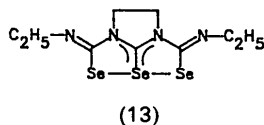(1.97 Å). These data indicate that the N(1)=C(1) and N(4)=C(3) bonds are not appreciably conjugated with the attached pairs of heteroatoms N(2), Se(1) and N(3), Se(3), respectively. The molecule of (8) can therefore be represented approximately by (13).

(13)

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Structure of a Covalently Linked Cross-Section Representative of a Hydrogen-Bonded dA·dT Base Pair

BY BALKRISHEN BHAT, SCOTT R. WILSON AND NELSON J. LEONARD*

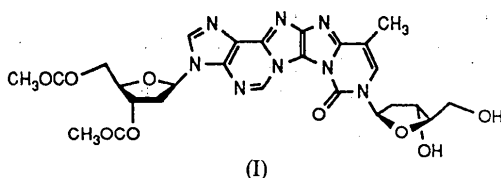*School of Chemical Sciences, University of Illinois, 1209 West California Street, Urbana, Illinois 61801-3731, USA*

Abstract. 3-(3′,5′-Di-O-acetyl-2′-deoxy-β-D-ribofuranosyl)-9-(2′-deoxy-β-D-ribofuranosyl)-11-methyl-3H-pyrimido[1″,6″:1′,2′]imidazo[4′,5′:4,5]imidazo-[2,1-i]purin-8(9H)-one acetonitrile solvate monohydrate, $C_{26}H_{28}N_8O_9 \cdot C_2H_3N \cdot H_2O$, $M_r = 655.63$ (596.56 + 41.05 + 18.02), monoclinic, $P2_1$, $a = 5.659$ (2), $b = 15.097$ (3), $c = 17.138$ (5) Å, $\beta = 96.73$ (3)°, $V = 1454$ (1) Å^3, $Z = 2$, $D_x = 1.497$ g cm^{-3}, $\lambda(\text{Mo }K\overline{\alpha}) = 0.71073$ Å, $\mu = 1.09$ cm^{-1}, $F(000) = 688$, $T = 198$ K, $R = 0.054$ and $wR = 0.056$ for 1532 observed reflections. The atoms of the central five-ring heteroaromatic array are coplanar with a root-mean-square deviation of ± 0.03 Å. The torsion angle of the glycosidic linkage, C(3a)—N(3)—C(1′)—O(1′), for attachment at the purine-N, is −174.4 (7)°, and the angle C(8)—N(9)—C(1″)—O(1″), for attachment at the pyrimidine-N, is −159.3 (7)°. Both are in the *anti* range. The N(12)···N(13) distance is 2.56 (1) Å, compared with the N—H···O distance of 2.85 Å in a dA·dT Watson–Crick base pair, and the N(6)···N(7) distance is 2.609 (10) Å, *cf.* N···H—N of 2.9 Å. Thus, compound (1) is a spatial mimic of a Watson–Crick double-helical dA·dT cross section. The sugar puckers are ^2E (C2′-*endo*), with $P = 169.8$ and $\tau_m = 37.2$, and ^3E (C3′-*endo*), with $P = 16.0$ and $\tau_m = 38.9$. Intermolecular hydrogen bonding in the crystal occurs between H(O5″) of one molecule and N(13) of an adjacent molecule, and likewise between H(O3″) and N(12) of the second.

Introduction. We have introduced the concept of covalently linked double-helical cross sections that are representative of A·U, dA·dU and dA·U duplexes (Devadas & Leonard, 1986, 1990). While comparison of the overall geometry of a Watson–Crick

$C_{26}H_{28}N_8O_9.C_2H_3N.H_2O$

A·U (dA·dT) base pair with that calculated from components of a double-helical cross section containing a 1,3,4,6-tetraazapentalene linking system showed close similarity, it was desirable to establish the validity of this comparison by means of an X-ray crystal-structure determination. One of the compounds we have synthesized for further investigation of the ligation, with T4 RNA ligase, of an oligodeoxyribonucleotide to covalently linked cross-sectional base-pair analogues (Petrič, Bhat, Leonard & Gumport, 1991), formed crystals that were satisfactory for structure analysis by X-ray diffraction. The compound is 3-(3',5'-di-O-acetyl-2'-deoxy-β-D-ribofuranosyl)-9-(2'-deoxy-β-D-ribofuranosyl)-11-methyl-3H-pyrimido[1'',6'':1',2']imidazo[4',5':4,5]-imidazo[2,1-i]purin-8(9H)-one (1) (Bhat & Leonard, 1992).

tions for all non-H atoms were deduced from an E map. Subsequent least-squares refinement and difference Fourier syntheses using the program SHELX76 (Sheldrick, 1976) revealed positions for C-attached H atoms; however, owing to the paucity of data, only the hydroxyl H-atom positions were refined. Solvate H atoms were not included in structure-factor calculations, but the remaining H atoms were included as fixed contributors in 'idealized' positions. In the final cycle of least-squares refinement, anisotropic thermal coefficients were refined for N and O atoms of the main molecule and the acetonitrile N atom [N(41)], isotropic thermal coefficients were refined for the remaining non-H atoms, and a common isotropic thermal parameter was varied for the H atoms. The atomic scattering factors, dispersion corrections and mass-attenuation

(I)

Experimental. Crystals of (1), suitable for X-ray investigations, were grown from 20% MeOH in undried acetonitrile at room temperature. A transparent colorless columnar crystal of approximately 0.1 × 0.2 × 0.4 mm was used for data collection on an Enraf–Nonius CAD-4 automated κ-axis diffractometer with graphite-monochromated Mo $K\alpha$ radiation. The crystal was mounted using oil (Paratone-N, Exxon) on a thin glass fiber and cooled to 198 K. The (10$\bar{2}$) scattering planes were approximately normal to the spindle axis. The crystal was bound approximately by {001}, {010} and {100}, and distances from the crystal center to these facial boundaries were 0.05, 0.09 and 0.24 mm, respectively. The lattice parameters were refined using 25 reflections with 2θ values between 16.2 and 23.9°. 2486 intensities were measured (h $-6\rightarrow6$, k $-16\rightarrow0$, l $0\rightarrow18$) to the limit of $2\theta < 46.0°$ (internal consistency, R_{int} = 0.023) using the ω/θ-scan technique, with scan rate 1 to 8 min^{-1}, scan width 1.50 (1.00 + 0.35tanθ)° with a scan background ratio of 0.33. Of 2107 unique intensities processed, 1532 reflections had $I > 1.96\sigma(I)$; $\sigma(F_o)^2$ based on counting statistics plus the term $0.02F_o^2$. The data were corrected numerically (Busing & Levy, 1957) for absorption (maximum and minimum transmission factors 0.989 and 0.980), and anomalous-dispersion, Lorentz and polarization corrections were applied. Three standard reflections monitored every 5400 s of exposure time showed no significant intensity variation.

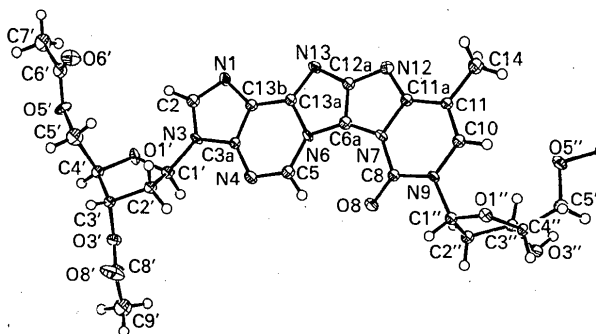The structure was solved using the direct-methods program SHELXS86 (Sheldrick, 1985). The posi-

Fig. 1. An ORTEP drawing (Johnson, 1965), with the atom numbering, of compound (1) as acetonitrile solvate monohydrate.
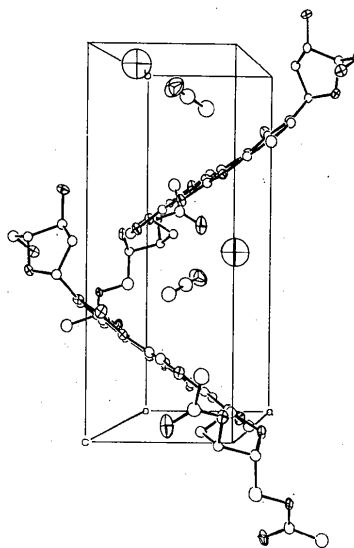

Fig. 2. Packing diagram of (1) with acetonitrile and water molecules, viewed along the cell edge with the origin and axes marked. O and N atoms are drawn with principal ellipsoids. H atoms have been removed for clarity.

coefficients used were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV). Successful convergence was indicated by the maximum shift/e.s.d. (0.02) in the final least-squares cycle. It was unnecessary for the absolute configuration to be determined crystallographically; the sugar moieties were known to be of the β-D-ribofuranosyl stereochemistry because of the synthetic precursors. The highest peaks in the final difference Fourier map were in the vicinity of the acetonitrile methyl C atom [C(42)]; the final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed no systematic errors. The final agreement factors for 1532 reflections were $R = 0.054$ and $wR = 0.056$ and goodness of fit $S = 1.55$; the range of residual electron density was 0.35 to -0.27 e Å^{-3}.

Discussion. An *ORTEP* view (Johnson, 1965) of compound (1), together with the standard atom numbering, is given in Fig. 1. It provides X-ray confirmation of the structure of this synthetic product (Bhat & Leonard, 1992) and indirectly of the structures of all the analogously synthesized compounds in the series of covalently linked cross sections (Devadas & Leonard, 1990). The near coplanarity of the atoms constituting the central pentacyclic N-aromatic system (root-mean-square deviation 0.03 Å) is illustrated clearly in the packing diagram of the unit cell (Fig. 2). Compound (1) thus fulfills a major requirement of comparability with a dA·dT base-paired DNA cross section that is devoid of propeller twist.

The final atomic coordinates for the non-H atoms are given in Table 1.* Selected bond lengths and angles are given in Table 2. Let us consider the bond lengths in the central 1,3,4,6-tetraazapentalene consisting of paired five-membered rings. The C—N and C—C distances in (1) are essentially the same, within the limit of error, as the corresponding distances in dipyrido[1,2-*a*:2′,1′-*f*]-1,3,4,6-tetraazapentalene (Groziak, Wilson, Clauson & Leonard, 1986) and 2,9-diethylpyrimido[1″,6″:1′,2′]imidazo[4′,5′:4,5]-imidazo[1,2-*c*]pyrimidine-1,10-dione (Leonard, Bhat, Wilson & Cruickshank, 1991). The N(12)···N(13) distance in (1) is 2.56 (1) Å compared with the value, 2.6 Å, calculated from X-ray structure results for the two 'halves' of the molecule (Devadas & Leonard, 1986, 1990) and the value, 2.85 Å, for the corre-

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters, torsion angles, deviations from aromatic planes and intra- and intermolecular hydrogen bonds have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55773 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: GR1001]

Table 1. *Final atomic coordinates and isotropic or equivalent isotropic thermal parameters* (Å^2)

For atoms refined anisotropically (indicated by an asterisk) equivalent isotropic U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{iso}/U_{eq}
N(1)	0.019 (1)	0.5432 (7)	0.2332 (4)	0.029 (4)*
C(2)	−0.061 (2)	0.5304 (7)	0.1589 (5)	0.029 (2)
N(3)	0.063 (1)	0.5736	0.1081 (3)	0.036 (4)*
C(3a)	0.245 (1)	0.6190 (7)	0.1529 (4)	0.020 (2)
N(4)	0.410 (1)	0.6696 (7)	0.1257 (3)	0.029 (4)*
C(5)	0.565 (2)	0.7023 (7)	0.1815 (5)	0.028 (2)
N(6)	0.559 (1)	0.6862 (7)	0.2590 (3)	0.022 (4)*
C(6a)	0.701 (1)	0.7112 (7)	0.3249 (5)	0.026 (2)
N(7)	0.905 (1)	0.7569 (6)	0.3525 (3)	0.023 (4)*
C(8)	1.047 (1)	0.8100 (7)	0.3130 (5)	0.022 (2)
O(8)	1.011 (1)	0.8211 (6)	0.2423 (3)	0.034 (4)*
N(9)	1.230 (1)	0.8488 (6)	0.3611 (3)	0.023 (4)*
C(10)	1.256 (1)	0.8382 (7)	0.4418 (5)	0.025 (2)
C(11)	1.110 (1)	0.7888 (7)	0.4806 (4)	0.021 (2)
C(11a)	0.924 (1)	0.7461 (7)	0.4362 (5)	0.023 (2)
N(12)	0.753 (1)	0.6949 (6)	0.4570 (4)	0.026 (4)*
C(12a)	0.613 (1)	0.6729 (7)	0.3870 (5)	0.024 (2)
N(13)	0.413 (1)	0.6237 (7)	0.3670 (4)	0.028 (4)*
C(13a)	0.382 (1)	0.6325 (7)	0.2887 (5)	0.023 (2)
C(13b)	0.213 (1)	0.5986 (7)	0.2298 (5)	0.024 (2)
C(1')	0.021 (1)	0.5768 (7)	0.0217 (4)	0.025 (2)
O(1')	−0.1931 (9)	0.5291 (6)	−0.0003 (3)	0.028 (3)*
C(2')	0.212 (1)	0.5306 (7)	−0.0196 (4)	0.025 (2)
C(3')	0.071 (1)	0.5019 (7)	−0.0952 (4)	0.022 (2)
O(3')	0.0254 (10)	0.5786 (6)	−0.1458 (3)	0.030 (3)*
C(4')	−0.168 (2)	0.4768 (7)	−0.0699 (5)	0.026 (2)
C(5')	−0.167 (2)	0.3795 (8)	−0.0497 (6)	0.045 (3)
O(5')	−0.3923 (9)	0.3538 (6)	−0.0256 (3)	0.031 (3)*
C(6')	−0.380 (2)	0.2873 (8)	0.0265 (5)	0.029 (2)
O(6')	−0.197 (1)	0.2577 (6)	0.0581 (3)	0.039 (4)*
C(7')	−0.622 (2)	0.2544 (8)	0.0395 (6)	0.045 (3)
C(8')	0.198 (2)	0.5996 (8)	−0.1889 (5)	0.037 (2)
O(8')	0.376 (1)	0.5588 (7)	−0.1896 (3)	0.060 (5)*
C(9')	0.136 (2)	0.6833 (8)	−0.2346 (6)	0.050 (3)
C(1'')	1.374 (1)	0.9157 (7)	0.3236 (5)	0.023 (2)
O(1'')	1.5951 (9)	0.9252 (6)	0.3701 (3)	0.024 (3)*
C(2'')	1.259 (1)	1.0061 (7)	0.3212 (5)	0.026 (2)
C(3'')	1.373 (1)	1.0499 (7)	0.3950 (5)	0.023 (2)
O(3'')	1.364 (1)	1.1439 (6)	0.3904 (4)	0.032 (3)*
C(4'')	1.621 (1)	1.0154 (7)	0.3983 (4)	0.022 (2)
C(5'')	1.774 (2)	1.0164 (8)	0.4764 (5)	0.030 (2)
O(5'')	1.658 (1)	0.9752 (6)	0.5373 (3)	0.032 (4)*
C(14)	1.137 (2)	0.7810 (8)	0.5689 (5)	0.034 (2)
N(41)	1.477 (2)	1.4039 (9)	0.1714 (7)	0.097 (9)*
C(41)	1.404 (2)	1.3844 (9)	0.2281 (7)	0.054 (3)
C(42)	1.295 (2)	1.3571 (9)	0.2982 (7)	0.064 (3)
O(43)	1.178 (3)	0.979 (1)	0.637 (1)	0.208 (9)

sponding N—H···O distance in a Watson–Crick A·U(T) base pair (Saenger, 1983). The N(6)···N(7) distance in (1) is 2.609 (10) Å, which may be compared with the value, 2.90 Å, for the corresponding N···H—N Watson–Crick hydrogen-bonding distance in A·U(T). There is some compression of the five-ring N-heterocyclic system in (1), probably owing to the additional aromatic conjugation. The distance C(1')···C(1'') in (1) is 10.11 (1) Å and the angles N(3)—C(1')···C(1'') and N(9)—C(1'')···C(1') are 58.6 (9) and 57.2 (9)°, respectively. These values differ slightly from the corresponding values observed for A·U(T) base pairs, 10.4 Å and 57° (Saenger, 1983). The atom O(8) is out of the plane of the pentacyclic ring system by 0.122 (8) Å, and the C(5)···O(8) and H(5)···O(8) distances are 3.17 (1) and 2.44 (1) Å, respectively.

In (1), the diacetyldeoxyribosyl and deoxyribosyl units are both *anti* in conformation with respect to

Table 2. *Selected bond lengths* (Å) *and bond angles* (°)

N(1)—C(2)	1.32 (1)	C(2)—N(3)	1.35 (1)
N(3)—C(3a)	1.39 (1)	C(3a)—N(4)	1.34 (1)
N(4)—C(5)	1.32 (1)	C(5)—N(6)	1.35 (1)
N(6)—C(6a)	1.36 (1)	C(6a)—N(7)	1.38 (1)
N(7)—C(8)	1.37 (1)	C(8)—O(8)	1.216 (10)
C(8)—N(9)	1.38 (1)	N(9)—C(10)	1.383 (10)
C(10)—C(11)	1.34 (1)	N(7)—C(11a)	1.434 (10)
C(11)—C(11a)	1.39 (1)	C(11a)—N(12)	1.32 (1)
C(6a)—C(12a)	1.35 (1)	N(12)—C(12a)	1.40 (1)
C(12a)—N(13)	1.36 (1)	N(6)—C(13a)	1.43 (1)
N(13)—C(13a)	1.338 (10)	N(1)—C(13b)	1.39 (1)
C(3a)—C(13b)	1.39 (1)	C(13a)—C(13b)	1.40 (1)
N(3)—C(1')	1.472 (9)	C(1')—O(1')	1.42 (1)
C(1')—C(2')	1.53 (1)	C(2')—C(3')	1.50 (1)
C(3')—O(3')	1.45 (1)	O(1')—C(4')	1.45 (1)
C(3')—C(4')	1.51 (1)	C(4')—C(5')	1.51 (2)
C(5')—O(5')	1.44 (1)	O(5')—C(6')	1.34 (1)
C(6')—O(6')	1.20 (1)	C(6')—C(7')	1.50 (1)
O(3')—C(8')	1.33 (1)	C(8')—O(8')	1.18 (1)
C(8')—C(9')	1.51 (2)	N(9)—C(1'')	1.49 (1)
C(1'')—O(1'')	1.412 (9)	C(1'')—C(2'')	1.51 (1)
C(2'')—C(3'')	1.50 (1)	C(3'')—O(3'')	1.42 (1)
O(1'')—C(4'')	1.45 (1)	C(3'')—C(4'')	1.50 (1)
C(4'')—C(5'')	1.51 (1)	C(5'')—O(5'')	1.44 (1)
C(11)—C(14)	1.51 (1)	N(41)—C(41)	1.14 (2)
C(41)—C(42)	1.47 (2)		

C(2)—N(1)—C(13b)	103.5 (7)	N(1)—C(2)—N(3)	114.0 (8)
C(2)—N(3)—C(3a)	106.8 (6)	C(2)—N(3)—C(1')	129.0 (6)
C(3a)—N(3)—C(1')	124.2 (6)	N(3)—C(3a)—N(4)	126.4 (7)
N(3)—C(3a)—C(13b)	104.2 (7)	N(4)—C(3a)—C(13b)	129.4 (8)
C(3a)—N(4)—C(5)	113.3 (7)	N(4)—C(5)—N(6)	123.6 (8)
C(5)—N(6)—C(6a)	133.1 (8)	C(5)—N(6)—C(13a)	123.6 (7)
C(6a)—N(6)—C(13a)	103.3 (6)	N(6)—C(6a)—N(7)	144.3 (8)
N(6)—C(6a)—C(12a)	107.3 (8)	N(7)—C(6a)—C(12a)	108.3 (7)
C(6a)—N(7)—C(8)	129.8 (7)	C(6a)—N(7)—C(11a)	104.3 (7)
C(8)—N(7)—C(11a)	125.5 (7)	N(7)—C(8)—O(8)	122.1 (8)
N(7)—C(8)—N(9)	113.4 (7)	O(8)—C(8)—N(9)	124.6 (8)
C(8)—N(9)—C(10)	122.3 (7)	C(8)—N(9)—C(1'')	116.1 (6)
C(10)—N(9)—C(1'')	120.8 (7)	N(9)—C(10)—C(11)	124.1 (8)
C(10)—C(11)—C(11a)	117.2 (7)	C(10)—C(10)—C(14)	123.0 (8)
C(11a)—C(11)—C(14)	119.8 (8)	N(7)—C(11a)—C(11)	117.3 (8)
N(7)—C(11a)—N(12)	111.5 (7)	C(11)—C(11a)—N(12)	131.1 (7)
C(11a)—N(12)—C(12a)	105.4 (7)	C(6a)—C(12a)—N(12)	110.3 (8)
C(6a)—C(12a)—N(13)	113.9 (7)	N(12)—C(12a)—N(13)	135.7 (8)
C(12a)—N(13)—C(13a)	101.8 (7)	N(6)—C(13a)—N(13)	113.6 (7)
N(6)—C(13a)—C(13b)	113.4 (7)	N(13)—C(13a)—C(13b)	133.0 (8)
N(1)—C(13b)—C(3a)	111.4 (7)	N(1)—C(13b)—C(13a)	131.8 (7)
C(3a)—C(13b)—C(13a)	116.7 (8)	N(3)—C(1')—O(1')	106.5 (6)
N(3)—C(1')—C(2')	114.3 (7)	O(1')—C(1')—C(2')	105.8 (8)
C(1')—O(1')—C(4')	109.4 (6)	C(1')—C(2')—C(3')	101.4 (6)
C(2')—C(3')—O(3')	108.9 (8)	C(2')—C(3')—C(4')	103.1 (6)
O(3')—C(3')—C(4')	105.7 (7)	C(3')—O(3')—C(8')	115.6 (7)
O(1')—C(4')—C(3')	105.9 (7)	O(1')—C(4')—C(5')	109.8 (7)
C(3')—C(4')—C(5')	109.3 (8)	C(4')—C(5')—O(5')	110.5 (8)
C(5')—O(5')—C(6')	114.5 (7)	O(5')—C(6')—O(6')	123.8 (8)
O(5')—C(6')—C(7')	111.7 (8)	O(6')—C(6')—C(7')	124.5 (9)
O(3')—C(8')—O(8')	124 (1)	O(3')—C(8')—C(9')	110.3 (9)
O(8')—C(8')—C(9')	125.2 (10)	N(9)—C(1'')—O(1'')	108.6 (7)
N(9)—C(1'')—C(2'')	111.8 (7)	O(1'')—C(1'')—C(2'')	105.9 (8)
C(1'')—O(1'')—C(4'')	109.5 (7)	C(1'')—C(2'')—C(3'')	103.7 (7)
C(2'')—C(3'')—O(3'')	112.6 (7)	C(2'')—C(3'')—C(4'')	100.7 (7)
O(3'')—C(3'')—C(4'')	111.9 (7)	O(1'')—C(4'')—C(3'')	104.8 (7)
O(1'')—C(4'')—C(5'')	109.4 (8)	C(3'')—C(4'')—C(5'')	118.0 (7)
C(4'')—C(5'')—O(5'')	112.2 (7)	N(41)—C(41)—C(42)	176 (1)

the adenine and thymine portions, respectively, of the pentacyclic system. The torsion angle of the glycosidic linkage, C(3a)—N(3)—C(1')—O(1'), for attachment at the purine-N is $-174.4\ (7)°$ and that for attachment at the pyrimidine-N, C(8)—N(9)—C(1'')—O(1''), is $-159.3\ (7)°$. The sugar torsion angles ν_0 through ν_4 [*i.e.* those for the ring bonds O(1')—C(1'), C(1')—C(2') and clockwise around the diacetyldeoxyribose ring] are $-18.2\ (9)$, $34.4\ (8)$,

$-36.6\ (8)$, $27.0\ (9)$ and $-5.4\ (9)°$. Torsion angles considered in the same order around the deoxyribose ring are $1.6\ (9)$, $-25.0\ (9)$, $37.4\ (8)$, $-36.9\ (8)$ and $22.7\ (9)°$. The corresponding pseudorotational angles (P) calculated from these torsion angles are 169.8 and 16.0°, which indicate that the sugar conformation is ^2E (C2'-*endo*) in the diacetyldeoxyribose unit and ^3E (C3'-*endo*) in the deoxyribose unit. The degrees of pucker (τ_m) as defined by Altona & Sundaralingam (1972) are, respectively, 37.2 and 38.9°.

The positions of the hydroxyl H atoms were refined. Crystal packing revealed paired hydrogen bonding between sequential adjacent molecules: O(5'')—H(O5'')···N(13) distance 2.84 (1) Å and angle 126 (5)° [bifurcated O(5'')—H(O5'')···O(43) distance 3.23 (2) Å and angle 101 (4)°; O(3'')—H(O3'')···N(12) distance 2.878 (9) Å and angle 168 (8)°]. The H(O5'')···N(13) and H(O3'')···N(12) hydrogen-bond lengths between adjacent molecules are 1.79 (8) and 1.94 (8) Å, respectively.

The dimensions of (1) indicate that the corresponding deacetylated compound is a satisfactory spatial and structural mimic of a dA·dT double-helical cross section.

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