



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:00 pm BST

PDB ID : 5W0O  
Title : Structure of human TUT7 catalytic module (CM) in complex with dsRNA  
Authors : Faehnle, C.R.; Walleshauser, J.; Joshua-Tor, L.  
Deposited on : 2017-05-31  
Resolution : 2.49 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

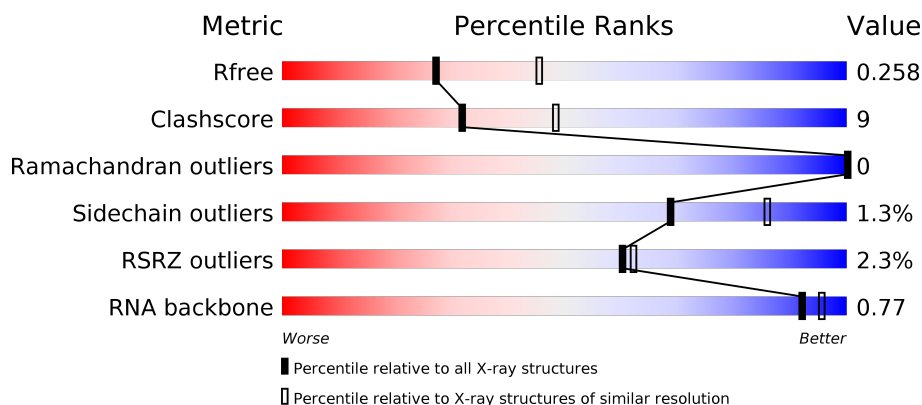
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)
RNA backbone	3102	1002 (2.82-2.14)

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 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	389	
1	B	389	
2	C	15	
2	D	15	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6085 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 Terminal uridylyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2746	1786	455	491	14			
1	B	317	Total	C	N	O	S	0	0	0
			2591	1683	433	462	13			

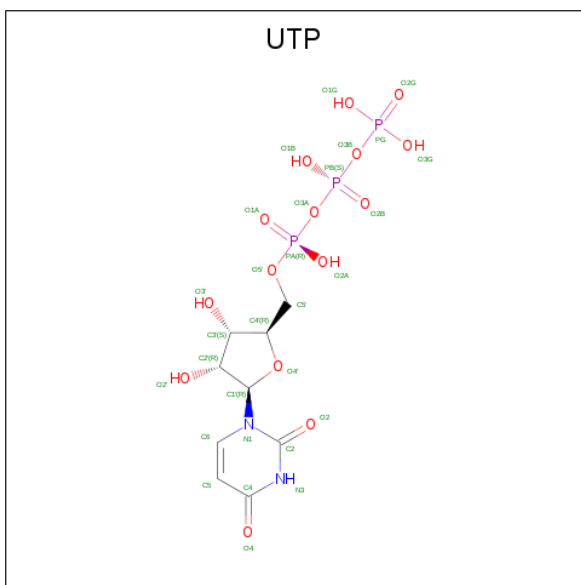
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	977	GLY	-	expression tag	UNP Q5VYS8
A	978	ALA	-	expression tag	UNP Q5VYS8
A	979	GLY	-	expression tag	UNP Q5VYS8
A	980	ALA	-	expression tag	UNP Q5VYS8
A	981	GLY	-	expression tag	UNP Q5VYS8
A	982	SER	-	expression tag	UNP Q5VYS8
B	977	GLY	-	expression tag	UNP Q5VYS8
B	978	ALA	-	expression tag	UNP Q5VYS8
B	979	GLY	-	expression tag	UNP Q5VYS8
B	980	ALA	-	expression tag	UNP Q5VYS8
B	981	GLY	-	expression tag	UNP Q5VYS8
B	982	SER	-	expression tag	UNP Q5VYS8

- Molecule 2 is a RNA chain called double-stranded RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			320	142	56	107	15			
2	D	15	Total	C	N	O	P	0	0	0
			320	142	56	107	15			

- 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 29	C 9	N 2	O 15	P 3	0	0
3	B	1	Total 29	C 9	N 2	O 15	P 3	0	0

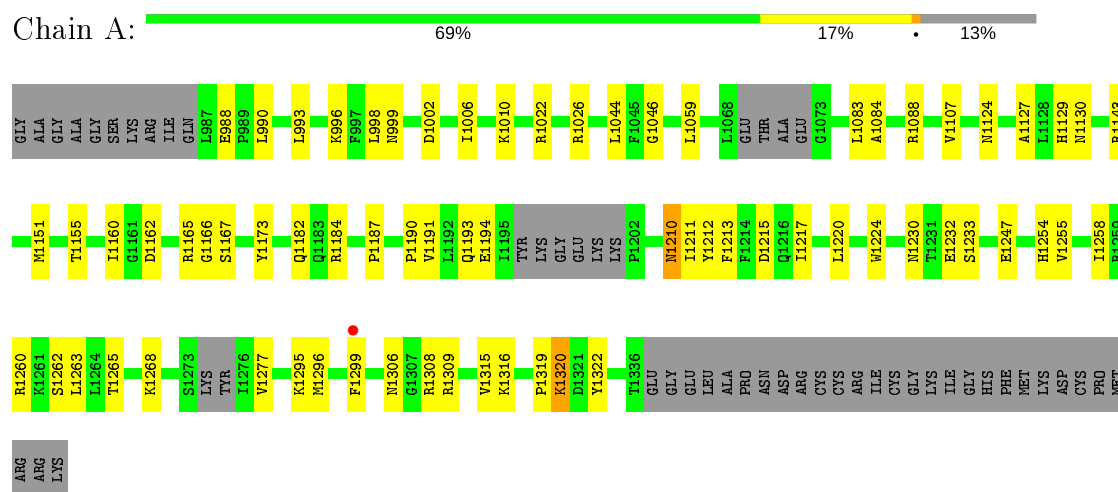
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	16	Total O 16 16	0	0
4	C	5	Total O 5 5	0	0
4	D	1	Total O 1 1	0	0

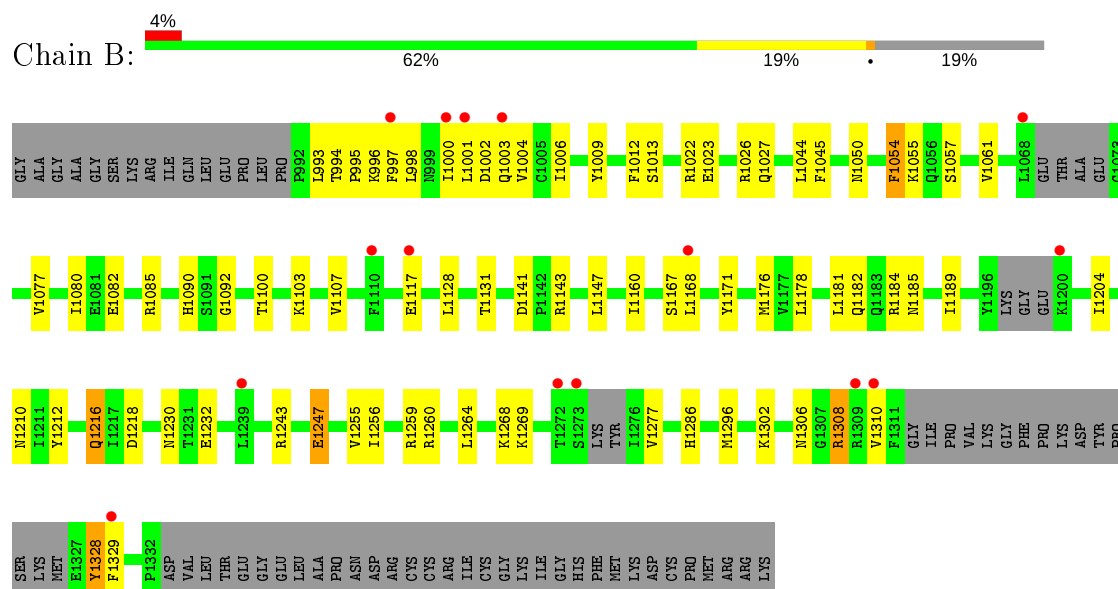
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

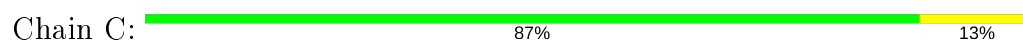
#### • Molecule 1: Terminal uridylyltransferase 7



#### • Molecule 1: Terminal uridylyltransferase 7



#### • Molecule 2: double-stranded RNA





- Molecule 2: double-stranded RNA

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.83Å 80.85Å 181.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.46 – 2.49 90.92 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.46-2.49) 99.3 (90.92-2.49)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.10 _2155	Depositor
R, $R_{free}$	0.205 , 0.254 0.207 , 0.258	Depositor DCC
$R_{free}$ test set	1778 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/2813	0.54	1/3804 (0.0%)
1	B	0.37	0/2651	0.54	0/3578
2	C	0.64	1/356 (0.3%)	0.82	0/551
2	D	0.71	1/356 (0.3%)	0.92	1/551 (0.2%)
All	All	0.41	2/6176 (0.0%)	0.59	2/8484 (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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	G	OP3-P	-10.56	1.48	1.61
2	C	1	G	OP3-P	-10.42	1.48	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	13	G	N3-C4-N9	-5.43	122.74	126.00
1	A	1151	MET	CG-SD-CE	5.03	108.25	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	996	LYS	Peptide

## 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	2746	0	2762	47	0
1	B	2591	0	2601	53	0
2	C	320	0	163	1	0
2	D	320	0	163	7	0
3	A	29	0	11	1	0
3	B	29	0	11	1	0
4	A	28	0	0	0	0
4	B	16	0	0	1	0
4	C	5	0	0	0	0
4	D	1	0	0	0	0
All	All	6085	0	5711	104	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 (104) 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:1103:LYS:HZ1	2:D:13:G:H5'	1.31	0.96
1:B:994:THR:HB	1:B:997:PHE:HB2	1.50	0.94
2:D:12:C:H2'	2:D:13:G:H5''	1.65	0.78
1:B:1255:VAL:HG13	1:B:1277:VAL:HG12	1.68	0.75
1:B:1247:GLU:OE1	1:B:1308:ARG:NH2	2.19	0.74
1:B:1103:LYS:HZ1	2:D:13:G:C5'	2.00	0.73
1:B:1103:LYS:NZ	2:D:13:G:H5'	2.02	0.73
1:B:1090:HIS:HD1	1:B:1092:GLY:H	1.37	0.71
1:B:1216:GLN:OE1	1:B:1218:ASP:N	2.23	0.71
1:B:1204:ILE:H	1:B:1210:ASN:ND2	1.88	0.70
1:A:1182:GLN:HE22	1:A:1258:ILE:HA	1.58	0.69
1:A:1265:THR:HG23	1:A:1268:LYS:H	1.58	0.69
1:A:1230:ASN:ND2	1:A:1232:GLU:OE2	2.27	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1143:ARG:NH2	1:B:1230:ASN:OD1	2.28	0.66
1:B:993:LEU:HB3	1:B:998:LEU:HD21	1.76	0.66
1:B:1176:MET:HG2	1:B:1256:ILE:HD13	1.78	0.66
1:B:993:LEU:HD23	1:B:998:LEU:HD11	1.77	0.65
1:A:1184:ARG:NH1	1:A:1232:GLU:OE1	2.30	0.65
1:A:1295:LYS:HE2	1:A:1299:PHE:HZ	1.63	0.63
1:A:1210:ASN:ND2	1:A:1212:TYR:H	1.98	0.62
1:B:1082:GLU:OE2	1:B:1085:ARG:NH2	2.32	0.61
1:A:1296:MET:HA	1:A:1299:PHE:CD1	2.36	0.61
1:A:1084:ALA:O	1:A:1088:ARG:HG3	2.02	0.60
1:B:1230:ASN:ND2	1:B:1232:GLU:OE2	2.27	0.60
1:A:1260:ARG:HH12	1:A:1263:LEU:C	2.06	0.59
1:B:994:THR:HB	1:B:997:PHE:CB	2.27	0.59
1:A:1083:LEU:HB3	1:A:1107:VAL:HG21	1.85	0.58
1:A:1255:VAL:HG13	1:A:1277:VAL:HG12	1.85	0.58
1:A:1295:LYS:HG2	1:A:1299:PHE:CZ	2.39	0.57
1:A:996:LYS:HD3	1:A:999:ASN:ND2	2.19	0.57
1:B:1302:LYS:HE2	1:B:1306:ASN:HD21	1.69	0.57
1:A:1129:HIS:CE1	1:A:1211:ILE:HD13	2.40	0.56
1:B:1259:ARG:HG3	1:B:1260:ARG:HG3	1.86	0.56
1:B:1167:SER:HB2	1:B:1296:MET:HG2	1.88	0.56
1:B:1000:ILE:HG13	1:B:1001:LEU:N	2.21	0.55
1:A:1022:ARG:HG2	1:A:1059:LEU:HD13	1.88	0.55
1:A:1166:GLY:O	1:A:1296:MET:HG2	2.06	0.55
1:A:996:LYS:HD3	1:A:999:ASN:HD22	1.70	0.55
1:A:1191:VAL:HG23	1:A:1194:GLU:HB2	1.87	0.55
1:A:1320:LYS:HD2	1:A:1320:LYS:H	1.72	0.55
1:A:988:GLU:O	1:A:1308:ARG:NH2	2.35	0.54
1:B:1023:GLU:O	1:B:1027:GLN:HG3	2.08	0.54
1:B:1077:VAL:HG22	1:B:1100:THR:HB	1.89	0.53
1:B:1264:LEU:HD21	1:B:1269:LYS:HD3	1.90	0.53
1:A:1217:ILE:HA	1:A:1220:LEU:HD11	1.90	0.53
1:A:1193:GLN:HG2	1:A:1213:PHE:HB3	1.92	0.52
1:B:1328:TYR:CD2	1:B:1329:PHE:CE1	2.99	0.51
1:A:1006:ILE:HG22	1:A:1010:LYS:HE2	1.93	0.51
1:A:1026:ARG:HB2	1:A:1044:LEU:HD21	1.93	0.50
1:B:1141:ASP:OD1	1:B:1143:ARG:HD3	2.11	0.50
1:A:993:LEU:HD13	1:A:998:LEU:HD13	1.93	0.50
1:A:1046:GLY:HA2	3:A:1401:UTP:O3'	2.12	0.50
1:A:1162:ASP:OD2	1:A:1165:ARG:NH1	2.44	0.50
1:A:990:LEU:HD11	1:A:1308:ARG:HG2	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:994:THR:O	1:B:998:LEU:HD22	2.13	0.49
1:B:1160:ILE:O	1:B:1167:SER:OG	2.30	0.49
1:B:1204:ILE:HD12	1:B:1212:TYR:HB2	1.94	0.49
1:A:1254:HIS:CE1	1:A:1263:LEU:HD12	2.48	0.49
1:A:1213:PHE:CE2	1:A:1215:ASP:HB3	2.48	0.49
1:B:1167:SER:OG	1:B:1168:LEU:N	2.46	0.48
1:B:997:PHE:CD1	1:B:1000:ILE:HD11	2.49	0.48
1:A:1247:GLU:OE2	1:A:1308:ARG:NH1	2.47	0.48
1:B:1184:ARG:HG3	1:B:1185:ASN:N	2.28	0.48
1:B:1147:LEU:HD12	1:B:1181:LEU:HD11	1.96	0.47
1:B:1050:ASN:HB3	1:B:1131:THR:HG23	1.96	0.47
1:A:1306:ASN:ND2	1:A:1309:ARG:HH22	2.12	0.47
1:A:1319:PRO:HG2	1:A:1322:TYR:CD2	2.50	0.46
1:A:1190:PRO:HB3	1:A:1224:TRP:CD1	2.50	0.46
1:B:995:PRO:HA	1:B:998:LEU:HD23	1.97	0.46
1:A:1124:ASN:ND2	2:C:15:U:O2	2.46	0.46
1:B:1080:ILE:HG23	1:B:1107:VAL:HG22	1.98	0.45
1:B:1306:ASN:O	1:B:1310:VAL:HG22	2.17	0.45
1:A:1306:ASN:HD22	1:A:1309:ARG:NH2	2.14	0.45
1:A:1315:VAL:O	1:A:1316:LYS:HG2	2.15	0.45
1:B:1022:ARG:NH2	1:B:1057:SER:O	2.41	0.45
1:B:1001:LEU:O	1:B:1004:VAL:HG12	2.16	0.45
1:B:1178:LEU:O	1:B:1182:GLN:HG3	2.17	0.45
1:A:1155:THR:HG21	1:A:1173:TYR:CD2	2.52	0.45
1:B:1003:GLN:HA	1:B:1006:ILE:HB	1.99	0.45
1:B:1117:GLU:N	1:B:1117:GLU:OE2	2.50	0.44
1:B:1009:TYR:O	1:B:1013:SER:OG	2.27	0.44
2:D:10:U:H2'	2:D:11:U:C6	2.53	0.44
1:B:1012:PHE:O	1:B:1055:LYS:HG3	2.17	0.44
1:B:1044:LEU:HD23	1:B:1061:VAL:HG22	1.99	0.43
1:A:1315:VAL:O	1:A:1316:LYS:CG	2.65	0.43
1:A:1260:ARG:NH1	1:A:1262:SER:O	2.46	0.43
1:B:1171:TYR:HB2	3:B:1401:UTP:O2A	2.19	0.43
1:A:1306:ASN:HD22	1:A:1309:ARG:HH22	1.67	0.43
1:A:1187:PRO:HB2	1:A:1224:TRP:HZ2	1.84	0.42
1:B:1268:LYS:HB2	1:B:1268:LYS:HE3	1.85	0.42
2:D:12:C:C2'	2:D:13:G:H5''	2.43	0.42
2:D:9:C:H2'	2:D:10:U:C6	2.55	0.42
1:A:1160:ILE:O	1:A:1167:SER:OG	2.35	0.42
1:B:1054:PHE:HB3	1:B:1057:SER:OG	2.20	0.42
1:B:1181:LEU:HB3	1:B:1189:ILE:HG12	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:ARG:NH1	1:A:1230:ASN:OD1	2.36	0.42
1:A:1191:VAL:CG2	1:A:1194:GLU:HB2	2.50	0.41
1:B:1243:ARG:O	1:B:1247:GLU:HG3	2.21	0.41
1:B:1286:HIS:HD2	4:B:1506:HOH:O	2.03	0.41
1:B:997:PHE:HA	1:B:1000:ILE:HG12	2.02	0.41
1:B:1026:ARG:HD3	1:B:1044:LEU:HG	2.02	0.41
1:B:1045:PHE:HB3	1:B:1128:LEU:HD23	2.02	0.41
1:A:1127:ALA:HA	1:A:1130:ASN:ND2	2.35	0.41
1:A:1002:ASP:OD1	1:A:1233:SER:HB2	2.21	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	330/389 (85%)	319 (97%)	11 (3%)	0	100	100
1	B	307/389 (79%)	299 (97%)	8 (3%)	0	100	100
All	All	637/778 (82%)	618 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	308/349 (88%)	306 (99%)	2 (1%)	86	94
1	B	289/349 (83%)	283 (98%)	6 (2%)	53	76
All	All	597/698 (86%)	589 (99%)	8 (1%)	69	86

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

Mol	Chain	Res	Type
1	A	1210	ASN
1	A	1320	LYS
1	B	1002	ASP
1	B	1054	PHE
1	B	1216	GLN
1	B	1247	GLU
1	B	1308	ARG
1	B	1328	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	999	ASN
1	A	1182	GLN
1	A	1210	ASN
1	A	1286	HIS
1	A	1306	ASN
1	B	1028	ASN
1	B	1210	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	14/15 (93%)	0	0
2	D	14/15 (93%)	1 (7%)	0
All	All	28/30 (93%)	1 (3%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	13	G

There are no RNA pucker outliers to report.

## 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 ⓘ

2 ligands are modelled in this entry.

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	B	1401	-	26,30,30	2.18	4 (15%)	34,47,47	1.73	9 (26%)
3	UTP	A	1401	-	26,30,30	2.23	5 (19%)	34,47,47	1.86	8 (23%)

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	B	1401	-	-	4/22/38/38	0/2/2/2
3	UTP	A	1401	-	-	0/22/38/38	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	UTP	C6-N1	-7.18	1.34	1.47
3	B	1401	UTP	C6-N1	-6.93	1.34	1.47
3	A	1401	UTP	C6-C5	-4.85	1.39	1.52
3	B	1401	UTP	C6-C5	-4.77	1.39	1.52
3	A	1401	UTP	C5-C4	-4.58	1.39	1.50
3	B	1401	UTP	C5-C4	-4.47	1.39	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1401	UTP	C2-N1	4.02	1.41	1.35
3	A	1401	UTP	C2-N1	4.00	1.41	1.35
3	A	1401	UTP	C2-N3	-2.51	1.33	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	UTP	C4-N3-C2	-6.59	120.32	125.79
3	B	1401	UTP	C4-N3-C2	-5.60	121.15	125.79
3	B	1401	UTP	N3-C2-N1	3.81	120.68	116.65
3	A	1401	UTP	N3-C2-N1	3.75	120.62	116.65
3	A	1401	UTP	C5-C4-N3	3.54	120.62	116.65
3	A	1401	UTP	O2-C2-N1	-2.87	119.51	123.11
3	B	1401	UTP	C5-C4-N3	2.81	119.81	116.65
3	B	1401	UTP	C5-C6-N1	2.65	120.36	111.61
3	B	1401	UTP	O4'-C1'-N1	2.39	112.55	109.30
3	A	1401	UTP	PB-O3A-PA	-2.37	124.70	132.83
3	B	1401	UTP	PB-O3A-PA	-2.31	124.90	132.83
3	B	1401	UTP	O3G-PG-O1G	2.31	116.45	107.64
3	B	1401	UTP	O2-C2-N1	-2.30	120.21	123.11
3	A	1401	UTP	O2A-PA-O1A	2.27	123.47	112.24
3	A	1401	UTP	C5-C6-N1	2.27	119.08	111.61
3	A	1401	UTP	PB-O3B-PG	-2.24	125.13	132.83
3	B	1401	UTP	PB-O3B-PG	-2.17	125.36	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

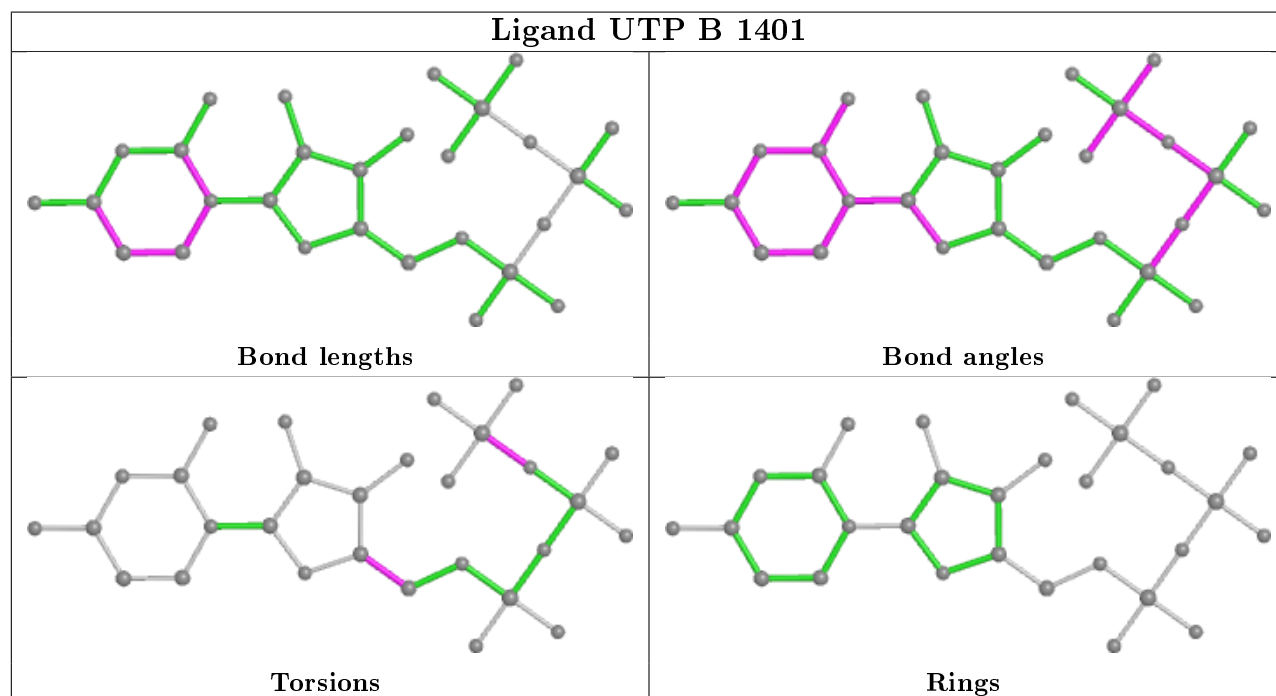
Mol	Chain	Res	Type	Atoms
3	B	1401	UTP	O4'-C4'-C5'-O5'
3	B	1401	UTP	C3'-C4'-C5'-O5'
3	B	1401	UTP	PB-O3B-PG-O1G
3	B	1401	UTP	PB-O3B-PG-O3G

There are no ring outliers.

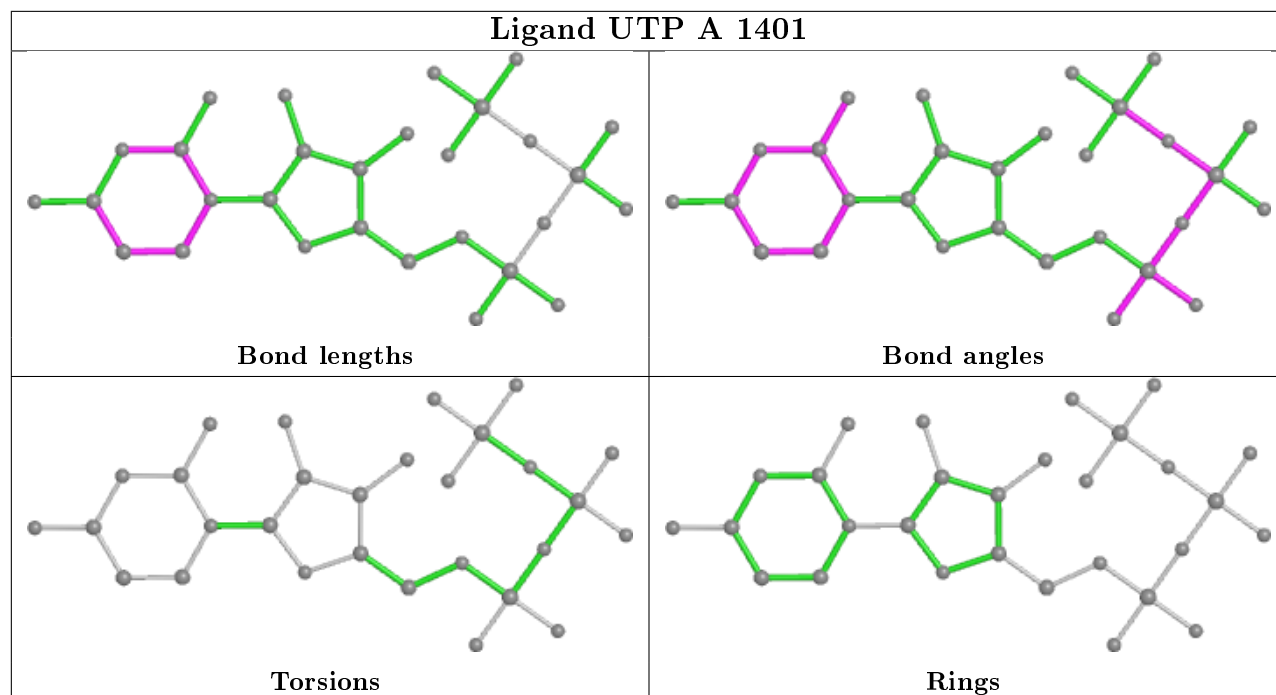
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1401	UTP	1	0
3	A	1401	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, 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	338/389 (86%)	0.30	1 (0%) 94 94	44, 70, 112, 137	0
1	B	317/389 (81%)	0.40	15 (4%) 31 33	48, 75, 119, 161	0
2	C	15/15 (100%)	-0.10	0 100 100	69, 83, 102, 111	0
2	D	15/15 (100%)	0.09	0 100 100	70, 89, 104, 111	0
All	All	685/808 (84%)	0.33	16 (2%) 60 62	44, 73, 115, 161	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1329	PHE	3.8
1	B	1001	LEU	3.4
1	B	1003	GLN	3.3
1	B	1239	LEU	3.3
1	B	997	PHE	2.9
1	B	1200	LYS	2.9
1	B	1117	GLU	2.6
1	B	1068	LEU	2.5
1	A	1299	PHE	2.5
1	B	1168	LEU	2.3
1	B	1309	ARG	2.2
1	B	1110	PHE	2.2
1	B	1272	THR	2.1
1	B	1000	ILE	2.1
1	B	1273	SER	2.1
1	B	1310	VAL	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 [i](#)

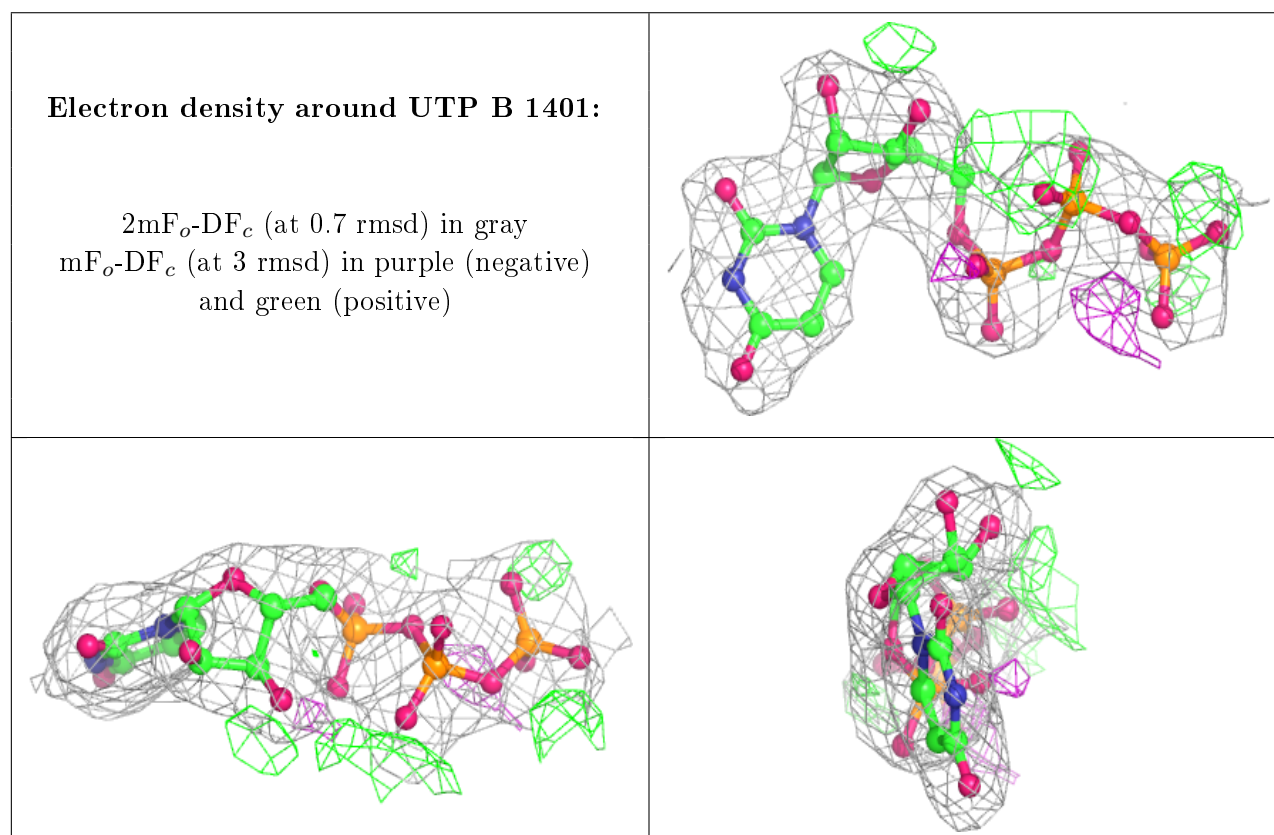
There are no carbohydrates in this entry.

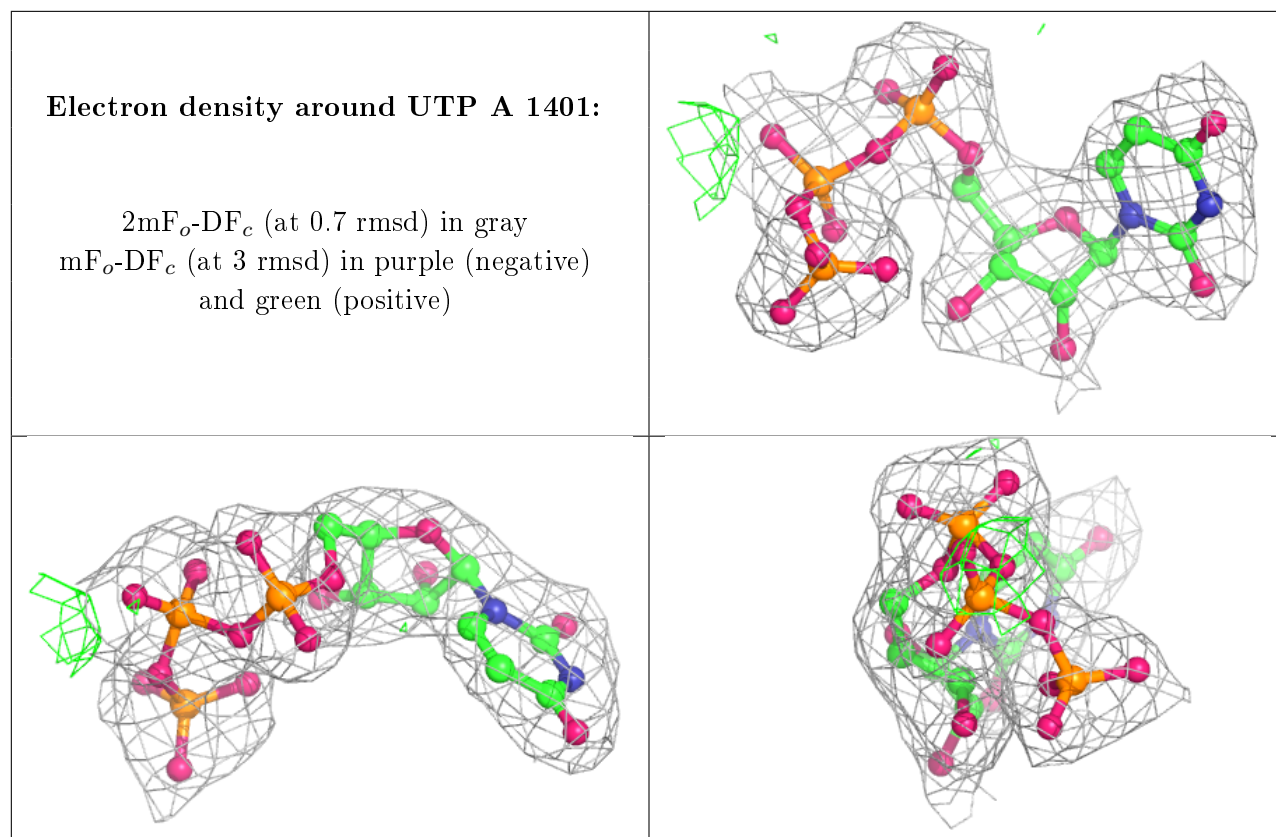
## 6.4 Ligands [i](#)

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UTP	B	1401	29/29	0.94	0.16	48,59,105,112	0
3	UTP	A	1401	29/29	0.97	0.17	46,53,66,70	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.