Discussion. The atomic coordinates and thermal parameters of the non-H atoms are given in Table 1. Fig. 1 depicts a perspective view of the molecule with its atom numbering. The unit-cell contents are presented in Fig. 2. The interatomic bond distances and angles are summarized in Table 2. The most conspicuous features of the structure are two inter- and two intramolecular symmetrically independent hydrogen bridges between the amidine nitrogens and the carboxylic oxygens. The intramolecular bridges are realized through H1N1 and H1N2 and intermolecular contacts are mediated by H2N1 and H2N2 hydrogens. Intermolecular hydrogen bonds give rise to infinite chains of molecules parallel to the **c** direction and thus form the arrangement of the structure. The chains are interconnected by van der Waals forces. A comparison of the N···O contacts in the title compound with the structures of methylguanidinium formate and L-arginine dihydrate shows no significant differences in bond lengths. Atoms of the amidine group (H1N1, N1, C4, N2 and H1N2) are situated nearly in one plane with a maximum deviation of 0·032 (2) Å for N2. This plane deviates from that of the benzene ring by 35·2 (3)°. The torsion angle C6—C5—C4—N2 is 35·1° and C10—C5—C4—N1 is 36·5 (2)°. The differences between N1···O1 and N2···O2 distances are due to the influence of the C2=O3 group in the pyruvic acid moiety. The same effect is probably responsible for the mutual orientation of amidine and carboxylic planes. The angle between the H1N1, N1, C4, N2, H1N2 and the H1N1, O1, C1, O2, H1N2 planes is 5·6 (3)°. The torsion angles O3—C2—C1—O2 and O3—C2—C1—O1 are 5·8 (3) and 5·2 (2)° respectively.

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Structure of 3′-*O*-Acetyl-2′-deoxyadenosine

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Abstract. $C_{12}H_{15}N_5O_4$, $M_r = 293\cdot3$, monoclinic, $P2_1$, $a = 8\cdot363\,(9)$, $b = 7\cdot33\,(1)$, $c = 11\cdot52\,(1)$ Å, $\beta = 106\cdot8\,(9)°$, $U = 676$ Å^3, $Z = 2$, $D_x = 1\cdot44$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0\cdot71069$ Å, $\mu = 0\cdot7$ mm^{-1}, $F(000) = 308$, $T = 293$ K, $R = 0\cdot044$ for 1901 unique observed $[F > 3\sigma(F)]$ reflections. The molecule is *anti*, with χ(C4—N9—C1′—O4′) = −165·7 (3)°, has sugar pucker $_3E$, with $P = 197°$, and C4′—C5′ conformation of +*sc* (*gauche–gauche*). The structure has base-paired symmetry-related molecules, with hydrogen bonds between the 6-amino group and N1 and N7. The structure differs from that of 3′-*O*-acetyladenosine [Rao & Sundaralingam (1970). *J. Am. Chem. Soc.* **92**, 4963–4970] in which there is no interbase hydrogen bonding. The base-pair shows a propeller twist, defined as the angle between the base planes about a line joining them, of 28°. There is also a hydrogen bond between N3 and O5′ of a symmetry-related molecule, similar to that found for 3′-*O*-acetyladenosine, with N···O = 2·811 (4), N···H = 1·847 Å and N···H—O = 153·2 (2)°.

Introduction. The structural study was undertaken in continuation of our studies of acetylated nucleosides, induced base-pairing and studies of propeller-twisting in mononucleoside crystals.

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Experimental. Crystals were obtained from aqueous solution. Space group and initial cell dimensions were obtained from Weissenberg photographs. Data were collected on a Nicolet *P*3 (four-circle) diffractometer in Aberdeen by RAH. The crystal was of cubic shape with sides of 0·5 mm. Cell parameters were measured on the diffractometer using the $50\bar{6}$, 034, 322, $31\bar{5}$ and their symmetry-related reflections ($20 < 2\theta < 30°$). Range of indices: $0 \leq h \leq 11$; $0 \leq k \leq 10$; $-15 \leq l \leq 15$. Data measured using $\theta/2\theta$ scans in the range $0 < 2\theta < 60°$. Standard reflections 034 and 322 were measured every 50 reflections. No significant change in the intensities of these reflections was found throughout data collection. 2056 independent reflections measured, giving 1901 observed [$F > 3\sigma(F)$] reflections used in the refinement. The 013 reflection for which no reliable measurement was obtained is included as one of the unobserved. No absorption or extinction corrections were made. The structure was solved using the direct-methods package *MITHRIL* (Gilmore, 1983). The *E* map with the highest combined figure of merit revealed all non-hydrogen atoms except C5′ and O5′. Fourier recycling completed the definition of the structure. Refinement (on *F*) was carried out using the program *SHELX*76 (Sheldrick, 1976). The positions of

Table 1. *Coordinates* ($\times 10^4$) *for non-hydrogen atoms with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}\textstyle\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i . \mathbf{a}_j .$$

	x	y	z	U_{eq}(Å$^2 \times 10^3$)
N1	8084 (2)	1130	−1343 (2)	41 (1)
C2	6483 (3)	1580 (5)	−1878 (2)	45 (1)
N3	5119 (2)	579 (4)	−2012 (2)	41 (1)
C4	5495 (2)	−1097 (4)	−1540 (2)	32 (1)
C5	7087 (2)	−1762 (4)	−966 (2)	33 (1)
C6	8428 (2)	−555 (4)	−862 (2)	34 (1)
N6	10020 (2)	−988 (4)	−307 (2)	42 (1)
N7	7008 (2)	−3546 (4)	−596 (2)	42 (1)
C8	5411 (3)	−3939 (5)	−946 (2)	42 (1)
N9	4434 (2)	−2517 (4)	−1518 (2)	36 (1)
C1′	2611 (2)	−2534 (5)	−2089 (2)	38 (1)
C2′	2135 (3)	−2834 (5)	−3452 (2)	40 (1)
C3′	487 (2)	−3844 (4)	−3687 (2)	37 (1)
O3′	−803 (2)	−2479 (4)	−3840 (1)	43 (1)
C3′1	−2379 (3)	−3119 (5)	−4219 (2)	46 (1)
C3′2	−3628 (3)	−1600 (6)	−4422 (3)	62 (1)
O3′1	−2704 (3)	−4710 (5)	−4362 (3)	72 (1)
C4′	688 (2)	−4939 (5)	−2523 (2)	37 (1)
O4′	1989 (2)	−4035 (4)	−1596 (1)	47 (1)
C5′	1141 (3)	−6926 (5)	−2618 (3)	49 (1)
O5′	2487 (3)	−7048 (5)	−3139 (2)	73 (1)

Table 2. *Interatomic distances* (Å) *and angles* (°)

C2—N1	1·344 (3)	C6—N1—C2	118·6 (2)
C6—N1	1·350 (3)	N3—C2—N1	128·8 (2)
N3—C2	1·328 (3)	C4—N3—C2	111·4 (2)
C4—N3	1·343 (3)	C5—C4—N3	126·3 (2)
C5—C4	1·392 (3)	N9—C4—N3	128·6 (2)
N9—C4	1·373 (3)	N9—C4—C5	105·1 (2)
C6—C5	1·406 (3)	C6—C5—C4	116·8 (2)
N7—C5	1·383 (3)	N7—C5—C4	110·7 (2)
N6—C6	1·338 (3)	N7—C5—C6	132·5 (2)
C8—N7	1·311 (3)	C5—C6—N1	118·0 (2)
N9—C8	1·370 (3)	N6—C6—N1	118·5 (2)
C1′—N9	1·476 (2)	N6—C6—C5	123·4 (2)
C2′—C1′	1·521 (3)	C8—N7—C5	104·3 (2)
O4′—C1′	1·405 (3)	N9—C8—N7	113·2 (2)
C3′—C2′	1·518 (3)	C8—N9—C4	106·7 (2)
O3′—C3′	1·444 (3)	C1′—N9—C4	126·0 (2)
C4′—C3′	1·530 (3)	C1′—N9—C8	127·2 (2)
C3′1—O3′	1·348 (3)	C2′—C1′—N9	113·0 (2)
C3′2—C3′1	1·497 (4)	O4′—C1′—N9	106·3 (2)
O3′1—C3′1	1·197 (4)	O4′—C1′—C2′	106·7 (2)
O4′—C4′	1·446 (3)	C3′—C2′—C1′	102·0 (2)
C5′—C4′	1·516 (4)	O3′—C3′—C2′	106·9 (2)
O5′—C5′	1·424 (3)	C4′—C3′—C2′	103·6 (2)
C4′—C3′—O3′	111·1 (2)		
C3′1—O3′—C3′	115·1 (2)		
C3′2—C3′1—O3′	111·4 (3)		
O3′1—C3′1—O3′	123·1 (3)		
O3′1—C3′1—C3′2	125·5 (3)		
O4′—C4′—C3′	106·1 (2)		
C5′—C4′—C3′	114·0 (2)		
C5′—C4′—O4′	110·1 (2)		
C4′—O4′—C1′	110·3 (2)		
O5′—C5′—C4′	109·6 (2)		

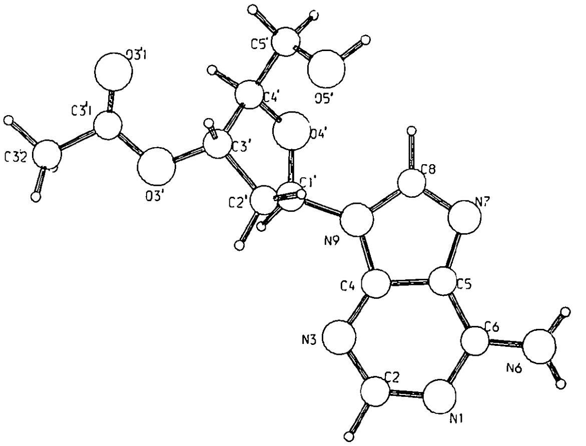

Fig. 1. View of the molecule with atom numbering.

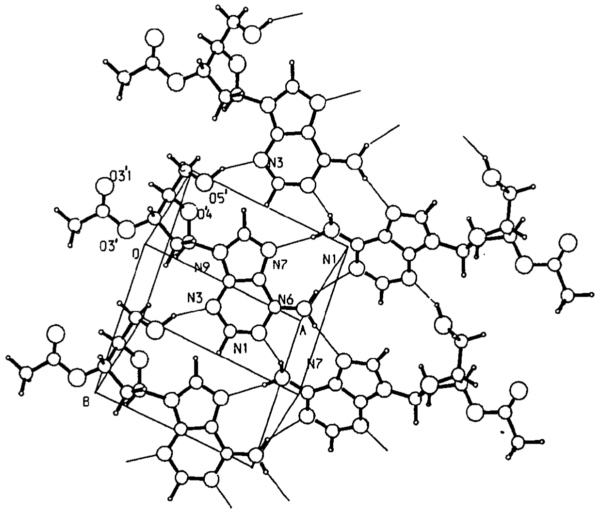

Fig. 2. Perspective view of the unit cell showing the hydrogen bonding.

the H atoms attached to N6 and O5′ were obtained from a difference Fourier map and their positions fixed after constrained refinement. The other H atoms were included at calculated positions. All H atoms were given fixed isotropic temperature factors of approximately 1·5 times that of the parent atom. Anisotropic temperature factors were used for all non-hydrogen atoms, and the refinement converged at $R = 0{\cdot}044$, $wR = 0{\cdot}060$, $w = 0{\cdot}9675/[\sigma^2(F) + 0{\cdot}001669F^2]$. 189 refined parameters; max. shift/e.s.d. $< 0{\cdot}05$; max. difference peak, 0·24, min. difference peak $-0{\cdot}23$ e Å^{-3}.

Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). The program packages *XANADU* (Roberts & Sheldrick, 1975) and *PLUTO* (Motherwell & Clegg, 1978) were also used. All calculations were carried out on the Dundee University DEC-10 computer.

Discussion. The atomic numbering is shown in the perspective drawing (Fig. 1), and tables of atomic parameters, bond lengths and angles are given (Tables 1 and 2).* The *N*-glycosidic torsion angle χ has value $-165{\cdot}7$ (1)°, in the *anti* range. The sugar pucker is $_3E$ (C3′-*exo*), with $P = 197$ (1)°, and $\psi_m = 21$ (1)°. The C4′—C5′ conformation, with $\gamma = 48{\cdot}3$ (3) and $\gamma' = -70{\cdot}7$ (3)°, is +*sc* (*gauche–gauche*). The conformational parameters used follow the guidelines of the IUPAC–IUB Joint Commission on Biochemical Nomenclature (1983). There are three hydrogen bonds present in the structure (see Fig. 2); N6—(0·894 Å)—H61···(2·134 Å)···N1($2-x$, $y-\frac{1}{2}$, $-z$) 2·974 (4) Å, H angle 156·2 (2)°; N6—(0·896 Å)—H62···(2·106 Å)···N7($2-x$, $\frac{1}{2}+y$, $-z$) 2·994 (4) Å, H angle 170·9 (2)° and O5′—(1·036 Å)—H5′···(1·847 Å)···N3(x, $y-1$, z) 2·811 (4) Å, H angle 153·2 (2)°. The bases are thus self base-paired in ribbons as in 2′,3′,5′-tri-*O*-acetyladenosine (Wilson, Tollin & Howie, 1986) and 8-bromo-2′,3′,5′-tri-*O*-acetyladenosine (Boyd, Low & Tollin, 1987). There is a propeller twist (Dickerson, 1983) of 28° between the planes of the two paired bases. This large propeller twist fits into the pattern observed for self-base-paired adenine bases (Wilson & Tollin, 1987).

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44180 (17 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of Hexamethyl Benzenehexacarboxylate

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Abstract. $C_{18}H_{18}O_{12}$, $M_r = 426{\cdot}33$, triclinic, $P\bar{1}$, $a = 11{\cdot}233$ (1), $b = 18{\cdot}940$ (1), $c = 10{\cdot}341$ (1) Å, $\alpha = 92{\cdot}29$ (1), $\beta = 105{\cdot}59$ (1), $\gamma = 75{\cdot}98$ (1)°, $U = 2055{\cdot}3$ (3) Å^3, $Z = 4$, $D_x = 1{\cdot}38$ Mg m^{-3}, λ(Cu $K\alpha$) $= 1{\cdot}5418$ Å, μ(Cu $K\alpha$) $= 0{\cdot}981$ mm^{-1}, $F(000) = 888$. Final $R = 0{\cdot}067$ for 4662 reflexions. The two symmetry-independent molecules present the same geometry in terms of bond lengths and angles, but

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