



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:57 AM UTC

PDB ID : 2IKF / pdb_00002ikf
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

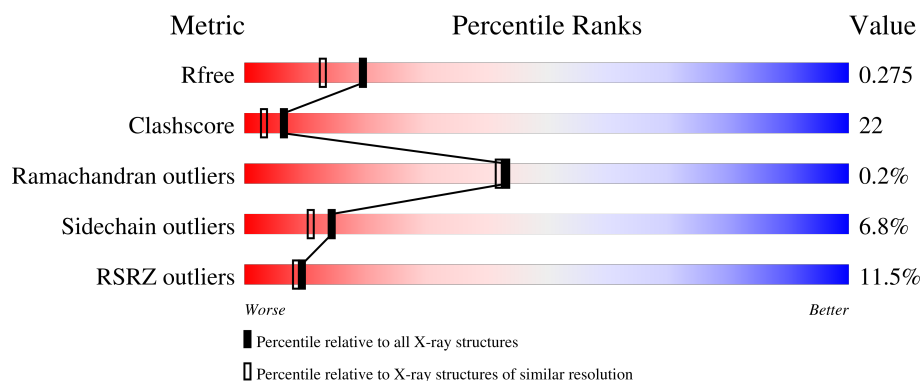
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	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

Continued on next page...

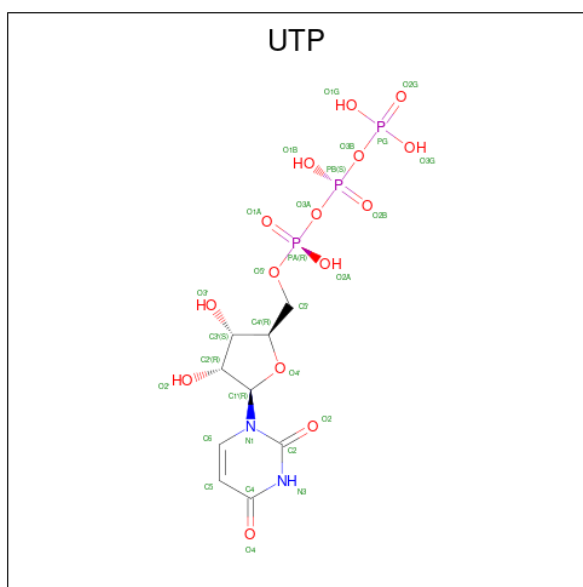
Continued from previous page...

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



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, α , β , γ	78.77Å 41.52Å 103.79Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	51.71 – 2.00 51.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (51.71-2.00) 94.3 (51.71-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.92	1/2658 (0.0%)	1.26	23/3605 (0.6%)
1	B	0.72	0/2541	1.21	20/3444 (0.6%)
All	All	0.83	1/5199 (0.0%)	1.23	43/7049 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	VAL	CA-CB	5.84	1.62	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ILE	N-CA-C	-17.18	97.39	113.71
1	A	120	THR	N-CA-C	9.73	123.08	110.53
1	B	4	SER	N-CA-C	9.31	120.30	109.60
1	B	231	ALA	N-CA-C	-8.99	99.38	110.88
1	A	159	PRO	N-CA-C	7.58	119.95	110.70
1	B	41	ALA	N-CA-C	-7.47	103.12	111.71
1	A	43	VAL	N-CA-C	-7.38	104.79	113.42
1	A	289	VAL	N-CA-C	-7.33	97.61	108.97
1	B	94	GLN	N-CA-C	-7.22	103.34	111.07
1	B	110	LEU	N-CA-C	7.00	120.71	111.75
1	A	259	ILE	N-CA-C	-6.80	99.86	108.84
1	A	266	ILE	N-CA-C	6.65	118.97	108.87
1	B	65	SER	N-CA-C	6.58	118.80	110.24
1	A	79	ASP	N-CA-C	-6.47	102.49	111.81
1	A	32	THR	N-CA-C	-6.42	104.20	111.07
1	A	232	ASP	N-CA-C	-6.37	102.89	111.87
1	B	297	ASP	CA-C-N	6.31	126.22	119.28
1	B	297	ASP	C-N-CA	6.31	126.22	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	PRO	N-CA-C	-6.09	99.92	112.47
1	B	143	ASN	N-CA-C	6.06	117.89	111.28
1	B	331	THR	N-CA-C	-6.05	106.03	113.41
1	B	98	LEU	N-CA-C	-5.96	105.50	112.89
1	B	257	GLN	N-CA-C	5.90	119.28	110.14
1	A	44	ASP	CA-C-N	5.86	125.54	119.56
1	A	44	ASP	C-N-CA	5.86	125.54	119.56
1	A	112	TRP	N-CA-C	5.74	119.27	110.20
1	A	220	PRO	N-CA-C	-5.72	105.58	113.53
1	A	276	LYS	N-CA-C	-5.72	105.05	111.28
1	B	135	PHE	N-CA-C	5.53	117.49	108.76
1	B	106	ARG	N-CA-C	-5.48	105.00	110.97
1	B	159	PRO	N-CA-C	5.43	117.33	110.70
1	A	143	ASN	N-CA-C	5.42	117.18	111.28
1	B	8	VAL	N-CA-C	-5.40	105.23	110.42
1	A	224	HIS	N-CA-C	-5.38	103.03	110.35
1	A	38	ASP	N-CA-C	-5.37	105.11	110.97
1	A	113	ASN	N-CA-C	-5.35	100.45	108.96
1	A	250	HIS	N-CA-C	5.34	121.55	114.12
1	B	72	LEU	N-CA-C	5.33	117.59	108.90
1	A	293	TRP	N-CA-C	-5.26	98.65	108.02
1	B	248	PHE	N-CA-C	5.18	119.22	113.01
1	B	294	CYS	N-CA-C	5.16	117.15	109.25
1	A	54	SER	N-CA-C	5.14	117.55	111.33
1	A	67	VAL	N-CA-C	-5.13	100.81	108.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	84	0
1	B	2486	0	2489	141	0
2	A	1	0	0	0	0
3	A	29	0	11	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	156	0	0	5	0
4	B	60	0	0	2	0
All	All	5333	0	5104	223	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 22.

All (223) 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:HH11	1:B:126:ARG:CB	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:19:PHE:CZ	1:B:166:MET:HE1	2.14	0.82
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:63:LYS:HE2	1:A:64:GLY:N	2.01	0.75
1:B:91:LYS:HD2	1:B:91:LYS:C	2.12	0.74
1:A:191:PHE:HA	1:A:194:MET:HE3	1.67	0.74
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:A:131:GLY:C	1:A:133:VAL:H	1.99	0.70
1:A:44:ASP:HB3	1:A:47:MET:HE2	1.73	0.69
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:B:47:MET:HE2	1:B:73:ASN:HB2	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ASP:HA	1:B:221:LEU:HD21	1.76	0.66
1:B:158:ASN:HD22	1:B:160:PRO:HD2	1.60	0.66
1:B:100:LYS:O	1:B:104:VAL:HG23	1.95	0.65
1:A:327:THR:C	1:A:332:ILE:HG22	2.21	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:70:VAL:HG23	1:B:138:THR:HG23	1.80	0.62
1:B:98:LEU:HB3	1:B:125:VAL:HG23	1.79	0.62
1:B:194:MET:HG2	1:B:259:ILE:HD13	1.81	0.62
1:B:124:VAL:HG23	1:B:137:ILE:C	2.24	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: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:3:PRO:HD3	1:A:326:ASP:HA	1.83	0.59
1:A:324:ALA:HB1	1:A:329:LEU:HD23	1.84	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:131:GLY:C	1:A:133:VAL:N	2.59	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:A:40:VAL:HG13	1:A:47:MET:HE3	1.85	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:A:295:ILE:HB	1:A:305:VAL:HB	1.86	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:198:TYR:OH	1:A:243:ASP:HB3	2.04	0.57
1:B:16:PHE:O	1:B:20:VAL:HG23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:47:MET:HG2	1:B:73:ASN:OD1	2.05	0.56
1:B:124:VAL:HG23	1:B:137:ILE:O	2.04	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
1:A:249:LEU:HD21	1:A:321:LEU:HB2	1.88	0.55
1:B:32:THR:O	1:B:36:VAL:HG23	2.06	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:A:254:SER:O	1:A:269:LYS:HE3	2.09	0.53
1:B:25:HIS:CE1	1:B:27:ARG:HG3	2.44	0.53
1:B:74:LYS:HD2	1:B:140:TYR:HB3	1.90	0.53
1:B:142:ARG:O	1:B:145:VAL:CG2	2.54	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:115:GLU:CD	1:B:117:VAL:HG13	2.35	0.52
1:B:47:MET:CE	1:B:73:ASN:HB2	2.38	0.52
1:B:146:ARG:NH1	1:B:146:ARG:HG2	2.25	0.51
1:B:90:ALA:C	1:B:92:GLY:N	2.68	0.51
1:A:78:GLU:C	1:A:80:GLY:H	2.19	0.51
1:B:14:ASN:HA	1:B:17:LYS:HG2	1.91	0.51
1:B:92:GLY:O	1:B:95:ALA:HB3	2.10	0.51
1:B:295:ILE:HB	1:B:305:VAL:HB	1.93	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:49:LEU:HD11	1:A:69:PHE:HB3	1.91	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:165:SER:OG	1:A:192:ASN:ND2	2.45	0.49
1:A:233:GLU:HG3	1:A:233:GLU:O	2.12	0.49
1:B:73:ASN:CB	1:B:140:TYR:HE1	2.26	0.49
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.77	0.49
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:198:TYR:OH	1:B:243:ASP:OD2	2.27	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: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:59:GLY:HA3	1:B:225:LEU:HB2	1.96	0.48
1:A:170:ARG:O	1:A:174:GLN:HG3	2.13	0.48
1:B:73:ASN:HD22	1:B:73:ASN:HA	1.54	0.48
1:B:163:TRP:CZ2	1:B:227:LEU:CD1	2.95	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: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:312:LEU:HD11	1:A:316:PHE:CZ	2.50	0.47
1:A:332:ILE:O	1:A:332:ILE:CG2	2.61	0.47
1:B:232:ASP:O	1:B:233:GLU:CG	2.63	0.47
1:B:244:PHE:CD1	1:B:244:PHE:C	2.92	0.47
1:A:11:SER:O	1:A:14:ASN:HB3	2.15	0.46
1:A:109:HIS:NE2	4:A:585:HOH:O	2.36	0.46
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:B:236:GLU:O	1:B:240:GLN:HG3	2.15	0.46
1:A:106:ARG:CZ	1:B:266:ILE:HD12	2.46	0.46
1:A:19:PHE:CZ	1:A:166:MET:HE1	2.50	0.46
1:B:89:VAL:HG13	1:B:90:ALA:N	2.30	0.46
1:A:30:ASP:OD2	1:A:221:LEU:HD21	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:CD	1:A:288:LYS:HZ1	2.24	0.46
1:A:314:ARG:NH2	1:A:318:ARG:HH21	2.13	0.46
1:A:333:VAL:OXT	1:A:333:VAL:HG13	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:178:ASN:O	1:B:184:GLY:HA3	2.16	0.45
1:B:252:PHE:CZ	1:B:259:ILE:HG13	2.51	0.45
1:B:91:LYS:HD2	1:B:91:LYS:O	2.15	0.45
1:A:53:GLY:HA2	3:A:501:UTP:O3'	2.17	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:B:283:ARG:NH1	1:B:284:MET:HE2	2.32	0.45
1:A:181:VAL:O	1:A:184:GLY:N	2.46	0.44
1:B:145:VAL:HG23	1:B:146:ARG:N	2.30	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:A:19:PHE:CE1	1:A:166:MET:HE1	2.53	0.44
1:A:146:ARG:HG3	1:A:215:VAL:HG23	1.98	0.44
1:B:159:PRO:HB2	1:B:160:PRO:HD3	1.99	0.44
1:A:254:SER:O	1:A:269:LYS:CE	2.65	0.44
1:B:225:LEU:HD12	1:B:225:LEU:HA	1.84	0.44
1:B:227:LEU:HD13	1:B:227:LEU:O	2.18	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:A:78:GLU:C	1:A:80:GLY:N	2.76	0.43
1:A:44:ASP:C	1:A:44:ASP:OD1	2.61	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:A:131:GLY:O	1:A:133:VAL:N	2.52	0.42
1:B:215:VAL:O	1:B:218:VAL:HG12	2.19	0.42
1:B:332:ILE:HG22	1:B:332:ILE:O	2.19	0.42
1:A:58:TYR:HB3	1:A:60:VAL:HG22	2.00	0.42
1:B:47:MET:SD	1:B:71:VAL:HG21	2.59	0.42
1:A:43:VAL:HG21	1:A:101:LEU:HA	2.01	0.42
1:A:282:ALA:HB3	1:A:289:VAL:HG22	2.01	0.42
1:B:156:GLU:CG	1:B:225:LEU:HD21	2.49	0.42
1:B:307:ARG:HG2	1:B:307:ARG:HH11	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLY:HA3	4:A:574:HOH:O	2.19	0.42
1:B:307:ARG:HG2	1:B:307:ARG:NH1	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:A:158:ASN:OD1	1:A:160:PRO:HD2	2.21	0.41
1:B:113:ASN:N	1:B:128:LYS:O	2.49	0.41
1:A:35:LEU:HD23	1:A:35:LEU:HA	1.92	0.41
1:B:73:ASN:HB2	1:B:140:TYR:HE1	1.85	0.41
1:B:327:THR:O	1:B:328:ALA:C	2.63	0.41
1:A:98:LEU:HB3	1:A:125:VAL:HG23	2.02	0.41
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.89	0.41
1:B:43:VAL:O	1:B:43:VAL:HG23	2.21	0.41
1:B:12:LEU:O	1:B:16:PHE:CD1	2.74	0.41
1:B:93:LEU:O	1:B:97:ILE:HB	2.21	0.41
1:A:253:ASP:HB3	1:A:257:GLN:HG3	2.01	0.41
1:A:327:THR:HA	1:A:332:ILE:CG2	2.51	0.41
1:B:19:PHE:CE2	1:B:166:MET:HE1	2.54	0.41
1:B:12:LEU:CD1	1:B:241:VAL:HG21	2.51	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: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:HD12	1:B:301:LEU:HA	1.75	0.40
1:A:44:ASP:HA	1:A:45:PRO:HD2	1.88	0.40
1:A:127:VAL:HG21	1:A:135:PHE:CE1	2.56	0.40
1:B:241:VAL:CG1	1:B:329:LEU:HD21	2.51	0.40
1:B:107:GLN:O	1:B:110:LEU:HD21	2.22	0.40
1:B:145:VAL:CG2	1:B:146:ARG:N	2.85	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	322/353 (91%)	312 (97%)	10 (3%)	0	100	100
1	B	302/353 (86%)	288 (95%)	13 (4%)	1 (0%)	36	35
All	All	624/706 (88%)	600 (96%)	23 (4%)	1 (0%)	43	42

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%)	270 (95%)	15 (5%)	20	18
1	B	274/309 (89%)	251 (92%)	23 (8%)	10	7
All	All	559/618 (90%)	521 (93%)	38 (7%)	14	11

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	47	MET
1	A	63	LYS
1	A	71	VAL
1	A	93	LEU
1	A	111	SER
1	A	133	VAL
1	A	134	ASP
1	A	145	VAL
1	A	169	LYS
1	A	200	LEU
1	A	227	LEU
1	A	237	LEU
1	A	259	ILE
1	A	273	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	24	LEU
1	B	35	LEU
1	B	44	ASP
1	B	47	MET
1	B	71	VAL
1	B	73	ASN
1	B	75	THR
1	B	97	ILE
1	B	103	ARG
1	B	114	VAL
1	B	117	VAL
1	B	126	ARG
1	B	141	ARG
1	B	146	ARG
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	315	ASP
1	B	329	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	107	GLN
1	A	192	ASN
1	A	203	ASN
1	A	320	HIS
1	B	73	ASN
1	B	113	ASN
1	B	143	ASN
1	B	158	ASN
1	B	174	GLN
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 oligosaccharides 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	29,30,30	1.86	5 (17%)	43,47,47	1.81	8 (18%)

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	-	3/22/38/38	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	5.40	1.35	1.24
3	A	501	UTP	PB-O3A	-4.66	1.54	1.59
3	A	501	UTP	C4-N3	-4.47	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	UTP	C6-C5	2.41	1.40	1.35
3	A	501	UTP	C6-N1	-2.32	1.32	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	UTP	C4-N3-C2	-4.61	120.89	126.61
3	A	501	UTP	N3-C2-N1	4.24	120.41	114.89
3	A	501	UTP	C5-C4-N3	4.16	120.63	114.80
3	A	501	UTP	O2-C2-N3	-3.76	114.55	121.49
3	A	501	UTP	O3'-C3'-C4'	3.17	120.20	111.08
3	A	501	UTP	O4'-C1'-N1	2.99	115.13	108.36
3	A	501	UTP	O1B-PB-O3B	2.33	113.58	107.27
3	A	501	UTP	O4-C4-C5	-2.05	121.62	125.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

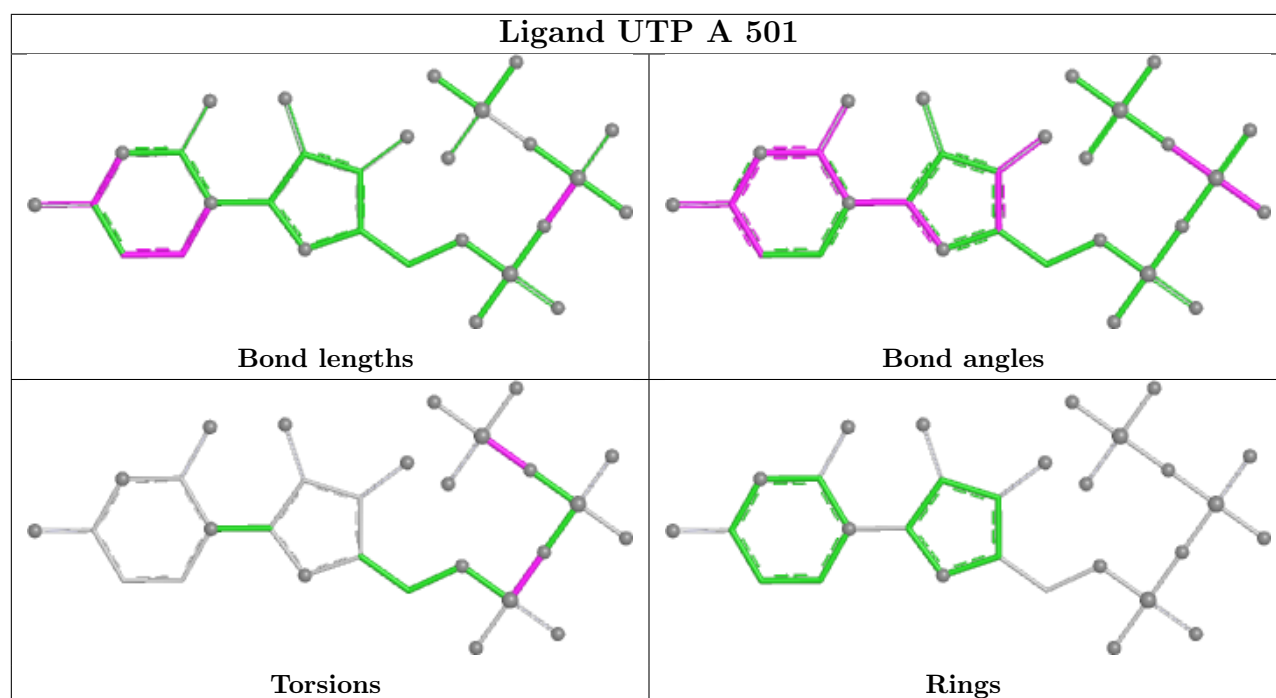
Mol	Chain	Res	Type	Atoms
3	A	501	UTP	PB-O3B-PG-O3G
3	A	501	UTP	PB-O3B-PG-O1G
3	A	501	UTP	PB-O3A-PA-O2A

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th 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 ²)	Q<0.9
1	A	326/353 (92%)	0.36	21 (6%) 25 24	10, 28, 51, 69	0
1	B	310/353 (87%)	0.97	52 (16%) 4 4	19, 42, 74, 85	0
All	All	636/706 (90%)	0.66	73 (11%) 9 8	10, 34, 69, 85	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	VAL	6.2
1	B	110	LEU	4.3
1	B	93	LEU	4.1
1	B	75	THR	3.9
1	B	92	GLY	3.8
1	B	97	ILE	3.8
1	B	137	ILE	3.8
1	B	7	VAL	3.8
1	B	36	VAL	3.7
1	B	123	PRO	3.7
1	B	35	LEU	3.5
1	A	133	VAL	3.5
1	B	99	ALA	3.3
1	A	28	HIS	3.3
1	A	232	ASP	3.2
1	A	18	GLN	3.2
1	A	132	ALA	3.1
1	B	326	ASP	3.1
1	B	140	TYR	3.0
1	A	17	LYS	3.0
1	B	98	LEU	3.0
1	B	96	ASP	2.9
1	B	102	ALA	2.9
1	A	129	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	231	ALA	2.8
1	B	40	VAL	2.8
1	B	135	PHE	2.7
1	B	24	LEU	2.7
1	B	127	VAL	2.7
1	B	30	ASP	2.7
1	B	270	GLU	2.7
1	A	332	ILE	2.7
1	B	43	VAL	2.7
1	B	131	GLY	2.7
1	B	101	LEU	2.6
1	B	105	ILE	2.6
1	B	38	ASP	2.6
1	B	114	VAL	2.6
1	B	90	ALA	2.6
1	B	95	ALA	2.6
1	B	3	PRO	2.6
1	B	33	TYR	2.6
1	B	117	VAL	2.6
1	B	21	SER	2.6
1	B	111	SER	2.6
1	B	73	ASN	2.5
1	A	333	VAL	2.5
1	A	331	THR	2.5
1	B	39	CYS	2.5
1	A	19	PHE	2.5
1	B	332	ILE	2.5
1	A	284	MET	2.4
1	A	107	GLN	2.4
1	B	37	LEU	2.4
1	B	71	VAL	2.4
1	B	26	THR	2.4
1	A	130	GLY	2.4
1	B	104	VAL	2.3
1	B	301	LEU	2.3
1	A	21	SER	2.3
1	A	281	PHE	2.3
1	B	25	HIS	2.2
1	B	72	LEU	2.2
1	A	285	ASN	2.2
1	B	94	GLN	2.1
1	A	16	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	125	VAL	2.1
1	A	43	VAL	2.1
1	B	134	ASP	2.1
1	B	91	LYS	2.1
1	B	215	VAL	2.0
1	B	112	TRP	2.0
1	A	119	ARG	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](#)

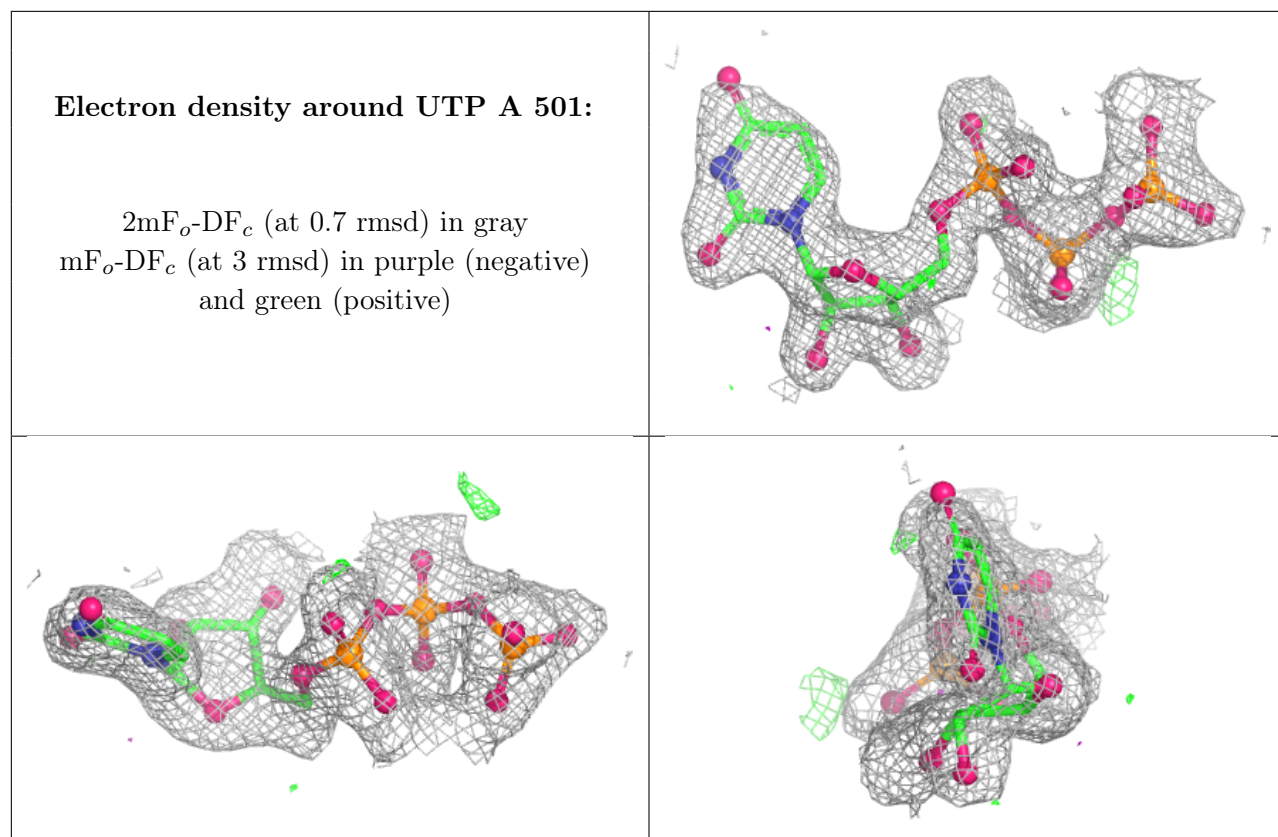
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	401	1/1	0.97	0.05	21,21,21,21	0
3	UTP	A	501	29/29	0.97	0.07	18,26,32,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.