A very weak stacking interaction of the 2'-acetyl group with a neighbouring base occurs, but is less pronounced than others in this series (Wilson, Low & Tollin, 1985) and, unusually, is above the indole ring of the purine base, rather than above the six-membered ring. Details are given in Table 3.

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Structure of 2',3',5'-Tri-O-acetylguanosine (Orthorhombic Form)

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Abstract. $C_{16}H_{19}N_5O_8$, $M_r = 409.4$, orthorhombic, $P2_12_12_1$, $a = 14.346$ (4), $b = 11.135$ (4), $c = 22.606$ (9) Å, $U = 3611.1$ Å^3, $Z = 8$, $D_x = 1.51$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0.71069$ Å, $\mu = 0.79$ cm^{-1}, $F(000) = 1712$, $T = 293$ K, $R = 0.091$ for 2835 unique observed reflections (Friedel pairs merged). The asymmetric unit consists of two molecules, A and B, of the title compound. A: the N-glycosidic torsion angle, χ, is -158 (1)°, in the *anti* range, the sugar pucker is ^2_3T, with $P = 147(1)°$, $\psi_m = 44(1)°$ and the C(4')–C(5') conformation is $+sc$ with $\gamma = 49$ (1)°. B: χ is 179 (1)°, in the *anti* range, the sugar pucker is $_4T^3$, with $P = 44$ (1)°, $\psi_m = 42$ (1)° and the C(4')–C(5') conformation is $+sc$ with $\gamma = 46$ (1)°. Each of these molecules is base-paired to one of their symmetry-related molecules by hydrogen bonds involving O(6)···N(2) [2.87 (1) Å (*A*), 2.82 (1) Å (*B*)] and N(7)···N(1) [2.83 (1) Å (*A*), 2.87 (1) Å (*B*)]. These base-paired molecules form ribbons which run through the crystal parallel to **b**.

Introduction. The structure determination resulted from an experiment in which an attempt was made to co-crystallize the title compound, designated TAG, with 3-deazauracil (Low & Wilson, 1983), to find out if the latter could intercalate between the stacked bases of TAG. This did not happen, an orthorhombic form of TAG with two molecules in the asymmetric unit being formed instead. This continues our study of conformations and base-pairing patterns of acetyl-substituted nucleosides. A monoclinic form of TAG has already been described by Wilson, Low & Tollin (1985).

Experimental. Crystals grown from an aqueous solution containing equal quantities of TAG and 3-deazauracil. Cell dimensions obtained by diffractometry from crystals mounted along **a** and **b**. These same crystals used in the collection of intensity data. Crystal dimensions approximately $0.5 \times 0.5 \times 0.5$ mm. Stoe Stadi II diffractometer (two-circle). Data collected in the range $h = 0$ to 6 from the a-axis crystal and $k = 0$ to 6 from the b-axis crystal. Max $\sin\theta/\lambda = 0.65$ Å^{-1}. Range of indices: $-18 < h < 18$, $-14 < k < 14$, $-25 < l < 25$. No absorption corrections. One standard reflection measured every 100 reflections; intensity variation $<5\%$ from the mean. 16 213 reflections measured; 4040 unique; $R_{int} = 0.026$; 1205 with $F < 4\sigma(F)$ regarded as unobserved; structure solved using the *MAGEX* module of the direct-methods program *MITHRIL* (Gilmore, 1983). Only a partial structure containing 21 atoms obtained from the E map; the other atoms obtained after Fourier recycling. Refinement (on F) by blocked-matrix least squares with *SHELX*76 (Sheldrick, 1976). Non-hydrogen atoms refined anisotropically; H atoms included at calculated positions with isotropic temperature factors approximately 1.5 times that of the parent atom. 523 parameters refined, $R = 0.091$, $wR = 0.082$, $w = 4.3851/[\sigma^2(F) + 0.000816F^2]$; max $\Delta/\sigma = 0.08$; max. difference-map peak 0.42, min. -0.46 e Å^{-3}. Other programs used; *XANADU* (Roberts & Sheldrick, 1975) and *PLUTO* (Motherwell & Clegg, 1978). Scattering factors from *International Tables for X-ray Crystallography* (1974). No correction for secondary extinction.

The intensity of the data falls off rapidly at a $\sin\theta/\lambda$ corresponding to a resolution of 1 Å and hence the thermal parameters are ill defined and the R factor is consequently higher than might be expected from the internal consistency of the data.

Discussion. Atomic coordinates are given in Table 1,* bond lengths and angles in Table 2. The atomic numbering is given in Fig. 1 which shows perspective views perpendicular to the purine bases of the two molecules in the asymmetric unit. The two independent molecules have similar bond lengths and angles.

The essential differences between the two molecules are in the glycosidic torsion angles and sugar-ring puckers, there being very little difference in the exocyclic torsion angles of the sugar ring, as is shown below, values for molecule A first: $\chi = -158$ (1), 179 (1)°; $P = 147$ (1), 44 (1)°; $\psi_m = 44$ (1), 42 (1)°; O(2')1—C(2')1—O(2')—C(2') = 3 (1), 5 (1)°; O(3')1—

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* Lists of structure amplitudes, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42724 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

C(3')1—O(3')—C(3') = 0 (1), 2 (1)°; and γ[C(3')—C(4')—C(5')—O(5')] = 49 (1), 46 (1)°. The conformational parameters used follow the guidelines of the IUPAC–IUB Joint Commission on Biochemical Nomenclature (1983).

The molecules are base-paired in ribbons, A with A and B with B. These ribbons extend along **b**. The base-pairing, like that of the monoclinic form of TAG, is a model of Hoogsteen G/C pairing (Hoogsteen, 1959), with propeller twists (Dickerson, 1983) of 9 (1)° for pair A and 11 (1)° for pair B. The molecules in the

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature factors* (Å$^2 \times 10^3$) *with e.s.d.'s in parentheses*

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

	x	y	z	U_{eq}
Molecule A				
N(1)	5520 (3)	12128 (5)	2616 (2)	28 (1)
C(2)	6337 (4)	12428 (7)	2863 (3)	32 (2)
N(2)	6476 (4)	13575 (6)	2966 (3)	47 (2)
N(3)	6945 (3)	11621 (6)	3022 (2)	32 (1)
C(4)	6683 (4)	10484 (7)	2906 (3)	30 (2)
C(5)	5882 (4)	10121 (6)	2661 (3)	28 (2)
C(6)	5229 (4)	10956 (7)	2497 (3)	30 (2)
O(6)	4488 (3)	10783 (4)	2265 (2)	43 (1)
N(7)	5856 (3)	8875 (6)	2642 (2)	36 (1)
C(8)	6624 (5)	8529 (6)	2871 (3)	28 (2)
N(9)	7166 (3)	9477 (5)	3029 (2)	29 (1)
C(1')	7983 (4)	9462 (6)	3374 (3)	30 (2)
C(2')	7851 (4)	9323 (6)	4028 (3)	30 (2)
O(2')	7537 (3)	10401 (4)	4308 (2)	37 (1)
C(2')1	6637 (5)	10457 (8)	4397 (3)	46 (2)
C(2')2	6358 (5)	11614 (8)	4644 (4)	67 (3)
O(2')1	6146 (3)	9641 (6)	4274 (3)	71 (2)
C(3')	8781 (4)	8931 (6)	4237 (3)	30 (2)
O(3')	9346 (3)	9979 (4)	4272 (2)	34 (1)
C(3')1	10174 (4)	9752 (9)	4521 (3)	45 (2)
C(3')2	10719 (5)	10895 (8)	4537 (3)	54 (2)
O(3')1	10387 (4)	8776 (6)	4693 (3)	67 (2)
C(4')	9066 (4)	8122 (6)	3715 (3)	31 (2)
C(5')	9010 (4)	6811 (7)	3846 (3)	38 (2)
O(5')	8124 (3)	6582 (4)	4106 (2)	41 (1)
C(5')1	7510 (5)	5994 (7)	3758 (3)	38 (2)
C(5')2	6586 (5)	6030 (8)	4034 (3)	60 (3)
O(5')1	7703 (3)	5552 (6)	3301 (2)	67 (2)
O(4')	8472 (3)	8408 (4)	3226 (2)	36 (1)
Molecule B				
N(1)	9649 (3)	7983 (5)	2200 (2)	36 (1)
C(2)	8835 (5)	8317 (8)	1970 (3)	37 (2)
N(2)	8688 (4)	9465 (7)	1885 (3)	54 (2)
N(3)	8186 (4)	7528 (7)	1832 (2)	41 (2)
C(4)	8426 (5)	6390 (7)	1938 (3)	37 (2)
C(5)	9214 (4)	5936 (8)	2169 (3)	42 (2)
C(6)	9881 (5)	6807 (8)	2346 (3)	44 (2)
O(6)	10603 (3)	6590 (5)	2603 (2)	59 (2)
N(7)	9169 (4)	4724 (6)	2239 (3)	45 (2)
C(8)	8356 (5)	4425 (7)	2038 (3)	42 (2)
N(9)	7882 (3)	5412 (5)	1836 (2)	35 (1)
C(1')	6943 (4)	5505 (7)	1652 (3)	41 (2)
C(2')	6843 (4)	6172 (7)	1060 (3)	40 (2)
O(2')	6124 (3)	7036 (5)	1137 (2)	47 (1)
C(2')1	6221 (6)	8138 (9)	890 (3)	57 (3)
C(2')2	5514 (6)	9006 (8)	1070 (3)	61 (3)
O(2')1	6860 (5)	8352 (6)	585 (3)	103 (3)
C(3')	6552 (5)	5150 (7)	652 (3)	44 (2)
O(3')	6011 (3)	5563 (5)	160 (2)	49 (1)
C(3')1	6489 (6)	6007 (7)	−308 (3)	42 (2)
C(3')2	5863 (6)	6459 (8)	−787 (3)	70 (3)
O(3')1	7290 (4)	6017 (5)	−321 (2)	58 (2)
C(4')	6036 (4)	4319 (7)	1060 (3)	46 (2)
C(5')	5923 (5)	3054 (8)	867 (3)	56 (3)
O(5')	6761 (4)	2571 (5)	643 (2)	58 (2)
C(5')1	7231 (6)	1791 (8)	981 (3)	59 (3)
C(5')2	8126 (7)	1509 (9)	707 (4)	89 (4)
O(5')1	6975 (5)	1394 (6)	1438 (3)	83 (2)
O(4')	6610 (3)	4340 (5)	1581 (2)	46 (1)

A ribbon are also linked, as in the monoclinic form, by an additional hydrogen bond between N(2) and the acetyl atom O(5')1 in a symmetry-related molecule. The hydrogen bonds involving *A* are N(1)···N(7)-

$(1 - x, \frac{1}{2} + y, \frac{1}{2} - z)$ 2·83 (1), N(2)···O(6)$(1 - x, \frac{1}{2} + y, \frac{1}{2} - z)$ 2·87 (1) and N(2)···O(5')1$(x, 1 + y, z)$ 2·92 (1) Å. Those involving *B* are N(1)···N(7)$(2 - x, \frac{1}{2} + y, \frac{1}{2} - z)$ 2·87 (1) and N(2)···O(6)$(2 - x, \frac{1}{2} + y, \frac{1}{2} - z)$ 2·82 (1) Å. Fig. 2 gives views of molecules *A* and *B*, separated for clarity, showing the proposed hydrogen-bonding scheme.

The acetyl oxygen O(2')1 of *A* takes up a 'scorpion-tail' position above its parent base, sitting 3·14 (1) Å above the base mean plane and 3·32 (1) Å from C(4) and 3·17(1)Å from N(9). Atoms O(4') and O(5')1 of *A* stack at 2·82 (1) and 3·12 (1) Å, respectively, above the mean plane of the base of *B* in the asymmetric unit. Atom O(4') lies at 2·91 (1), 2·89 (1) and 3·27 (1) Å from atoms N(1), C(2) and N(2), respectively, of molecule *B*, while O(5')1 lies at 3·26 (1) Å from C(8) of molecule *B*. This type of close contact of O(4') of the ribose with the base is discussed by Bugg, Thomas, Sundaralingam & Rao (1971). Acetyl stacking above base rings is once again found to be of importance in the structure, as will be discussed elsewhere in more

Table 2. *Bond lengths* (Å) *and angles* (°)

|	*A*	*B*
C(2)–N(1)	1·340 (8)	1·331 (8)
C(6)–N(1)	1·397 (9)	1·391 (11)
N(2)–C(2)	1·314 (10)	1·310 (11)
N(3)–C(2)	1·303 (9)	1·317 (10)
C(4)–N(3)	1·346 (10)	1·335 (11)
C(5)–C(4)	1·339 (9)	1·344 (10)
N(9)–C(4)	1·347 (9)	1·360 (10)
C(6)–C(5)	1·371 (9)	1·421 (11)
N(7)–C(5)	1·389 (9)	1·360 (11)
O(6)–C(6)	1·200 (7)	1·212 (8)
C(8)–N(7)	1·277 (8)	1·294 (9)
N(9)–C(8)	1·358 (8)	1·370 (9)
C(1')–N(9)	1·408 (7)	1·413 (8)
C(2')–C(1')	1·498 (8)	1·537 (10)
O(4')–C(1')	1·408 (8)	1·391 (9)
O(2')–C(2')	1·430 (8)	1·422 (8)
C(3')–C(2')	1·481 (8)	1·524 (10)
C(2')–O(2')	1·307 (8)	1·355 (11)
C(2')2–C(2')1	1·460 (12)	1·459 (12)
O(2')1–C(2')1	1·183 (10)	1·170 (11)
O(3')–C(3')	1·423 (8)	1·430 (8)
C(4')–C(3')	1·539 (9)	1·503 (10)
C(3')–O(3')	1·338 (8)	1·355 (8)
C(3')2–C(3')1	1·494 (12)	1·493 (11)
O(3')1–C(3')1	1·194 (11)	1·150 (10)
C(5')–C(4')	1·491 (10)	1·483 (12)
O(4')–C(4')	1·433 (7)	1·438 (8)
O(5')–C(5')	1·423 (7)	1·412 (9)
C(5')1–O(5')	1·350 (8)	1·339 (10)
C(5')2–C(5')1	1·467 (10)	1·460 (13)
O(5')1–C(5')1	1·177 (9)	1·182 (10)
C(6)–N(1)–C(2)	125·1 (5)	124·5 (6)
N(2)–C(2)–N(1)	116·8 (6)	118·1 (7)
N(3)–C(2)–N(1)	121·9 (6)	121·7 (7)
N(3)–C(2)–N(2)	121·3 (6)	120·2 (6)
C(4)–N(3)–C(2)	114·1 (5)	114·1 (6)
C(5)–C(4)–N(3)	127·1 (6)	130·1 (7)
N(9)–C(4)–N(3)	126·9 (5)	125·5 (6)
N(9)–C(4)–C(5)	106·0 (6)	104·4 (7)
C(6)–C(5)–C(4)	119·6 (7)	114·8 (8)
N(7)–C(5)–C(4)	109·7 (6)	112·2 (7)
N(7)–C(5)–C(6)	130·6 (6)	132·7 (7)
C(5)–C(6)–N(1)	112·1 (5)	114·5 (6)
O(6)–C(6)–N(1)	120·0 (6)	120·5 (7)
O(6)–C(6)–C(5)	127·9 (7)	125·0 (8)
C(8)–N(7)–C(5)	105·4 (5)	104·9 (6)
N(9)–C(8)–N(7)	111·5 (6)	111·0 (6)
C(8)–N(9)–C(4)	107·4 (5)	107·5 (5)
C(1')–N(9)–C(4)	123·4 (5)	122·6 (6)
C(1')–N(9)–C(8)	127·8 (5)	129·1 (6)
C(2')–C(1')–N(9)	116·3 (5)	112·4 (5)
O(4')–C(1')–N(9)	107·0 (5)	107·0 (6)
O(4')–C(1')–C(2')	102·2 (5)	108·6 (5)
O(2')–C(2')–C(1')	112·9 (5)	106·7 (5)
C(3')–C(2')–C(1')	103·4 (5)	101·1 (6)
C(3')–C(2')–O(2')	113·0 (5)	112·4 (5)
C(2')1–O(2')–C(2')	114·8 (5)	119·2 (6)
C(2')2–C(2')1–O(2')	111·9 (7)	114·4 (7)
O(2')1–C(2')1–O(2')	121·0 (8)	120·5 (8)
O(2')1–C(2')1–C(2')2	127·1 (7)	125·0 (9)
O(3')–C(3')–C(2')	106·8 (5)	112·2 (6)
C(4')–C(3')–C(2')	99·6 (5)	102·9 (6)
C(4')–C(3')–O(3')	111·8 (5)	114·1 (5)
C(3')1–O(3')–C(3')	112·0 (6)	116·7 (5)
C(3')2–C(3')1–O(3')	108·3 (7)	112·7 (7)
O(3')1–C(3')1–O(3')	122·4 (7)	121·9 (6)
O(3')1–C(3')1–C(3')2	129·3 (6)	125·4 (7)
C(5')–C(4')–C(3')	114·0 (5)	117·2 (6)
O(4')–C(4')–C(3')	107·7 (5)	102·2 (5)
O(4')–C(4')–C(5')	109·8 (5)	108·6 (6)
O(5')–C(5')–C(4')	107·8 (5)	112·0 (6)
C(5')1–O(5')–C(5')	115·3 (5)	118·1 (6)
C(5')2–C(5')1–O(5')	109·2 (6)	109·9 (7)
O(5')1–C(5')1–O(5')	124·1 (6)	125·8 (8)
O(5')1–C(5')1–C(5')2	126·6 (7)	124·3 (8)
C(4')–O(4')–C(1')	107·3 (4)	107·8 (5)

(*a*)

(*b*)
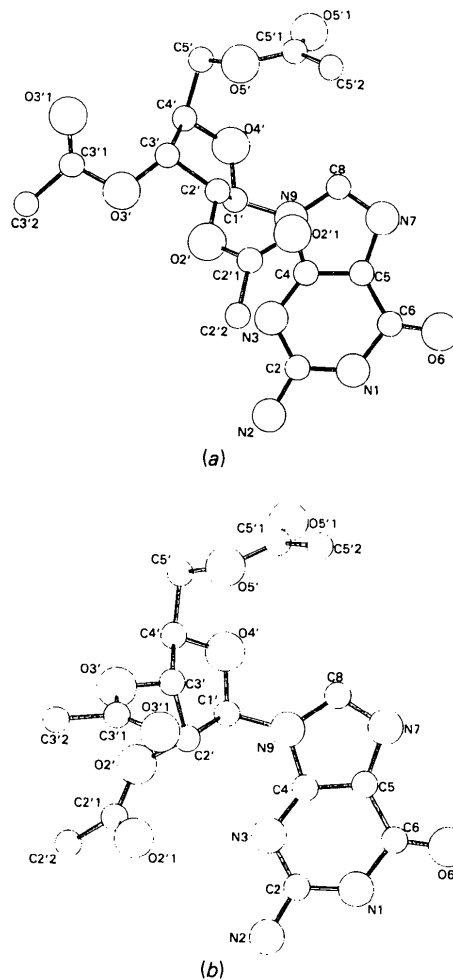
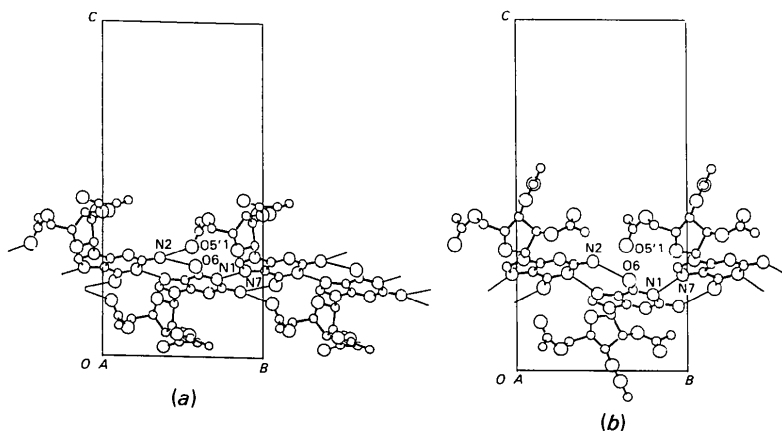Fig. 1. Perspective view of (*a*) molecule *A* and (*b*) molecule *B*.

Fig. 2. Proposed hydrogen bonding of (a) molecule A and (b) molecule B.

detail (Wilson, Low & Tollin, to be published). In the structure of monoclinic TAG (Wilson, Low & Tollin, 1985), the acetyl O(2′)1 intercalates between two parallel bases, separated by 6·2 Å, with possible biological implications (Wilson & Tollin, 1985). However, while the 'scorpion-tail' shape of monoclinic TAG is repeated in molecule A of the present structure, O(2′)1 in this case does not intercalate. Instead, there is very strong stacking of O(4′) and acetyl O(5′)1 of molecule A above the base of B, on the opposite side of the base ring to O(2′)1. The existence of this second stacking contact involving these two O atoms with molecule B precludes the extended base–acetyl–base stacking structure noted in monoclinic TAG.

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Structure of 1,2:7,8-Dibenzo[2.2]paracyclophane

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Abstract. $C_{24}H_{16}$, $M_r = 304\cdot39$, monoclinic, $P2_1/c$, $a = 7\cdot074$ (2), $b = 17\cdot761$ (4), $c = 12\cdot925$ (3) Å, $\beta = 98\cdot55$ (2)°, $V = 1605\cdot9$ (7) Å^3, $Z = 4$, $D_m = 1\cdot25$ (1), $D_x = 1\cdot259$ g cm^{-3}, Mo $K\alpha$, $\bar{\lambda} = 0\cdot71069$ Å, $\mu = 0\cdot66$ cm^{-1}, $F(000) = 639\cdot92$, $T = 295$ K, $R = 0\cdot093$ for 1064 observed data and 157 parameters. The two *para*-fused benzenoid rings are boat-shaped, and the innermost (bridging) bond of each *ortho*-fused ring is significantly lengthened to $1\cdot431$ (10) Å. The molecule departs very slightly from idealized D_{2h} symmetry.

Introduction. Compounds possessing orthogonal benzenoid rings are decidedly rare. Jacobson & Boekelheide (1978) reported the isolation and