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2,2'-Anhydro-1-(3',5'-di-O-acetyl- β -D-arabinofuranosyl)uracil, a cyclouridine nucleoside with a C4'-endo furanosyl conformation

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2,2'-Anhydro-1-(3',5'-di-O-acetyl- β -D-arabinofuranosyl)uracil, C₁₃H₁₄N₂O₇, was obtained by refluxing 2',3'-O-(methoxymethylene)uridine in acetic anhydride. The structure exhibits a nearly perfect C4'-endo (⁴E) conformation. The best four-atom plane of the five-membered furanose ring is O-C-C-C, involving the C atoms of the fused fivemembered oxazolidine ring, and the torsion angle is only -0.4 (2)°. The oxazolidine ring is essentially coplanar with the six-membered uracil ring [r.m.s. deviation = 0.012 (5) Å and dihedral angle = -3.2 (3)°]. The conformation at the exocyclic C-C bond is gauche-trans which is stabilized by various C-H··· π and C-O·· π interactions.

Comment

Conformationally restricted cyclonucleoside analogues are of considerable importance in biochemistry, medicinal chemistry and nucleoside-based drug discovery (Wnuk *et al.*, 2002; Bennett & Swayze, 2010). These compounds are key intermediates for the synthesis of a considerable number of nucleoside analogues (Dai *et al.*, 2008; Belostotskii *et al.*, 2012). Besides their utility in synthetic chemistry, cyclonucleosides, with a rigid fused polycyclic system, are good reference compounds to correlate X-ray data with dihedral angles obtained from proton–proton coupling constants (Jardetzky, 1960; Cross & Schleich, 1973) and circular dichroism (Miles *et al.* 1979).

In our attempt to synthesize deoxyuridine derivatives, we tried to make use of a pivotal intermediate, 1-(5-O-acetyl-2,3-dideoxy- β -D-glycero-pent-2-enofuranosyl)uracil, (II), which was reported to be readily obtained from 2',3'-O-(methoxymethylene)uridine, (III) (Shiragami *et al.*, 1988).

However, when repeating this procedure in our laboratory, we found that 2,2'-anhydro-1-(3',5'-di-O-acetyl- β -D-arabinofuranosyl)uracil, (I), was the main product instead of (II). The expected product (II) formed but in low yield (23%) and was found to be unstable in boiling acetic anhydride. 3',5'-Diacetylated cyclouridine, (I), was obtained in 65% yield after



boiling for 5 h. To confirm its molecular structure, as well as to provide the solid-state conformation of this fused polycyclic



Figure 1

The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.



system, we report here the crystal structure of (I) (Fig. 1) and compare it with those of related cyclouridine molecules.

The preferred sugar puckering modes in nucleosides are C2'-endo and C3'-endo (Saenger, 1984), whereas the C4'-endo $({}^{4}E)$ conformation was considered to be unlikely given the short O2' - O3' distance and the fact that some adjacent bonds would be in an eclipsed conformation (Jardetzky, 1960). However, with the cyclization of O2' and C2', the ribosyl furanose ring changes to the arabinosyl configuration, thus eliminating the steric congestion at O3'. The fused oxazolidine ring demands C1'-N1 and C2'-O2' to be eclipsed in order to conform to the sp^2 character of atoms N1 and C2 in the pyrimidine ring. The X-ray study of (I) shows that the fivemembered furanosyl ring adopts a nearly perfect C4'-endo puckered conformation. The best four-atom plane, comprised of atoms O4', C1', C2' and C3', is planar, as the O4'-C1'-C2' - C3' torsion angle is only -0.4 (2)°. Atom C4' is displaced by 0.491 (3) Å to the same side of this plane as C5'. A quantitative analysis of the ring conformations was performed using the method of Cremer & Pople (1975) for the calculation of puckering parameters. The polar parameters for the furanose ring are Q = 0.316 (2) Å and $\varphi = 143.3 (4)^{\circ}$, comparable with an ideal envelope C4'-endo conformation (ideal $\varphi = 144^{\circ}$). This conformation is also found in cyclonucleosides such as 2,2'-anhydro-1-(β -D-arabinofuranosyl)uracil (Suck & Saenger, 1973) and 1,2-di-O-isopropylidenepentofuranose (Doboszewski et al. 2012).

The exocyclic C4'-C5' bond adopts a *gauche-trans* conformation instead of the *gauche-gauche* conformation commonly observed in nucleosides (Shefter & Trueblood, 1965). The corresponding dihedral angles, as defined by Shefter & Trueblood (1965), are $\varphi_{OO} = 55.2$ (3)° and $\varphi_{OC} = 172.5$ (2)°. This geometric arrangement may lessen the short contacts that would occur if the conformation were *gauche-gauche* and *syn* (Seshadri *et al.*, 1983). In addition, a significant intramolecular $C5'-H5'2\cdots\pi$ (pyrimidine) hydrogen bond and a $C7-O7\cdots\pi$ (pyrimidine) interaction were observed in this molecule, which we believe are the other main forces stabilizing the C4'-C5' *gauche-trans* configuration. The present geometry is very similar to that of the 5'-O-tosyl and 5'-O-acetylated analogues (Gautham *et al.*, 1983; Seshadri *et al.*, 1983).

The uracil ring and the five-membered oxazolidine ring fused at atoms N1 and C2 are both essentially planar. The interplanar angle between the six- and five-membered rings is about 2°. The glycosidic torsion angle χ (O4'-C1'-N1-C6) is -63.5 (3)°, reflecting a *syn* conformation. The value agrees well with those for the similar fused-ring systems 2,2'-anhydro-1- β -D-*arabino*-furanosyl cytosine hydrochloride ($\chi_{CN} = -61^{\circ}$; Sundaralingam, 1973) and 2,2'-anhydro-1- β -D-*arabino*-furanosyl uracil ($\chi_{CN} = -65.5^{\circ}$; Delbaere & James, 1973).

For the 5'-O-acetyl group, the C8–C7–O5'–C5' and O7– C7–O5'–C5' torsion angles are 177.0 (3) and -3.2 (4)°, respectively, and thus the C8–C7 bond is *trans* and the C7–O7 bond *cis* to the arabinose C5'–O5' bond. This is the same for the 3'-O-acetyl group, as the C10–C9–O3'–C3' and O9–C9–O3'–C3' torsion angles are 178.4 (2) and





 $-2.1 (4)^{\circ}$, respectively, indicating that the C10-C9 bond is *trans* and the C9-O9 bond *cis* to the C3'-O3' bond.

Various $C-O\cdots\pi$, $C-H\cdots\pi$, $C-H\cdots0$ and $C-H\cdotsN$ hydrogen bonds are present in the structure of (I). The $C-O\cdots\pi$ interactions that can be observed are an intramolecular $C7-O7\cdots Cg$ interaction $[O7\cdots Cg = 3.595 (2) \text{ Å}; Cg$ is the centroid of the N1/C2/N3/C4-C6 ring] and an intermolecular $C9-O9\cdots Cg^{i}$ interaction $[O9\cdots Cg^{i} = 3.3036 (12) \text{ Å};$ symmetry code: (i) x - 1, y, z]. Molecules are arranged in chains in a head-to-tail fashion via $C6-H6\cdots N3^{ii}$ hydrogen bonds and $C1'-H1'\cdots O4^{iii}$ short contacts [symmetry codes: (ii) x + 2, $y - \frac{1}{2}, -z$; (iii) $-x + 2, y + \frac{1}{2}, -z$] along the [010] direction (Table 1 and Fig. 2). These chains are further connected via weak $C8-H8B\cdots O7^{iv}$ hydrogen bonds [symmetry code: (iv) $x + 1, y + \frac{1}{2}, -z + 1$] into a sheet and these sheets are in turn further connected via various weak $C-H\cdots O$ short contacts into a three-dimensional network.

Experimental

2',3'-O-(Methoxymethylene)uridine, (III) (see Scheme), was prepared according to a previously reported method (Shiragami *et al.*, 1988). All other chemicals were obtained commercially and used without further purification. The title compound, (I), was prepared according to a similar procedure used for the synthesis of 1-(5-Oacetyl-2,3-dideoxy- β -D-glycero-pent-2-enofuranosy1)uracil, (II). A solution of (III) (7.0 g, 21.3 mmol) in acetic anhydride (50 ml) was boiled gently and the acetic acid which formed was boiled off. After the disappearance of the starting material (about 5 h), the remaining acetic anhydride was evaporated under reduced pressure, and the residue was dissolved in chloroform (100 ml) and washed with aqueous NaHCO₃ (50 ml). The aqueous layer was extracted with CHCl₃ (50 ml). The combined organic layers were dried over Na₂SO₄, concentrated and purified by silica-gel column chromatography (CHCl₃-MeOH 10:1 ν/ν) to give (I) (yield: 4.3 g, 65%; m.p. 461– 463 K). Crystals suitable for X-ray diffraction analysis were crystallized from a petroleum ether–ethyl acetate mixture (4:1 ν/ν).

V = 719.21 (5) Å³

Mo $K\alpha$ radiation

 $0.3 \times 0.3 \times 0.3$ mm

H-atom parameters constrained

Absolute structure: Flack (1983),

 $\Delta \rho_{\text{max}} = 0.14 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

933 Friedel pairs

Flack parameter: -0.2 (12)

 $\mu = 0.12 \text{ mm}^{-1}$

T = 294 K

Z = 2

Crystal data

 $C_{13}H_{14}N_2O_7$ $M_r = 310.26$ Monoclinic, P2₁ a = 8.1032 (3) Å b = 10.0065 (3) Å c = 8.8704 (4) Å $\beta = 90.609$ (4)°

Data collection

Agilent SuperNova (Dual, Cu at
zero, Eos) diffractometer2985 measured reflections
2483 independent reflections
2160 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.015$ Absorption correction: multi-scan
(CrysAlis PRO; Agilent, 2012)
 $T_{min} = 0.710, T_{max} = 1.000$ 2985 measured reflections
2483 independent reflections
2160 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.015$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.091$ S = 1.092483 reflections 201 parameters 1 restraint

Table 1

Hydrogen-bond geometry (Å, °).

Cg is the centroid of the N1/C2/N3/C4-C6 ring.

$D - H \cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - H \cdot \cdot \cdot A$
$C1' - H1' \cdots O4^i$	0.98	2.36	3,308 (3)	162
$C5' - H5'A \cdots O4^{ii}$	0.97	2.59	3.537 (3)	166
$C5' - H5'B \cdots Cg$	0.97	2.50	3.026 (2)	114
C6−H6···O9 ⁱⁱⁱ	0.93	2.42	3.313 (3)	162
$C8-H8C\cdots O4^{iv}$	0.96	2.48	3.272 (4)	140
$C6-H6\cdots N3^i$	0.93	2.68	3.226 (3)	118
$C3' - H3' \cdots O4'^v$	0.98	2.37	3.311 (3)	161
$C4' - H4' \cdots O2'^{iii}$	0.98	2.62	3.340 (3)	130

Symmetry codes: (i) $-x + 2, y + \frac{1}{2}, -z$; (ii) x - 1, y, z; (iii) $-x + 1, y + \frac{1}{2}, -z$; (iv) $-x + 2, y + \frac{1}{2}, -z + 1$; (v) $-x + 1, y - \frac{1}{2}, -z$.

All H atoms were placed geometrically and refined using a riding model, with C–H = 0.93 (aromatic), 0.96 (methyl), 0.97 (methylene) and 0.98 Å (methine), and with $U_{\rm iso}({\rm H}) = 1.5 U_{\rm eq}({\rm C})$ for methyl H atoms and $1.2 U_{\rm eq}({\rm C})$ otherwise. The chirality of (I) was known from the synthetic route and the absolute structure was assigned on the basis of the known chirality of the uridine used in the chemical synthesis.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FN3123). Services for accessing these data are described at the back of the journal.

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supplementary materials

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2,2'-Anhydro-1-(3',5'-di-O-acetyl- β -D-arabinofuranosyl)uracil, a cyclouridine nucleoside with a C4'-*endo* furanosyl conformation

Ying Fu, Yin-Xia He, Hong-Xia Hou, Wen-Bo Zhu, Hu-Lin Li, Chao Wu and Fang-Yan Xian

2,2'-Anhydro-1-(2'-deoxy-3',5'-di-O-acety-β-D- arabinofuranosyl)uracil

Crystal data

 $C_{13}H_{14}N_2O_7$ $M_r = 310.26$ Monoclinic, $P2_1$ a = 8.1032 (3) Å b = 10.0065 (3) Å c = 8.8704 (4) Å $\beta = 90.609$ (4)° V = 719.21 (5) Å³ Z = 2F(000) = 324

Data collection

Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer Radiation source: SuperNova (Mo) X-ray Source Mirror monochromator Detector resolution: 16.0733 pixels mm⁻¹ ω scans Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)

Refinement

Refinement on F^2 Least-squares matrix: full $R[F^2 > 2\sigma(F^2)] = 0.039$ $wR(F^2) = 0.091$ S = 1.092483 reflections 201 parameters 1 restraint Primary atom site location: structure-invariant direct methods Secondary atom site location: difference Fourier map $D_x = 1.433 \text{ Mg m}^{-3}$ Melting point = 461–463 K Mo K α radiation, $\lambda = 0.7107 \text{ Å}$ Cell parameters from 1211 reflections $\theta = 3.1-28.4^{\circ}$ $\mu = 0.12 \text{ mm}^{-1}$ T = 294 KBlock, colourless $0.3 \times 0.3 \times 0.3 \text{ mm}$

 $T_{\min} = 0.710, T_{\max} = 1.000$ 2985 measured reflections
2483 independent reflections
2160 reflections with $I > 2\sigma(I)$ $R_{int} = 0.015$ $\theta_{\max} = 26.4^{\circ}, \theta_{\min} = 3.1^{\circ}$ $h = -6 \rightarrow 10$ $k = -12 \rightarrow 12$ $l = -11 \rightarrow 8$

Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained $w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.0609P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{max} < 0.001$ $\Delta\rho_{max} = 0.14 \text{ e } \text{Å}^{-3}$ $\Delta\rho_{min} = -0.17 \text{ e } \text{Å}^{-3}$ Absolute structure: Flack (1983), 933 Friedel pairs Flack parameter: -0.2 (12)

Special details

Experimental. Absorption correction: CrysAlisPro, Agilent Technologies, Version 1.171.36.20, Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2$ sigma(F^2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

0.7319(2) $0.7319(2)$ $0.39998(15)$ $-0.0785(2)$ $0.0440(4)$	
O3' 0.3797 (2) 0.55971 (17) -0.24786 (17) 0.0443 (4)	
O4 1.1202 (3) 0.37929 (19) 0.2971 (2) 0.0594 (6)	
O4' 0.5843 (2) 0.70443 (14) -0.02277 (19) 0.0424 (4)	
O5' 0.4859 (3) 0.6532 (2) 0.27176 (19) 0.0570 (6)	
O70.6470 (3)0.5328 (3)0.4235 (2)0.0886 (8)	
O9 0.1443 (2) 0.48121 (19) -0.1537 (2) 0.0605 (6)	
N1 0.8368 (2) 0.58738 (17) 0.0164 (2) 0.0365 (5)	
N3 0.9211 (3) 0.37845 (19) 0.1143 (2) 0.0416 (5)	
C1' 0.7165 (3) 0.6383 (2) -0.0916 (3) 0.0389 (6)	
H1' 0.7682 0.6938 -0.1689 0.047*	
C2 0.8376 (3) 0.4522 (2) 0.0244 (3) 0.0379 (6)	
C2' 0.6476 (3) 0.5074 (2) -0.1578 (3) 0.0396 (5)	
H2' 0.6637 0.5021 -0.2670 0.048*	
C3' 0.4659 (3) 0.5081 (2) -0.1176 (2) 0.0353 (5)	
H3' 0.4262 0.4195 -0.0882 0.042*	
C4 1.0285 (3) 0.4446 (2) 0.2130 (3) 0.0430 (6)	
C4' 0.4557 (3) 0.6092 (2) 0.0112 (3) 0.0382 (5)	
H4' 0.3485 0.6544 0.0059 0.046*	
C5 1.0296 (3) 0.5895 (3) 0.2110 (3) 0.0466 (6)	
H5 1.0980 0.6354 0.2780 0.056*	
C5' 0.4762 (3) 0.5453 (2) 0.1656 (2) 0.0433 (6)	
H5'A 0.3828 0.4882 0.1874 0.052*	
H5'B 0.5761 0.4919 0.1698 0.052*	
C6 0.9345 (3) 0.6582 (2) 0.1148 (3) 0.0412 (6)	
H6 0.9345 0.7511 0.1147 0.049*	
C7 0.5792 (4) 0.6352 (3) 0.3962 (3) 0.0526 (7)	
C8 0.5833 (5) 0.7582 (3) 0.4902 (4) 0.0828 (12)
H8A 0.5352 0.7397 0.5865 0.124*	
H8B 0.5218 0.8276 0.4406 0.124*	
H8C 0.6956 0.7865 0.5044 0.124*	
C9 0.2144 (3) 0.5409 (3) -0.2514 (3) 0.0469 (6)	
C10 0.1376 (4) 0.6010 (4) -0.3879 (3) 0.0728 (10)
H10A 0.1457 0.5396 -0.4707 0.109*	
H10B 0.1940 0.6824 -0.4125 0.109*	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\hat{A}^2)

supplementary materials

H10C	0.0236	0.61	99	-0.3690	0.109*		
Atomic displacement parameters $(Å^2)$							
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}	
02′	0.0470 (11)	0.0286 (8)	0.0562 (11)	0.0040 (8)	-0.0104 (9)	-0.0056 (8)	
O3′	0.0443 (10)	0.0488 (10)	0.0395 (9)	-0.0025 (8)	-0.0049 (7)	0.0081 (8)	
O4	0.0649 (14)	0.0506 (11)	0.0625 (12)	0.0135 (10)	-0.0152 (11)	0.0053 (10)	
O4′	0.0427 (10)	0.0265 (7)	0.0581 (11)	0.0009 (7)	0.0009 (8)	-0.0029 (7)	
O5′	0.0711 (14)	0.0549 (11)	0.0444 (11)	0.0133 (10)	-0.0170 (10)	-0.0116 (9)	
07	0.118 (2)	0.0762 (15)	0.0703 (14)	0.0182 (17)	-0.0367 (14)	0.0102 (14)	
09	0.0483 (12)	0.0631 (13)	0.0703 (13)	-0.0071 (10)	0.0032 (10)	0.0039 (11)	
N1	0.0367 (12)	0.0264 (10)	0.0464 (12)	0.0004 (9)	-0.0038 (9)	0.0014 (9)	
N3	0.0456 (13)	0.0306 (10)	0.0484 (13)	0.0065 (10)	-0.0023 (11)	0.0018 (9)	
C1′	0.0415 (15)	0.0307 (11)	0.0444 (15)	-0.0004 (11)	0.0012 (11)	0.0035 (10)	
C2	0.0381 (14)	0.0293 (12)	0.0463 (15)	0.0043 (10)	0.0067 (11)	-0.0015 (11)	
C2′	0.0460 (13)	0.0336 (12)	0.0393 (12)	0.0037 (12)	-0.0028 (10)	0.0008 (11)	
C3′	0.0424 (13)	0.0274 (11)	0.0360 (12)	-0.0002 (11)	-0.0057 (10)	0.0009 (10)	
C4	0.0451 (16)	0.0408 (14)	0.0430 (15)	0.0067 (12)	0.0031 (12)	0.0016 (11)	
C4′	0.0372 (14)	0.0342 (11)	0.0433 (13)	0.0004 (11)	-0.0029 (10)	-0.0031 (10)	
C5	0.0483 (16)	0.0447 (14)	0.0468 (15)	0.0002 (13)	-0.0052 (12)	-0.0053 (12)	
C5′	0.0465 (15)	0.0422 (14)	0.0410 (12)	0.0003 (12)	-0.0029 (11)	-0.0049 (11)	
C6	0.0477 (16)	0.0317 (12)	0.0442 (15)	-0.0029 (11)	0.0038 (12)	-0.0007 (11)	
C7	0.0574 (18)	0.0602 (18)	0.0401 (15)	-0.0141 (15)	-0.0092 (13)	0.0072 (13)	
C8	0.134 (4)	0.066 (2)	0.0477 (18)	-0.039 (2)	-0.021 (2)	0.0018 (15)	
C9	0.0467 (15)	0.0490 (15)	0.0450 (14)	0.0044 (13)	-0.0043 (12)	-0.0090 (13)	
C10	0.062 (2)	0.101 (3)	0.0542 (17)	0.019 (2)	-0.0174 (15)	-0.0010 (17)	

Geometric parameters (Å, °)

02′—C2	1.350 (3)	C2'—C3'	1.518 (3)
O2'—C2'	1.451 (3)	С3′—Н3′	0.9800
O3'—C3'	1.440 (3)	C3′—C4′	1.528 (3)
O3′—C9	1.353 (3)	C4—C5	1.450 (3)
O4—C4	1.234 (3)	C4′—H4′	0.9800
O4′—C1′	1.404 (3)	C4′—C5′	1.519 (3)
O4′—C4′	1.447 (3)	С5—Н5	0.9300
O5'—C5'	1.434 (3)	C5—C6	1.335 (3)
O5′—C7	1.343 (3)	С5'—Н5'А	0.9700
O7—C7	1.186 (4)	С5′—Н5′В	0.9700
О9—С9	1.200 (3)	С6—Н6	0.9300
N1—C1′	1.452 (3)	C7—C8	1.487 (4)
N1-C2	1.355 (3)	C8—H8A	0.9600
N1-C6	1.370 (3)	C8—H8B	0.9600
N3—C2	1.276 (3)	C8—H8C	0.9600
N3—C4	1.394 (3)	C9—C10	1.482 (4)
С1'—Н1'	0.9800	C10—H10A	0.9600
C1′—C2′	1.539 (3)	C10—H10B	0.9600
C2'—H2'	0.9800	C10—H10C	0.9600

C2—O2'—C2'	109.45 (18)	O4'—C4'—C5'	113.11 (18)
C9—O3'—C3'	116.16 (19)	C3'—C4'—H4'	109.0
C1'—O4'—C4'	109.56 (16)	C5'—C4'—C3'	112.91 (19)
C7—O5'—C5'	117.7 (2)	C5'—C4'—H4'	109.0
C2—N1—C1′	112.8 (2)	C4—C5—H5	119.4
C2—N1—C6	118.7 (2)	C6—C5—C4	121.3 (3)
C6—N1—C1′	128.20 (19)	С6—С5—Н5	119.4
C2—N3—C4	116.2 (2)	O5'—C5'—C4'	106.28 (19)
O4′—C1′—N1	112.9 (2)	O5'—C5'—H5'A	110.5
O4'—C1'—H1'	111.8	O5'—C5'—H5'B	110.5
O4'—C1'—C2'	107.0 (2)	C4'—C5'—H5'A	110.5
N1—C1′—H1′	111.8	C4'—C5'—H5'B	110.5
N1—C1′—C2′	101.02 (18)	H5'A—C5'—H5'B	108.7
C2'—C1'—H1'	111.8	N1—C6—H6	121.1
O2′—C2—N1	110.4 (2)	C5—C6—N1	117.9 (2)
N3—C2—O2′	121.8 (2)	С5—С6—Н6	121.1
N3—C2—N1	127.8 (2)	O5′—C7—C8	111.0 (3)
O2'—C2'—C1'	106.17 (17)	O7—C7—O5′	122.6 (3)
O2'—C2'—H2'	111.8	O7—C7—C8	126.3 (3)
O2'—C2'—C3'	110.04 (18)	C7—C8—H8A	109.5
C1'—C2'—H2'	111.8	С7—С8—Н8В	109.5
C3'—C2'—C1'	104.77 (19)	С7—С8—Н8С	109.5
C3'—C2'—H2'	111.8	H8A—C8—H8B	109.5
O3'—C3'—C2'	106.06 (17)	H8A—C8—H8C	109.5
O3'—C3'—H3'	112.3	H8B—C8—H8C	109.5
O3'—C3'—C4'	109.44 (19)	O3′—C9—C10	111.7 (3)
C2'—C3'—H3'	112.3	09—C9—O3′	121.9 (2)
C2'—C3'—C4'	103.84 (18)	O9—C9—C10	126.4 (3)
C4'—C3'—H3'	112.3	C9—C10—H10A	109.5
O4—C4—N3	119.7 (2)	C9—C10—H10B	109.5
O4—C4—C5	122.2 (3)	C9—C10—H10C	109.5
N3—C4—C5	118.1 (2)	H10A—C10—H10B	109.5
O4'—C4'—C3'	103.63 (18)	H10A—C10—H10C	109.5
O4'—C4'—H4'	109.0	H10B—C10—H10C	109.5
O2'—C2'—C3'—O3'	-149.97 (18)	C2—N3—C4—O4	-175.8(2)
O2'—C2'—C3'—C4'	94.7 (2)	C2—N3—C4—C5	3.3 (4)
O3'—C3'—C4'—O4'	-81.4 (2)	C2'—O2'—C2—N1	-2.7(3)
O3'—C3'—C4'—C5'	155.9 (2)	C2'—O2'—C2—N3	176.5 (2)
O4—C4—C5—C6	177.2 (2)	C2'—C3'—C4'—O4'	31.5 (2)
O4'—C1'—C2'—O2'	-116.8 (2)	C2'—C3'—C4'—C5'	-91.2 (2)
O4'—C1'—C2'—C3'	-0.4 (2)	C3'—O3'—C9—O9	-2.1(4)
O4'—C4'—C5'—O5'	55.2 (3)	C3'-O3'-C9-C10	178.4 (2)
N1—C1′—C2′—O2′	1.4 (2)	C3'—C4'—C5'—O5'	172.5 (2)
N1—C1′—C2′—C3′	117.88 (19)	C4—N3—C2—O2'	178.7 (2)
N3—C4—C5—C6	-1.9 (5)	C4—N3—C2—N1	-2.3 (4)
C1'—O4'—C4'—C3'	-33.6 (2)	C4—C5—C6—N1	-0.8(4)
C1'—O4'—C4'—C5'	89.1 (2)	C4'—O4'—C1'—N1	-88.8 (2)
C1'—N1—C2—O2'	3.9 (3)	C4'—O4'—C1'—C2'	21.4 (2)

supplementary materials

C1'—N1—C2—N3	-175.3 (2)	C5'—O5'—C7—O7	-3.2 (4)
C1′—N1—C6—C5	175.9 (2)	C5'—O5'—C7—C8	177.0 (3)
C1'—C2'—C3'—O3'	96.3 (2)	C6—N1—C1'—O4'	-63.5 (3)
C1'—C2'—C3'—C4'	-19.0 (2)	C6—N1—C1′—C2′	-177.4 (2)
C2—O2'—C2'—C1'	0.7 (2)	C6—N1—C2—O2'	178.7 (2)
C2—O2'—C2'—C3'	-112.2 (2)	C6—N1—C2—N3	-0.5 (4)
C2—N1—C1′—O4′	110.7 (2)	C7—O5'—C5'—C4'	-148.2 (2)
C2—N1—C1′—C2′	-3.2 (3)	C9—O3'—C3'—C2'	165.25 (19)
C2—N1—C6—C5	2.0 (4)	C9—O3'—C3'—C4'	-83.3 (2)

Hydrogen-bond geometry (Å, °)

Cg is the centroid of the N1/C2/N3/C4-C6 ring [Added text OK?].

D—H···A	D—H	H···A	$D \cdots A$	D—H···A
C1'—H1'····O4 ⁱ	0.98	2.36	3.308 (3)	162
C5′—H5′A····O4 ⁱⁱ	0.97	2.59	3.537 (3)	166
C5′—H5′ <i>B</i> ··· <i>Cg</i>	0.97	2.50	3.026 (2)	114
C6—H6····O9 ⁱⁱⁱ	0.93	2.42	3.313 (3)	162
C8—H8 <i>C</i> ···O4 ^{iv}	0.96	2.48	3.272 (4)	140
C6—H6…N3 ⁱ	0.93	2.68	3.226 (3)	118
C3′—H3′····O4′ ^v	0.98	2.37	3.311 (3)	161
C4′—H4′…O2′ ⁱⁱⁱⁱ	0.98	2.62	3.340 (3)	130

Symmetry codes: (i) -x+2, y+1/2, -z; (ii) x-1, y, z; (iii) -x+1, y+1/2, -z; (iv) -x+2, y+1/2, -z+1; (v) -x+1, y-1/2, -z.

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