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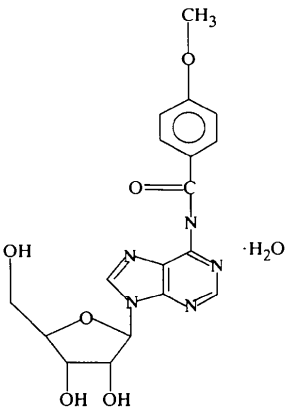

(I)

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N^6-Anisoyladenosine monohydrate

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Abstract

The title compound, $C_{18}H_{19}N_5O_6{\cdot}H_2O$, has a *syn* conformation about the glycosidic bond. Its furanose ring shows a C2′-*endo*–C3′-*exo* twist conformation and *trans-gauche* geometry about the C4′—C5′ bond. The angle between the adenine base and the phenyl ring of the anisoyl group is 22.9°. Adenine and anisoyl groups stack along the *b* axis at a separation of 3.4 Å.

Comment

The investigation of the title compound, (I), was carried out to study the effect of modifications of the base on the nucleoside conformation as part of our studies on modified nucleosides (Padiyar & Seshadri, 1996). The conformation of the adenine base with respect to the ribose is *syn* with $\chi_{CN} = -68.1\,(2)°$. This *syn* conformation is not accompanied by the N3—O5′ intramolecular hydrogen bond characteristically seen in several 2′- and 2′,5′-nucleotide structures (Padiyar & Seshadri, 1998; Krishnan & Seshadri, 1993, 1994). The furanose ring shows a C2′-*endo*–C3′-*exo* twist conformation which is evident from the pseudorotation angle $P = 174.3°$. The maximum amplitude of pucker is 39.4° (Altona & Sundaralingam, 1972; Saenger, 1984). The torsion angles φ_{oo}(O5′—C5′—C4′—O4′) and φ_{oc}(O5′—C5′—C4′—C3′) are 173.1 (2) and −69.2 (2)°, respectively. They indicate that the conformation about the C4′—C5′ bond is *trans-gauche*. The angle between the adenine base and the phenyl ring of the anisoyl group is 22.9° and these stack at a separation of 3.4 Å along the *b* axis. This column of nucleosides repeats along the *c* axis. An

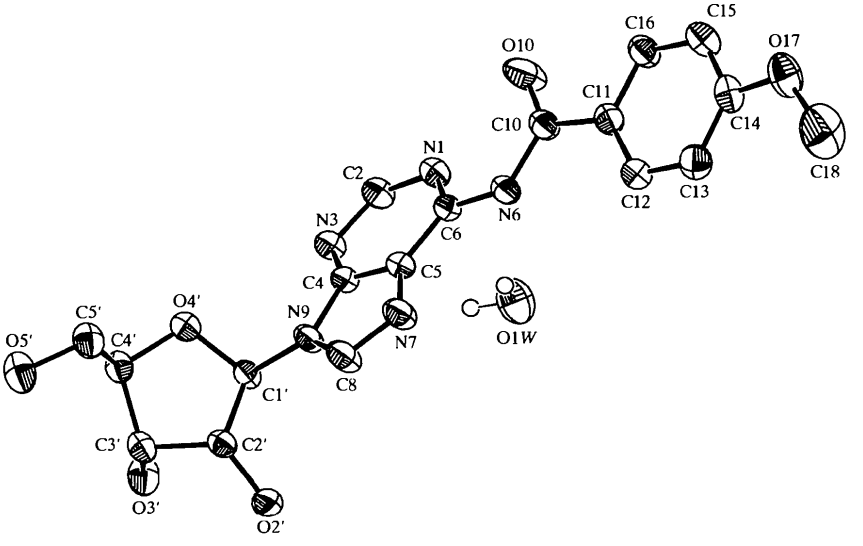

Fig. 1. Molecular structure of (I) showing 50% probability displacement ellipsoids.

important feature of this structure is the formation of hydrogen bonds between the carbonyl O atom O10, and the O2′, C2′ and C8 atoms (Desiraju, 1996).

Experimental

The title compound was obtained from the Sigma Chemical Company. Crystals were grown by evaporation of a solution of the compound in dimethylformamide.

Crystal data

$C_{18}H_{19}N_5O_6 \cdot H_2O$
$M_r = 419.40$
Monoclinic
$P2_1$
$a = 9.412\ (2)$ Å
$b = 6.914\ (1)$ Å
$c = 14.667\ (2)$ Å
$\beta = 102.89\ (2)°$
$V = 930.4\ (3)$ Å^3
$Z = 2$
$D_x = 1.497$ Mg m^{-3}
D_m not measured
Cu $K\alpha$ radiation
$\lambda = 1.5418$ Å
Cell parameters from 25 reflections
$\theta = 8–25°$
$\mu = 0.994$ mm^{-1}
$T = 293\ (2)$ K
Plate
0.80 × 0.20 × 0.05 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: none
2367 measured reflections
2026 independent reflections
1948 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 72.90°$
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 8$
$l = -18 \rightarrow 17$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.102$
$S = 1.009$
2026 reflections
301 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.303$ e Å^{-3}
$\Delta\rho_{min} = -0.186$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0120 (17)
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = 0.15 (21)

Table 1. *Selected torsion angles (°)*

C4—N9—C1′—O4′	−68.1 (2)	C2′—C1′—O4′—C4′	−16.9 (2)
O4′—C1′—C2′—C3′	35.3 (2)	C3′—C4′—O4′—C1′	−9.0 (2)
C1′—C2′—C3′—C4′	−39.1 (2)	O4′—C4′—C5′—O5′	173.1 (2)
C2′—C3′—C4′—O4′	30.6 (2)	C3′—C4′—C5′—O5′	−69.2 (2)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Data reduction: *CAD-4 Software*. Program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1997). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *Xtal_GX* (Hall & du Boulay, 1995). Software used to prepare material for publication: *SHELXL*93.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: VJ1092). Services for accessing these data are described at the back of the journal.

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N^3-Benzoyl-2′,3′-di-*O*-benzoyluridine

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Abstract

The structure of N^3-benzoyl-2′,3′-di-*O*-benzoyluridine, $C_{30}H_{24}N_2O_9$, has two molecules in the asymmetric unit. The uracil bases of both the molecules are in the *anti* conformation with respect to the ribose moiety and the furanosyl rings adopt a C3′-*endo* conformation. The orientation about the C4′—C5′ bond is *gauche-gauche*. The two crystallographically independent molecules are linked through several C—H···O hydrogen bonds. The nucleoside molecules pack as columns along the *a* axis and these columns repeat along the *c* axis.