We thank the CSIR and DST, India, for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1093). Services for accessing these data are described at the back of the journal.

References

Altona, C. & Sundaralingam, M. (1972). *J. Am. Chem. Soc.* **94**, 8205–8212.

Biosym Technologies (1995). *INSIGHT*II. Biosym Technologies Inc., San Diego, CA 92121-2777, USA.

Enraf–Nonius (1985*a*). *CAD-4 Diffractometer Control Software*. Enraf–Nonius, Delft, The Netherlands.

Enraf–Nonius (1985*b*). *Structure Determination Package*. Enraf–Nonius, Delft, The Netherlands.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Fujii, S., Fujiwara, T. & Tomita, K. I. (1976). *Nucleic Acids Res.* **3**, 1985–1989.

Hall, S. R. & du Boulay, D. (1995). *Xtal_GX*. University of Western Australia, Australia.

Krishnan, R. & Seshadri, T. P. (1992). *Nucleosides Nucleotides*, **11**, 1047–1057.

Mande, S. S., Seshadri, T. P. & Viswamitra, M. A. (1994). *Acta Cryst.* C**50**, 876–879.

North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.

Padiyar, G. S. & Seshadri, T. P. (1996). *Nucleosides Nucleotides*, **15**, 857–865.

Prusiner, P. & Sundaralingam, M. (1976). *Acta Cryst.* B**32**, 161–169.

Radwan, M. M. & Wilson, H. R. (1979). *Acta Cryst.* B**35**, 3072–3077.

Sheldrick, G. M. (1985). *SHELXS*86. *Program for the Solution of Crystal Structures*. University of Göttingen, Germany.

Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.

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N^4-Anisoylcytidine dihydrate

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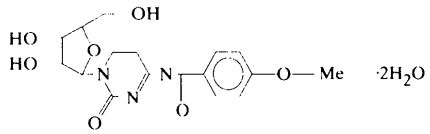
Abstract

The title compound, $C_{17}H_{19}N_3O_7\cdot 2H_2O$, has C2′-*endo*, C3′-*exo* puckering. The orientation of the base with respect to the sugar is *anti* and the geometry about C4′—C5′ is *gauche,trans*. The angle between the cytidine base and the phenyl ring of the anisoyl group is 15.5 (2)°.

Comment

This investigation of N^4-anisoylcytidine dihydrate, (I), was carried out to study the effect of modification of the base on the nucleoside conformation. The cytidine base is planar and is in an *anti* [χ = −158.1 (2)°] conformation with respect to the ribose moiety. The furanosyl ring shows C2′-*endo*, C3′-*exo* (Saenger, 1984) twist conformation, which is evident from the pseudorotation angle P = 184.1° (Altona & Sundaralingam, 1972). The puckering amplitude (Cremer & Pople, 1975) is 40.0°. The torsion angles φ_{oo} (O5′—C5′—C4′—O4′) and φ_{oc} (O5′—C5′—C4′—C3′) are 61.3 (3) and 179.5 (3)°, respectively, indicating that the conformation about C4′—C5′ bond is *gauche,trans*.



(I)

The phenyl ring of the anisoyl group makes an angle of 15.5 (2)° with the cytosine base. The three Watson–Crick sites (N3, N4 and O2) of the cytosine base are involved in hydrogen bonding with the water atoms O1*W* and O2*W*; further details are given in Table 2. There is also an intramolecular C—H···O hydrogen bond (Jeffrey & Saenger, 1991; Desiraju, 1996) between C5 of the cytosine base and O7 of the anisoyl group. A similar C—H···O intramolecular hydrogen bond has also been observed in the crystal structure of amicetin (Smith & Sundaralingam, 1981).

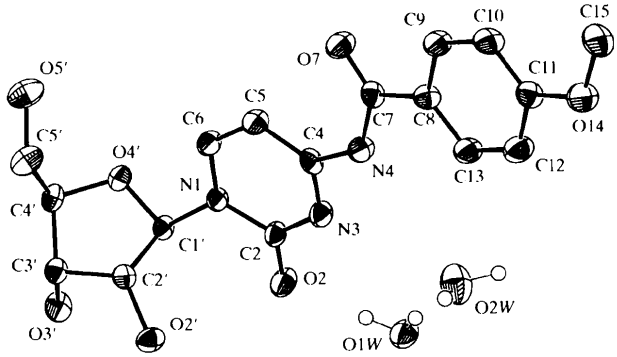


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme and 50% probability displacement ellipsoids. H atoms are omitted for clarity, except for those on the two water molecules which are drawn as circles of an arbitrary radius.

Comparison of amicetin with the structure of (I) shows that the two compounds, both with substitution at N^4, display similar deviations in geometrical parameters

from the average values. As in amicetin, there is also a shortening of the N3—C4 and lengthening of C4—N4 and C5—C6 bonds in (I). The N3—C4—C5 and C5—C4—N4 bond angles are increased, accompanied by a decrease in the C4—C5—C6 angle.

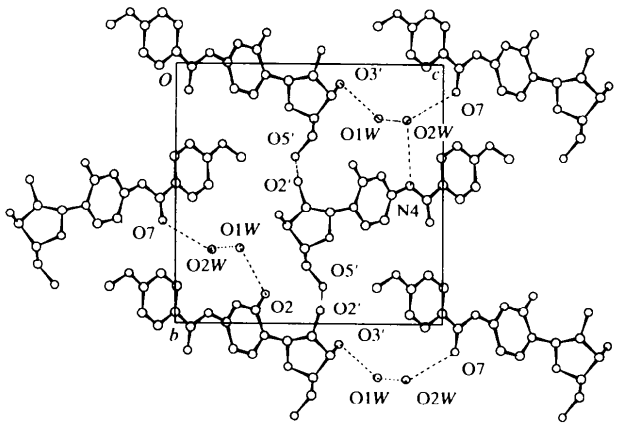


Fig. 2. Packing diagram for (I), viewed down the *a* axis.

Experimental

Crystals of (I) were grown by the diffusion method, from a dimethylformamide–toluene solution of the compound (Sigma Chemical Company, USA).

Crystal data

$C_{17}H_{19}N_3O_7 \cdot 2H_2O$
M_r = 413.38
Monoclinic
$P2_1$
a = 4.851 (2) Å
b = 13.535 (3) Å
c = 14.013 (5) Å
β = 97.28 (1)°
V = 912.7 (5) Å^3
Z = 2
D_x = 1.504 Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
λ = 1.5418 Å
Cell parameters from 25 reflections
θ = 6–20°
μ = 1.052 mm^{-1}
T = 293 (2) K
Needle
1.10 × 0.05 × 0.05 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2046 measured reflections
1864 independent reflections
1682 reflections with $I > 2\sigma(I)$

R_{int} = 0.060
θ_{max} = 71.87°
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 16$
$l = -17 \rightarrow 17$
3 standard reflections
every 100 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.132
S = 1.051
1857 reflections
284 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1042P)^2 + 0.0243P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005

$\Delta\rho_{max}$ = 0.392 e Å^{-3}
$\Delta\rho_{min}$ = −0.219 e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.0053 (16)
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = −0.3 (3)

Table 1. *Selected torsion angles (°)*

C2—N1—C1′—O4′	−158.1 (2)	C2′—C1′—O4′—C4′	−10.2 (3)
O4′—C1′—C2′—C3′	31.9 (3)	C3′—C4′—O4′—C1′	−16.0 (3)
C1′—C2′—C3′—C4′	−39.9 (3)	O4′—C4′—C5′—O5′	61.3 (3)
C2′—C3′—C4′—O4′	34.9 (2)	C3′—C4′—C5′—O5′	179.5 (3)

Table 2. *Hydrogen-bonding geometry (Å, °)*

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O7	0.93	2.29	2.839 (4)	118
N4—H4···O2W^{i}	0.86	2.54	3.374 (5)	165
O1W···O2^{ii}			2.787 (4)	
O1W···N3^{ii}			3.110 (5)	

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Data reduction: *CAD-4 Software*. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *INSIGHT*II (Biosym Technologies, 1995) and *Xtal_GX* (Hall & du Boulay, 1995). Software used to prepare material for publication: *SHELXL*93.

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References

Altona, C. & Sundaralingam, M. (1972). *J. Am. Chem. Soc.* **94**, 8205–8212.
Biosym Technologies (1995). *INSIGHT*II. Biosym Technologies Inc., San Diego, CA 92121-2777, USA.
Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.
Desiraju, G. R. (1996). *Acc. Chem. Res.* **29**, 441–449.
Enraf-Nonius (1989). *CAD-4 Software*. Version 5.0. Enraf-Nonius, Delft, The Netherlands.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Hall, S. R. & du Boulay, D. (1995). *Xtal_GX*. University of Western Australia, Australia.
Jeffrey, G. A. & Saenger, W. (1991). *Hydrogen Bonding in Biological Structures*, pp. 156–160. New York: Springer-Verlag.
Saenger, W. (1984). *Principles of Nucleic Acid Structures*, edited by C. R. Cantor, pp. 16–27. New York: Springer-Verlag.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures*. University of Göttingen, Germany.
Smith, J. L. & Sundaralingam, M. (1981). *Acta Cryst.* B**37**, 1095–1101.