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# 2′,3′,5′-Tri-*O*-benzoylinosine

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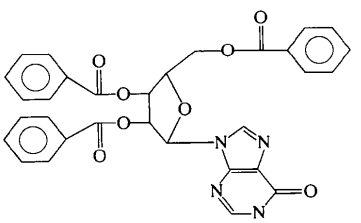
## Abstract

The title compound, $C_{31}H_{24}N_4O_8$, adopts a conformation generally consistent with those of published ribonucleoside crystal structures. The orientation of the base with respect to the furanose ring is *anti* [$\chi = -93.9\,(3)°$] and has a C3′-*endo*,C2′-*exo* twist. The geometry about the exocyclic C4′—C5′ bond is *gauche–gauche*.

## Comment

This investigation of the title compound, (I), is part of our structural studies on modified nucleosides and nucleotides (Krishnan & Seshadri, 1992; Prahadeeswaran & Seshadri, 1999). The presence of bulky moieties at the 2′, 3′ and 5′ positions of the ribose moiety modifies the hydrogen-bond donor–acceptor properties of the nucleotide. It is therefore interesting to study the effect of this bulky substitution on the conformation and hydrogen-bonding pattern of this nucleoside.



(I)

The inosine base in (I) is essentially planar and its conformation with respect to the furanose ring is *anti* with the glycosidic torsion angle $\chi$ (O4′—C1′—N9—C4) = $-93.9\,(3)°$, whereas the guanosine base is in the *syn* region in the 2′,3′,5′-tri-*O*-benzoylguanosine structure, with $\chi = -78.4\,(4)°$. The furanose ring assumes a C3′-*endo*,C2′-*exo* twist conformation with pseudorotation angle $P = 3.8°$ and a maximum amplitude of pucker of 22.1° (Altona & Sundaralingam, 1972; Saenger, 1984), similar to that in the 2′,3′,5′-tri-*O*-benzoylguanosine structure. The torsion angles $\varphi_{OO}$ (O5′—C5′—C4′—O4′) and $\varphi_{OC}$ (O5′—C5′—C4′—C3′) are $-65.4\,(3)$ and $55.6\,(3)°$, respectively, which shows that the conformation about the C4′—C5′ bond is *gauche–gauche*. It is noted that, despite the bulky aromatic group at the 5′ position, the nucleoside is in the $g^+$ conformation. The benzoyl groups attached to atoms O2′ and O3′ are not parallel, but inclined to each other at 77.0°. The inosine base is at 77.4° to the benzoyl ring attached to O5′. Hypoxanthine bases of two symmetry-related molecules form a pair of hydrogen bonds (N1—H···N7 and C2—H···O6) with an angle of 52° between them. A similar hydrogen-bonding pattern has been observed in the crystal structure of 2′,3′-*O*-isopropylideneinosine (Mande *et al.*, 1992), but the bases are nearly coplanar. The atoms C8 and C3′ form weak hydrogen bonds with O4′. The nucleoside molecules form infinite columns along the *b* axis and these columns repeat along the *c* axis. The packing of the 2′,3′,5′-tri-*O*-benzoylguanosine molecules is significantly different from that of the title compound.

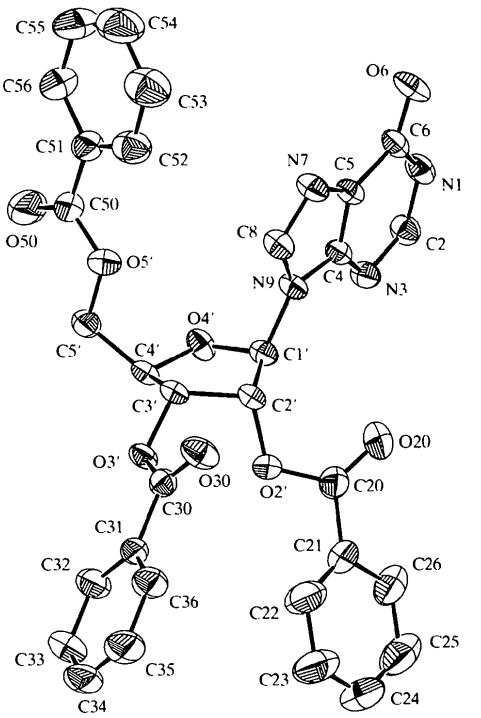



Fig. 1. The molecular structure of (I) showing 50% probability displacement ellipsoids.

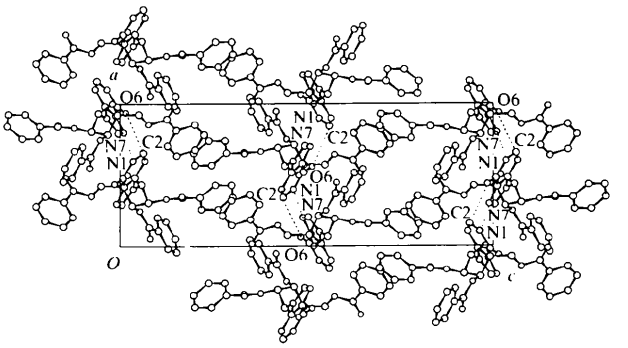



Fig. 2. Packing diagram viewed down the *a* axis.

## Experimental

Crystals were grown by diffusion of an acetonitrile solution of the title compound into water.

*Crystal data*

$C_{31}H_{24}N_4O_8$
$M_r$ = 580.54
Orthorhombic
$P2_12_12_1$
$a$ = 9.849 (2) Å
$b$ = 10.800 (2) Å
$c$ = 25.682 (3) Å
$V$ = 2731.8 (8) Å$^3$
$Z$ = 4
$D_x$ = 1.412 Mg m$^{-3}$
$D_m$ not measured

Cu $K\alpha$ radiation
$\lambda$ = 1.54180 Å
Cell parameters from 25 reflections
$\theta$ = 5–22°
$\mu$ = 0.868 mm$^{-1}$
$T$ = 293 (2) K
Plate
0.60 × 0.10 × 0.05 mm
Colourless

*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$–2$\theta$ scans
Absorption correction: none
3148 measured reflections
3026 independent reflections
2527 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.016
$\theta_{max}$ = 72.95°
$h = 0 \rightarrow 11$
$k = 0 \rightarrow 13$
$l = 0 \rightarrow 31$
3 standard reflections
every 100 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.117
$S$ = 0.691
3026 reflections
413 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1326P)^2 + 0.8103P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.023
$\Delta\rho_{max}$ = 0.164 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.166 e Å$^{-3}$
Extinction correction: *SHELXL*97 (Sheldrick, 1997*b*)
Extinction coefficient: 0.0032 (4)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Hydrogen-bonding geometry (Å, °)*

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···N7$^i$ | 0.86 | 2.15 | 2.956 (3) | 157 |
| C2—H2···O6$^i$ | 0.93 | 2.56 | 3.057 (4) | 114 |

Symmetry code: (i) $\frac{1}{2} + x, \frac{3}{2} - y, -z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Data reduction: *CAD-4 Software*. Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*b*). Molecular graphics: *INSIGHT*II (Biosym Technologies, 1995) and *Xtal_GX* (Hall & du Boulay, 1995). Software used to prepare material for publication: *SHELXL*97.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1094). Services for accessing these data are described at the back of the journal.

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# 1-Acetyl-5-(4-methoxyphenyl)-3-(4-methoxystyryl)-2-pyrazoline and 1-acetyl-5-(2-chlorophenyl)-3-(2-chlorostyryl)-2-pyrazoline

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## Abstract

The structural details of two methoxy- and chloro-substituted pyrazoline derivatives ($C_{21}H_{22}N_2O_3$ and $C_{19}H_{16}Cl_2N_2O$, respectively) are presented. The two structures show considerable differences in the orientation of the phenyl ring attached to the heterocyclic ring. While the packing of the molecules in the methoxy-substituted derivative is characterized by a C—H···O hydrogen bond, the packing in the chloro-substituted derivative is characterized by short Cl···Cl contacts and C—H···Cl intramolecular hydrogen bonds.

## Comment

Pyrazolines are known to exhibit important biological and industrial properties (Wang *et al.*, 1995; El-