The positions of five H atoms were computed; the remaining H atoms were located from a difference map. The computed H atoms were refined isotropically using a riding model, while the remaining H atoms were refined independently.

Data collection: *CAD-4/PC* (Kretschmar, 1996). Cell refinement: *CAD-4/PC*. Data reduction: *CFEO* (Solans, 1978). Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*b*). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*). Molecular graphics: *ORTEP* (Brueggemann & Schmid, 1990). Software used to prepare material for publication: *PLATON* (Spek, 1990).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GS1024). Services for accessing these data are described at the back of the journal.

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5′-*O*-(Toluenesulfonyl)adenosine

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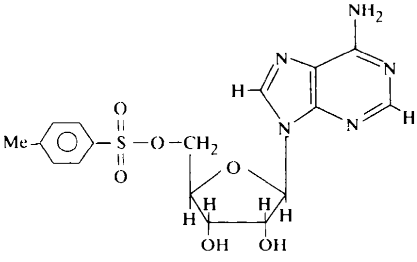
Abstract

The title compound, $C_{17}H_{19}N_5O_6S$, crystallizes from a water–acetone solution. The adenine base is in an *anti* conformation, with a glycosyl torsion angle of −166.5 (4)°. The ribose sugar adopts an envelope conformation (^3E). The toluenesulfonyl moiety is nearly perpendicular to the base. Both Watson–Crick and Hoogsteen sites, N1 and N6, and N6 and N7, of the adenine base are involved in a pair of hydrogen bonds, forming an *A.A.A* triplet pattern in the crystal lattice.

Comment

As part of our systematic X-ray studies on ribose/deoxyribose nucleosides and nucleotides (Padiyar & Seshadri, 1996; Mande *et al.*, 1994; Krishnan & Seshadri, 1992), we report here the crystal structure of 5′-*O*-(toluenesulfonyl)adenosine, (I). We were also interested in studying the effect of the bulky substituent on the conformation of the nucleoside molecule.



(I)

The glycosyl torsion angle [C4—N9—C1′—O4′] of −166.5 (4)° indicates an *anti* conformation. The ribofuranose ring is C3′-*endo* puckered. The pseudorotation parameters (Altona & Sundaralingam, 1972) are P = 19.1° and τ_m = 35.5°. The exocyclic torsion angle about the C4′—C5′ bond is g^+. The toluenesulfonyl moiety is nearly perpendicular to the adenine base.

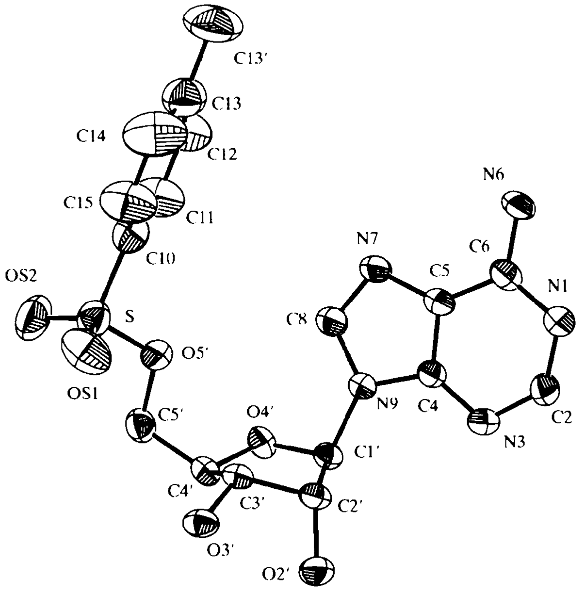


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms are omitted for clarity.

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The adenine base forms a self-pair. The N6 atom in (I) is hydrogen-bonded to atoms N1 and N7 of symmetry-related molecules. Thus, both the Watson–Crick and the Hoogsteen sites of adenine are occupied, giving rise to an *A.A.A* base triplet. A similar base-pairing pattern has been observed in other structures containing adenine, such as 8-bromo-2′,3′-*O*-isopropylidine adenosine (Fujii *et al.*, 1976), 2′-deoxyadenosine (Radwan & Wilson, 1979) and 2′-*O*-methyladenosine (Prusiner & Sundaralingam, 1976). The ribose hydroxyl O3′ atom forms a hydrogen bond with atom N3 of a symmetry-related molecule in the unit cell. The toluenesulfonyl moieties stack partially along the *a* axis in the crystal lattice. The hydrogen-bonding geometry is summarized in Table 2.

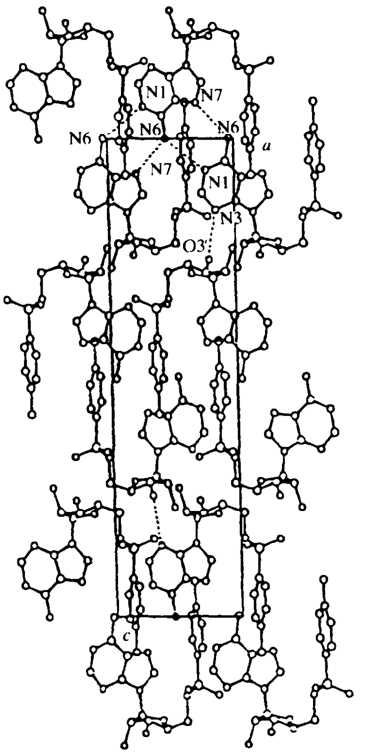

Fig. 2. Packing diagram of (I), viewed along the *b* axis, illustrating the *A.A.A* base-pairing pattern.

Experimental

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

Crystal data

$C_{17}H_{19}N_5O_6S$
$M_r = 421.43$
Orthorhombic
$P2_12_12_1$
$a = 8.045\ (2)$ Å
$b = 8.937\ (2)$ Å
$c = 26.773\ (3)$ Å
$V = 1924.9\ (7)$ Å^3
$Z = 4$
$D_x = 1.454$ Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
$\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 6\text{–}12°$
$\mu = 1.912$ mm^{-1}
$T = 293\ (2)$ K
Parallelepiped
0.35 × 0.25 × 0.20 mm
Colourless

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.627$, $T_{\max} = 0.682$
1960 measured reflections
1960 independent reflections

1573 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 69.96°$
$h = 0 \rightarrow 9$
$k = 0 \rightarrow 10$
$l = 0 \rightarrow 32$
3 standard reflections frequency: 60 min intensity decay: none

Refinement

Refinement on F^2
$R(F) = 0.039$
$wR(F^2) = 0.115$
$S = 1.049$
1960 reflections
285 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.1143P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = -0.001$
$\Delta\rho_{\max} = 0.267$ e Å^{-3}
$\Delta\rho_{\min} = -0.230$ e Å^{-3}
Extinction correction: none
Scattering factors from *International Tables for Crystallography* (Vol. C)
Absolute structure: Flack (1983)
Flack parameter = −0.08 (4)

Table 1. *Selected torsion angles (°)*

O4′—C1′—C2′—C3′	−21.4 (4)	C3′—C4′—C5′—O5′	53.2 (5)
C1′—C2′—C3′—C4′	33.5 (3)	C4′—C5′—O5′—S	−142.8 (3)
C2′—C3′—C4′—O4′	−34.8 (4)	C5′—O5′—S—C10	−170.0 (3)
C2′—C1′—O4′—C4′	−0.1 (4)	O5′—S—C10—C11	50.8 (6)
C3′—C4′—O4′—C1′	22.2 (4)	O5′—S—C10—C15	−132.5 (5)
O4′—C4′—C5′—O5′	−65.7 (4)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N6—H61···N7^{i}	0.860 (6)	2.082 (6)	2.937 (6)	172.2 (5)
N6—H62···N1^{ii}	0.860 (6)	2.310 (6)	3.131 (6)	159.8 (5)
O3′—HO3′···N3^{iii}	0.859 (4)	1.990 (5)	2.826 (4)	170.1 (2)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{5}{2} - y, -z$; (ii) $\frac{1}{2} + x, \frac{5}{2} - y, -z$; (iii) $-x, y - \frac{1}{2}, \frac{1}{2} - z$.

All H atom coordinates were refined, but not the occupancies or *U* values, as riding on the coordinates of the parent atom.

Data collection: *CAD-4 Diffractometer Control Software* (Enraf–Nonius, 1985*a*). Cell refinement: *CAD-4 Diffractometer Control Software*. Data reduction: *Structure Determination Package* (Enraf–Nonius, 1985*b*). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *INSIGHTII* (Biosym Technologies, 1995) and *Xtal_GX* (Hall & du Boulay, 1995). Software used to prepare material for publication: *SHELXL93*.

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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.

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N^4-Anisoylcytidine dihydrate

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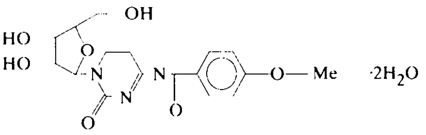
Abstract

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* [$\chi = -158.1\,(2)°$] 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).

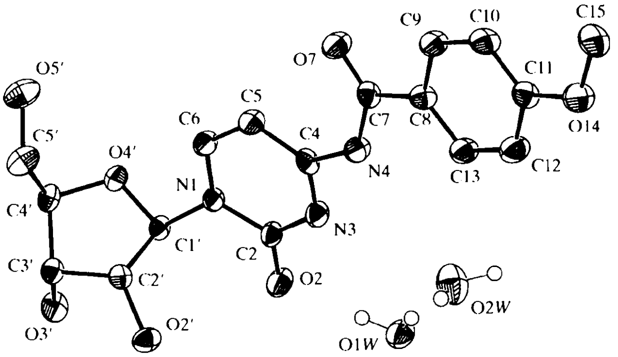


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme and 50% probability displacement ellipsoids. H atoms are omitted for clarity, except for those on the two water molecules which are drawn as circles of an arbitrary radius.

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

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