASN:OD1	2.05	0.56
1:B:105:ILE:HD11	1:B:114:VAL:HG21	1.88	0.56
1:A:81:LYS:HE3	1:A:214:ASP:HB2	1.88	0.55
1:B:281:PHE:O	1:B:285:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:O	1:B:36:VAL:HG23	2.06	0.55
1:A:249:LEU:HD21	1:A:321:LEU:HB2	1.88	0.55
1:A:101:LEU:O	1:A:105:ILE:HG12	2.07	0.54
1:B:152:ARG:CZ	1:B:222:PRO:HB2	2.38	0.53
1:A:4:SER:OG	1:A:7:VAL:HG23	2.08	0.53
1:B:66:ASP:OD1	1:B:134:ASP:HB3	2.08	0.53
1:B:25:HIS:CE1	1:B:27:ARG:HG3	2.44	0.53
1:A:254:SER:O	1:A:269:LYS:HE3	2.09	0.53
1:B:142:ARG:O	1:B:145:VAL:CG2	2.54	0.53
1:B:74:LYS:HD2	1:B:140:TYR:HB3	1.90	0.53
1:B:158:ASN:ND2	1:B:160:PRO:HD2	2.23	0.53
1:B:31:ALA:HA	1:B:34:ARG:CZ	2.39	0.52
1:B:162:ARG:O	1:B:166:MET:HG3	2.09	0.52
1:B:268:THR:O	1:B:271:GLU:HG2	2.09	0.52
1:A:88:GLN:HE22	1:A:91:LYS:HE2	1.75	0.52
1:B:47:MET:CE	1:B:73:ASN:HB2	2.38	0.52
1:A:131:GLY:C	1:A:133:VAL:N	2.59	0.52
1:B:146:ARG:NH1	1:B:146:ARG:HG2	2.25	0.51
1:B:295:ILE:HB	1:B:305:VAL:HB	1.93	0.51
1:B:92:GLY:O	1:B:95:ALA:HB3	2.10	0.51
1:B:14:ASN:HA	1:B:17:LYS:HG2	1.91	0.51
1:A:120:THR:HB	4:A:642:HOH:O	2.10	0.51
1:A:6:ALA:O	1:A:10:ARG:HG3	2.11	0.51
1:A:63:LYS:HE2	1:A:64:GLY:CA	2.39	0.51
1:B:222:PRO:HG2	4:B:362:HOH:O	2.11	0.51
1:A:49:LEU:HD11	1:A:69:PHE:HB3	1.91	0.51
1:A:174:GLN:CB	1:A:330:LEU:HD12	2.40	0.50
1:A:38:ASP:O	1:A:41:ALA:HB3	2.11	0.50
1:A:106:ARG:NH1	1:B:266:ILE:HD12	2.26	0.50
1:A:121:ARG:N	1:A:285:ASN:HD21	2.08	0.50
1:B:209:PRO:O	1:B:212:THR:HB	2.11	0.50
1:B:297:ASP:OD1	1:B:298:PRO:HD2	2.11	0.50
1:B:44:ASP:HB3	1:B:47:MET:N	2.26	0.50
1:B:178:ASN:HA	1:B:186:ILE:O	2.12	0.49
1:B:288:LYS:HD2	4:B:337:HOH:O	2.11	0.49
1:B:241:VAL:HG11	1:B:329:LEU:CD2	2.42	0.49
1:B:44:ASP:HB2	1:B:47:MET:HG3	1.95	0.49
1:A:233:GLU:HG3	1:A:233:GLU:O	2.12	0.49
1:A:165:SER:OG	1:A:192:ASN:ND2	2.45	0.49
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.77	0.49
1:B:73:ASN:CB	1:B:140:TYR:HE1	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:SER:HB3	1:B:313:LYS:CD	2.42	0.49
1:B:105:ILE:CD1	1:B:114:VAL:HB	2.43	0.49
1:A:142:ARG:O	1:A:146:ARG:HB2	2.13	0.48
1:B:254:SER:OG	1:B:314:ARG:CZ	2.61	0.48
1:A:164:LEU:O	1:A:168:ILE:HG12	2.14	0.48
1:B:59:GLY:HA3	1:B:225:LEU:HB2	1.96	0.48
1:A:12:LEU:HD23	1:A:331:THR:HG21	1.95	0.48
1:A:236:GLU:OE2	1:A:240:GLN:NE2	2.46	0.48
1:B:163:TRP:CZ2	1:B:227:LEU:CD1	2.95	0.48
1:B:73:ASN:HD22	1:B:73:ASN:HA	1.54	0.48
1:A:170:ARG:O	1:A:174:GLN:HG3	2.13	0.48
1:B:217:ARG:CZ	1:B:217:ARG:HB3	2.43	0.47
1:B:40:VAL:HA	1:B:43:VAL:HG22	1.97	0.47
1:B:115:GLU:CD	1:B:117:VAL:HG13	2.35	0.47
1:A:52:PHE:HA	1:A:56:VAL:HG21	1.95	0.47
1:B:282:ALA:CB	1:B:289:VAL:HG22	2.43	0.47
1:A:332:ILE:CG2	1:A:332:ILE:O	2.61	0.47
1:B:232:ASP:O	1:B:233:GLU:CG	2.63	0.47
1:A:312:LEU:HD11	1:A:316:PHE:CZ	2.50	0.47
1:B:90:ALA:C	1:B:92:GLY:N	2.68	0.47
1:B:106:ARG:CG	1:B:114:VAL:HG11	2.34	0.46
1:B:163:TRP:NE1	1:B:230:PRO:HD3	2.30	0.46
1:A:11:SER:O	1:A:14:ASN:HB3	2.15	0.46
1:B:236:GLU:O	1:B:240:GLN:HG3	2.15	0.46
1:A:109:HIS:NE2	4:A:585:HOH:O	2.36	0.46
1:A:106:ARG:CZ	1:B:266:ILE:HD12	2.46	0.46
1:B:89:VAL:HG13	1:B:90:ALA:N	2.30	0.46
1:A:78:GLU:C	1:A:80:GLY:H	2.19	0.46
1:A:314:ARG:NH2	1:A:318:ARG:HH21	2.13	0.46
1:A:333:VAL:HG13	1:A:333:VAL:OXT	2.16	0.46
1:A:30:ASP:OD2	1:A:221:LEU:HD21	2.16	0.46
1:A:186:ILE:HG21	1:A:194:MET:CE	2.46	0.46
1:B:199:LEU:HB2	1:B:205:LEU:HD12	1.97	0.46
1:A:230:PRO:HB3	4:A:608:HOH:O	2.16	0.46
1:B:252:PHE:CZ	1:B:259:ILE:HG13	2.51	0.45
1:B:178:ASN:O	1:B:184:GLY:HA3	2.16	0.45
1:B:91:LYS:O	1:B:91:LYS:HD2	2.15	0.45
1:B:12:LEU:O	1:B:16:PHE:HD1	2.00	0.45
1:B:152:ARG:HG2	1:B:156:GLU:OE1	2.17	0.45
1:A:53:GLY:HA2	3:A:501:UTP:O3'	2.17	0.45
1:B:145:VAL:HG23	1:B:146:ARG:N	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:O	1:A:184:GLY:N	2.46	0.44
1:A:147:ASN:O	1:A:151:LEU:HG	2.17	0.44
1:A:197:TYR:O	1:A:201:GLN:HG2	2.16	0.44
1:B:159:PRO:HB2	1:B:160:PRO:HD3	1.99	0.44
1:A:146:ARG:HG3	1:A:215:VAL:HG23	1.98	0.44
1:A:254:SER:O	1:A:269:LYS:CE	2.65	0.44
1:B:227:LEU:O	1:B:227:LEU:HD13	2.18	0.44
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.84	0.44
1:B:52:PHE:CZ	1:B:68:ASP:HB3	2.52	0.44
1:B:42:ALA:CB	1:B:104:VAL:HG11	2.48	0.43
1:B:196:VAL:HG12	1:B:200:LEU:HD22	2.00	0.43
1:B:9:GLY:O	1:B:13:VAL:HG23	2.18	0.43
1:B:115:GLU:CG	1:B:117:VAL:HG13	2.49	0.43
1:B:4:SER:OG	1:B:7:VAL:HG23	2.19	0.42
1:B:245:LEU:HD13	1:B:325:ARG:HG3	1.99	0.42
1:B:215:VAL:O	1:B:218:VAL:HG12	2.19	0.42
1:A:131:GLY:O	1:A:133:VAL:N	2.52	0.42
1:B:332:ILE:HG22	1:B:332:ILE:O	2.19	0.42
1:B:244:PHE:CD1	1:B:244:PHE:C	2.92	0.42
1:A:279:GLU:CD	1:A:288:LYS:HZ1	2.23	0.42
1:B:47:MET:SD	1:B:71:VAL:HG21	2.59	0.42
1:A:58:TYR:HB3	1:A:60:VAL:HG22	2.00	0.42
1:A:43:VAL:HG21	1:A:101:LEU:HA	2.01	0.42
1:B:156:GLU:CG	1:B:225:LEU:HD21	2.49	0.42
1:A:282:ALA:HB3	1:A:289:VAL:HG22	2.01	0.42
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.85	0.42
1:A:131:GLY:HA3	4:A:574:HOH:O	2.19	0.42
1:B:307:ARG:NH1	1:B:307:ARG:HG2	2.35	0.42
1:A:35:LEU:O	1:A:38:ASP:HB2	2.20	0.41
1:A:199:LEU:HB3	1:A:205:LEU:HG	2.01	0.41
1:B:113:ASN:N	1:B:128:LYS:O	2.49	0.41
1:A:158:ASN:OD1	1:A:160:PRO:HD2	2.21	0.41
1:B:73:ASN:HB2	1:B:140:TYR:HE1	1.85	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.92	0.41
1:A:98:LEU:HB3	1:A:125:VAL:HG23	2.02	0.41
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.89	0.41
1:B:43:VAL:O	1:B:43:VAL:HG23	2.21	0.41
1:B:93:LEU:O	1:B:97:ILE:HB	2.21	0.41
1:A:43:VAL:O	1:A:44:ASP:HB2	2.21	0.41
1:B:12:LEU:O	1:B:16:PHE:CD1	2.74	0.41
1:A:327:THR:HA	1:A:332:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:HB3	1:A:257:GLN:HG3	2.01	0.41
1:B:33:TYR:CE1	1:B:49:LEU:HD23	2.56	0.41
1:B:70:VAL:HA	1:B:138:THR:O	2.20	0.41
1:B:12:LEU:CD1	1:B:241:VAL:HG21	2.51	0.41
1:B:146:ARG:HD2	1:B:215:VAL:CG2	2.51	0.41
1:B:197:TYR:CE1	1:B:201:GLN:NE2	2.89	0.41
1:B:301:LEU:HA	1:B:301:LEU:HD12	1.75	0.40
1:A:127:VAL:HG21	1:A:135:PHE:CE1	2.56	0.40
1:A:44:ASP:HA	1:A:45:PRO:HD2	1.88	0.40
1:B:241:VAL:CG1	1:B:329:LEU:HD21	2.51	0.40
1:B:145:VAL:CG2	1:B:146:ARG:N	2.85	0.40
1:B:107:GLN:O	1:B:110:LEU:HD21	2.22	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	322/353 (91%)	312 (97%)	10 (3%)	0	100	100
1	B	302/353 (86%)	288 (95%)	13 (4%)	1 (0%)	46	41
All	All	624/706 (88%)	600 (96%)	23 (4%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	VAL

### 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	285/309 (92%)	272 (95%)	13 (5%)	33	28
1	B	274/309 (89%)	243 (89%)	31 (11%)	7	4
All	All	559/618 (90%)	515 (92%)	44 (8%)	15	9

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	PHE
1	A	20	VAL
1	A	47	MET
1	A	63	LYS
1	A	71	VAL
1	A	111	SER
1	A	134	ASP
1	A	146	ARG
1	A	169	LYS
1	A	200	LEU
1	A	227	LEU
1	A	237	LEU
1	A	273	ASP
1	B	24	LEU
1	B	35	LEU
1	B	38	ASP
1	B	44	ASP
1	B	47	MET
1	B	71	VAL
1	B	73	ASN
1	B	75	THR
1	B	91	LYS
1	B	96	ASP
1	B	97	ILE
1	B	103	ARG
1	B	114	VAL
1	B	117	VAL

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Mol	Chain	Res	Type
1	B	126	ARG
1	B	136	ASP
1	B	141	ARG
1	B	142	ARG
1	B	146	ARG
1	B	158	ASN
1	B	200	LEU
1	B	212	THR
1	B	228	GLU
1	B	233	GLU
1	B	237	LEU
1	B	270	GLU
1	B	312	LEU
1	B	314	ARG
1	B	315	ASP
1	B	319	ARG
1	B	329	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	88	GLN
1	A	192	ASN
1	A	203	ASN
1	B	73	ASN
1	B	109	HIS
1	B	113	ASN
1	B	158	ASN
1	B	201	GLN
1	B	224	HIS

### 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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	1.37	2 (10%)	30,47,47	1.72	3 (10%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	UTP	C6-N1	-2.30	1.32	1.35
3	A	501	UTP	O4-C4	4.32	1.35	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	UTP	O3'-C3'-C4'	3.05	120.20	111.05
3	A	501	UTP	O4'-C1'-N1	3.34	115.13	108.08
3	A	501	UTP	C4-N3-C2	6.82	120.89	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	UTP	1	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	326/353 (92%)	0.04	8 (2%) 61 61	10, 28, 51, 69	0
1	B	310/353 (87%)	0.56	43 (13%) 4 4	19, 42, 74, 85	0
All	All	636/706 (90%)	0.29	51 (8%) 15 16	10, 34, 69, 85	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	ALA	6.1
1	B	36	VAL	5.1
1	B	98	LEU	4.9
1	B	40	VAL	4.6
1	B	137	ILE	4.4
1	B	140	TYR	4.2
1	B	72	LEU	4.2
1	A	231	ALA	4.0
1	A	333	VAL	4.0
1	B	103	ARG	3.9
1	B	74	LYS	3.9
1	B	131	GLY	3.9
1	B	93	LEU	3.9
1	B	117	VAL	3.8
1	B	73	ASN	3.8
1	A	332	ILE	3.7
1	B	95	ALA	3.6
1	A	28	HIS	3.6
1	B	125	VAL	3.4
1	B	110	LEU	3.4
1	B	89	VAL	3.4
1	B	41	ALA	3.3
1	B	97	ILE	3.1
1	B	102	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLY	2.9
1	A	119	ARG	2.8
1	B	48	ARG	2.8
1	B	111	SER	2.8
1	B	37	LEU	2.7
1	B	100	LYS	2.7
1	B	75	THR	2.7
1	B	215	VAL	2.6
1	B	101	LEU	2.6
1	B	33	TYR	2.6
1	B	38	ASP	2.5
1	B	39	CYS	2.4
1	B	43	VAL	2.4
1	B	96	ASP	2.3
1	B	99	ALA	2.3
1	B	135	PHE	2.3
1	A	18	GLN	2.3
1	B	21	SER	2.2
1	B	105	ILE	2.2
1	B	130	GLY	2.2
1	B	7	VAL	2.1
1	A	132	ALA	2.1
1	B	30	ASP	2.1
1	B	71	VAL	2.1
1	B	217	ARG	2.0
1	B	116	GLU	2.0
1	B	47	MET	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](#)

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
3	UTP	A	501	29/29	0.98	0.09	-1.66	18,26,32,39	0
2	MG	A	401	1/1	0.97	0.10	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.