

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

C₁₈H₁₉N₅O₆·H₂O

M_r = 419.40

Monoclinic

*P*2₁

a = 9.412 (2) Å

b = 6.914 (1) Å

c = 14.667 (2) Å

β = 102.89 (2)°

V = 930.4 (3) Å³

Z = 2

D_x = 1.497 Mg m⁻³

D_m not measured

Cu Kα radiation

λ = 1.5418 Å

Cell parameters from 25 reflections

θ = 8–25°

μ = 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 > 2σ(*I*)

*R*_{int} = 0.021

θ_{max} = 72.90°

h = 0 → 11

k = 0 → 8

l = –18 → 17

3 standard reflections

every 100 reflections

intensity decay: none

Refinement

Refinement on *F*²

R[*F*² > 2σ(*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/[σ²(*F*_o²) + (0.1*P*)²]

where *P* = (*F*_o² + 2*F*_c²)/3

(Δ/σ)_{max} = 0.004

Δρ_{max} = 0.303 e Å⁻³

Δρ_{min} = –0.186 e Å⁻³

Extinction correction:

SHELXL93 (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: *SIR97* (Altomare *et al.*, 1997). Program(s) used to refine structure: *SHELXL93* (Sheldrick, 1993). Molecular graphics: *Xtal.GX* (Hall & du Boulay, 1995). Software used to prepare material for publication: *SHELXL93*.

We thank DST and CSIR, India, for financial assistance.

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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N³-Benzoyl-2',3'-di-O-benzoyluridine

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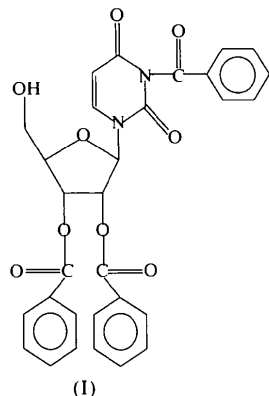
(Received 2 June 1998; accepted 19 November 1998)

Abstract

The structure of *N*³-benzoyl-2',3'-di-*O*-benzoyluridine, C₃₀H₂₄N₂O₉, 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.

Comment

The aim of the work is to study the effect of aromatic substituents on the structure of pyrimidine nucleosides and has been taken up as a sequel to our earlier studies



on modified purine nucleosides (Kolappan & Seshadri, 1999a). In the title compound, (I), the uracil bases are in the *anti* conformation with respect to the ribose moiety.

This contrasts with the *syn* geometry of the guanine base in 2',3',5'-tri-*O*-benzoylguanosine (Kolappan & Seshadri, 1999b). The furanosyl ring adopts a C3'-*endo* envelope pucker in both molecules *A* and *B* with pseudo-rotation angles of 10.6 and 15.7°, respectively. The maximum angles of pucker (Altona & Sundaralingam, 1972; Saenger, 1984) are 37.9 and 34.9° for *A* and *B*, respectively. The phenyl rings covalently linked to the uracil base at N3 are inclined at 74.5 and 86.9° to it. The phenyl rings at O2' and O3' are oriented at 51.5 and 75.5° with respect to each other and are separated by 6.8 and 5.7 Å in *A* and *B*, respectively. This is similar to the geometry seen in 2',3',5'-tri-*O*-benzoylguanosine and inosine (Kolappan & Seshadri, 1998c). The two nucleoside molecules *A* and *B* in the asymmetric unit are linked by several weak hydrogen bonds (Desiraju, 1996). The phenyl rings at O2' in the two molecules overlap at a separation of 3.7 Å. Nucleoside molecules pack as columns along the *a* axis and these columns repeat along the *c* axis. Also, there is partial overlapping of phenyl rings at O3' at a separation of 3.78 Å along the *a* axis.

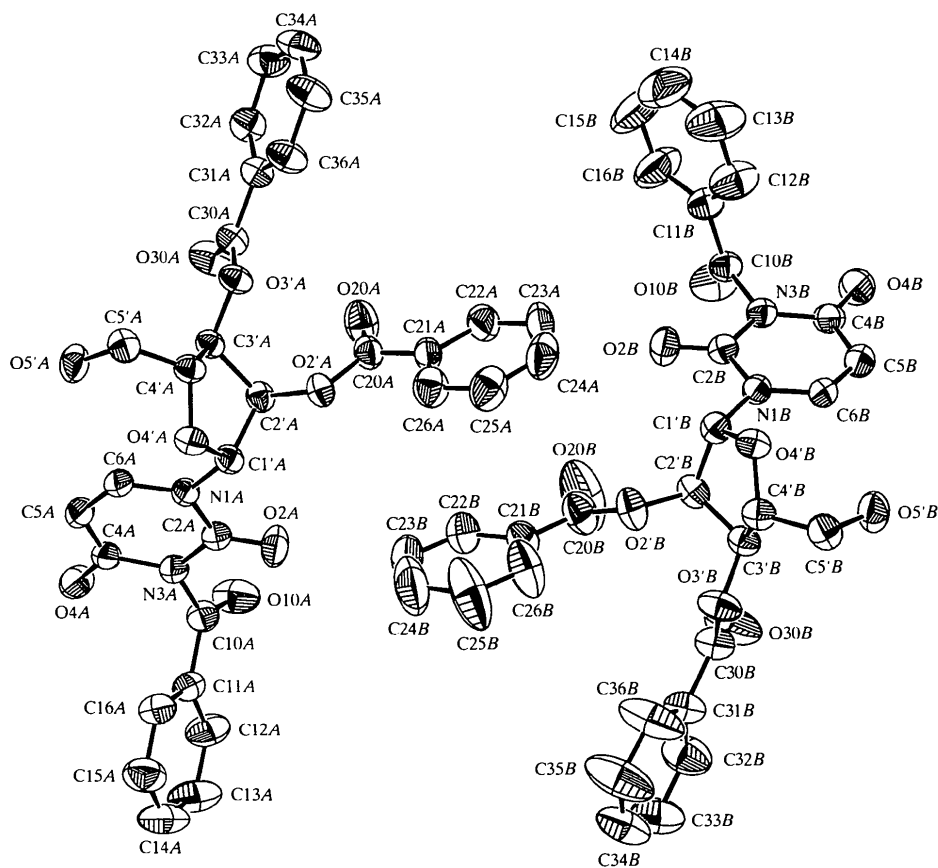


Fig. 1. The molecular structure of (I) showing 50% probability displacement ellipsoids. H atoms are omitted for clarity.

Experimental

The title compound was obtained from the Sigma Chemical Company. Crystals were grown by the diffusion method from an aqueous acetonitrile solution of the compound.

Crystal data

C ₃₀ H ₂₄ N ₂ O ₉	Cu K α radiation
$M_r = 556.51$	$\lambda = 1.5418 \text{ \AA}$
Monoclinic	Cell parameters from 25 reflections
$P2$	$\theta = 10\text{--}25^\circ$
$a = 14.202 (2) \text{ \AA}$	$\mu = 0.855 \text{ mm}^{-1}$
$b = 5.737 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 33.319 (5) \text{ \AA}$	Plate
$\beta = 92.93 (2)^\circ$	$0.90 \times 0.20 \times 0.05 \text{ mm}$
$V = 2711.5 (15) \text{ \AA}^3$	Colourless
$Z = 4$	
$D_x = 1.363 \text{ Mg m}^{-3}$	
D_m not measured	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{\text{int}} = 0.032$
ω - 2θ scans	$\theta_{\text{max}} = 69.9^\circ$
Absorption correction: none	$h = 0 \rightarrow 16$
6192 measured reflections	$k = 0 \rightarrow 6$
5536 independent reflections	$l = -40 \rightarrow 40$
4265 reflections with $I > 2\sigma(I)$	3 standard reflections every 100 reflections
	intensity decay: none

Refinement

Refinement on F^2	Extinction correction:
$R[F^2 > 2\sigma(F^2)] = 0.041$	<i>SHELXL93</i> (Sheldrick, 1993)
$wR(F^2) = 0.117$	Extinction coefficient:
$S = 1.055$	0.0016 (3)
5491 reflections	Scattering factors from <i>International Tables for Crystallography</i> (Vol. C)
789 parameters	Absolute structure: Flack (1983)
H atoms constrained	Flack parameter = 0.15 (22)
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$	
where $P = (F_o^2 + 2F_c^2)/3$	
$(\Delta/\sigma)_{\text{max}} = 0.009$	
$\Delta\rho_{\text{max}} = 0.278 \text{ e \AA}^{-3}$	
$\Delta\rho_{\text{min}} = -0.235 \text{ e \AA}^{-3}$	

Table 1. Selected torsion angles ($^\circ$)

C2A–N1A–C1'A–O4'A	–154.8 (3)
O4'A–C1'A–C2'A–C3'A	–27.1 (3)
C1'A–C2'A–C3'A–C4'A	37.5 (3)
C2'A–C3'A–C4'A–O4'A	–35.1 (3)
C2'A–C1'A–O4'A–C4'A	5.5 (3)
C3'A–C4'A–O4'A–C1'A	18.9 (3)
O4'A–C4'A–C5'A–O5'A	–60.8 (4)
C3'A–C4'A–C5'A–O5'A	56.7 (4)
C2B–N1B–C1'B–O4'B	–156.8 (3)
O4'B–C1'B–C2'B–C3'B	–22.7 (3)
C1'B–C2'B–C3'B–C4'B	34.1 (3)
C2'B–C3'B–C4'B–O4'B	–34.1 (3)
C2'B–C1'B–O4'B–C4'B	1.5 (3)
C3'B–C4'B–O4'B–C1'B	20.8 (3)
O4'B–C4'B–C5'B–O5'B	–62.3 (4)
C3'B–C4'B–C5'B–O5'B	55.4 (4)

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Data reduction: *CAD-4 Software*. Program(s) used to solve struc-

ture: *SHELXS86* (Sheldrick, 1990). 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*.

We thank DST and CSIR, India, for financial assistance.

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2'-O-Tosyladenosine

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Abstract

In the title compound, 2'-O-tosyl(toluenesulfonyl)-adenosine, C₁₇H₁₉N₅O₆S, the adenine base is in the *syn* conformation with a glycosidic torsion angle of 62.7 (4) $^\circ$. The ribose sugar adopts the envelope conformation (2E). The tosyl moiety is nearly parallel to the base. Both Watson–Crick and Hoogsteen sites of the adenine bases are involved in intermolecular hydrogen bonds.