



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 08:57 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 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/ValidationPDFNotes.html>

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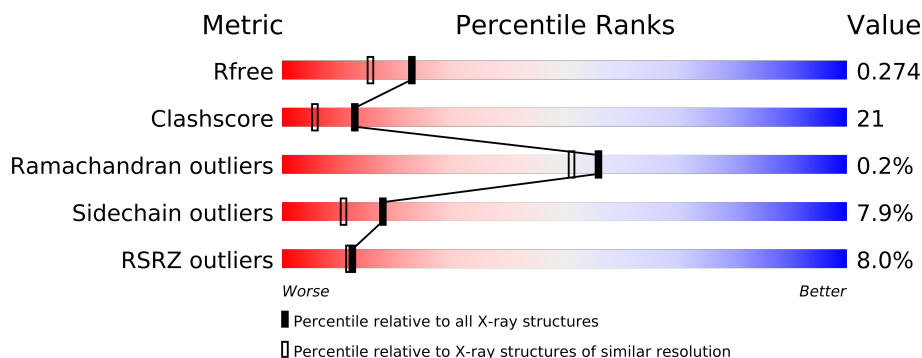
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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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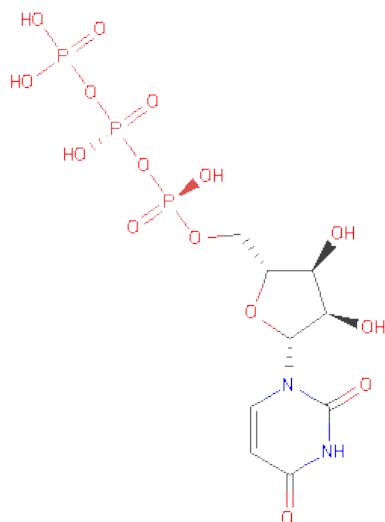
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-13	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-12	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-11	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-10	HIS	-	EXPRESSION TAG	UNP Q381M1
B	-9	SER	-	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 , 0.274	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> )	0.36 , 38.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5333	0	5104	213	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (213) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:281:PHE:O	1:B:285:ASN:HB2	2.06	0.55
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	Distance(Å)	Clash(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
1:A:181:VAL:O	1:A:184:GLY:N	2.46	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	50	44
All	All	624/706 (88%)	600 (96%)	23 (4%)	1 (0%)	56	51

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%)	37	30
1	B	274/309 (89%)	243 (89%)	31 (11%)	9	4
All	All	559/618 (90%)	515 (92%)	44 (8%)	18	11

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
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

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Mol	Chain	Res	Type
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 chains 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	30,30,30	1.64	5 (16%)	43,47,47	1.69	7 (16%)

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	-	0/20/38/38	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	UTP	O4-C4	5.37	1.35	1.24
3	A	501	UTP	C4-N3	-3.76	1.31	1.37
3	A	501	UTP	PB-O3A	-2.99	1.54	1.59
3	A	501	UTP	C6-C5	2.87	1.40	1.36
3	A	501	UTP	C6-N1	-2.01	1.32	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	UTP	N3-C2-N1	5.32	120.41	115.97
3	A	501	UTP	C2-N1-C1'	4.20	120.84	118.21
3	A	501	UTP	O3B-PB-O3A	3.93	109.65	101.66
3	A	501	UTP	O4'-C1'-N1	3.35	115.13	108.06
3	A	501	UTP	O3'-C3'-C4'	3.10	120.20	111.08
3	A	501	UTP	C3'-C2'-C1'	2.59	104.96	100.91
3	A	501	UTP	C5-C4-N3	2.08	120.63	116.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	326/353 (92%)	0.03	6 (1%) 65 66	10, 28, 51, 69	0
1	B	310/353 (87%)	0.57	45 (14%) 3 3	19, 42, 74, 85	0
All	All	636/706 (90%)	0.29	51 (8%) 12 12	10, 34, 69, 85	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	LEU	5.7
1	B	90	ALA	5.5
1	B	117	VAL	5.3
1	B	36	VAL	4.8
1	B	131	GLY	4.7
1	B	93	LEU	4.5
1	B	140	TYR	4.2
1	B	95	ALA	4.2
1	B	137	ILE	3.9
1	B	72	LEU	3.9
1	A	231	ALA	3.7
1	B	111	SER	3.7
1	B	110	LEU	3.7
1	B	40	VAL	3.6
1	B	73	ASN	3.5
1	B	74	LYS	3.5
1	B	125	VAL	3.5
1	B	103	ARG	3.3
1	B	97	ILE	3.2
1	A	28	HIS	3.2
1	B	75	THR	3.1
1	A	333	VAL	3.1
1	A	332	ILE	3.1
1	B	37	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	33	TYR	2.9
1	B	7	VAL	2.8
1	B	100	LYS	2.8
1	B	48	ARG	2.7
1	B	89	VAL	2.7
1	B	301	LEU	2.7
1	B	38	ASP	2.5
1	B	29	VAL	2.5
1	B	127	VAL	2.4
1	A	132	ALA	2.3
1	B	101	LEU	2.3
1	B	91	LYS	2.3
1	B	99	ALA	2.2
1	B	105	ILE	2.2
1	B	30	ASP	2.2
1	B	47	MET	2.2
1	B	41	ALA	2.2
1	B	43	VAL	2.2
1	B	49	LEU	2.1
1	B	102	ALA	2.1
1	B	92	GLY	2.1
1	B	71	VAL	2.1
1	B	124	VAL	2.1
1	B	135	PHE	2.1
1	B	215	VAL	2.0
1	B	116	GLU	2.0
1	A	130	GLY	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	401	1/1	0.12	0.85	21,21,21,21	0
3	UTP	A	501	29/29	0.08	-1.74	18,26,32,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.