distances and angles are summarized in Table 2. Fig. 1 shows the molecular structure and Fig. 2 the arrangement of the compound in the unit cell viewed along **a**.

Related literature. The structural parameters of the inorganic ring skeleton can be compared with those found in related structures $(NSOPh)_2NPXY$ (van Bolhuis, Cnossen-Voswijk & van de Grampel, 1981; van Bolhuis, van den Berg & van de Grampel, 1981; Meetsma, Spek, Olthof-Hazekamp, Winter, van de Grampel & de Boer, 1985; Meetsma, Spek, Winter, Cnossen-Voswijk, van de Grampel & de Boer, 1986; Meetsma, Spek, Winter, van de Grampel & de Boer, 1986; Winter, van de Grampel, de Boer, Meetsma & Spek, 1987).

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Structure of 3-{2-[4-(2-Methoxyphenyl)-1-piperazinyl]ethyl}-2,4(1*H*,3*H*)-quinazolinedione Monohydrate (SGB1534)

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Abstract. $C_{21}H_{24}N_4O_3.H_2O$, $M_r = 398{\cdot}47$, monoclinic, $P2_1/c$, $a = 19{\cdot}199$ (4), $b = 13{\cdot}667$ (2), $c = 7{\cdot}559$ (2) Å, $\beta = 97{\cdot}05$ (2)°, $V = 1968{\cdot}5$ Å^3, $Z = 4$, $D_x = 1{\cdot}344$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7{\cdot}36$ cm^{-1}, $F(000) = 848$, $T = 298$ K, final $R = 0{\cdot}059$ for 1295 unique reflections $[F_o^2 > 1{\cdot}8\sigma(F_o^2)]$. Phenyl and quinazolinedione moieties of an SGB1534 molecule are arranged parallel to each other, and attached to the N atoms of a piperazine ring (chair form) at equatorial positions. Water molecules are held in the hole running through the crystal along the direction [001].

Experimental. Colorless thin plates of SGB1534 grew from a mixed solvent of methanol/water (=2:1, v/v). Crystal size 0·33 × 0·25 × 0·03 mm, Enraf–Nonius CAD-4 κ-cradle diffractometer, Cu $K\alpha$ radiation, graphite monochromator, θ–2θ scan with scan speed 1·27–2·75° min^{-1} in θ, scan width (0·50 + 0·14tanθ)°. Range of indices, $-22 \le h \le 22$, $0 \le k \le 16$, $0 \le l \le 8$ ($2\theta < 130°$). Lattice parameters determined based on 22 2θ values ($24 < 2\theta < 64°$). Variation of standard <1·2%; 3338 reflections measured; 1295 observed reflections with $F_o^2 > 1{\cdot}8\sigma(F_o^2)$. Systematic absences $h0l$, l odd; $0k0$, k odd. No corrections for absorption. Structure solved by direct methods with *MULTAN*11/82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982). Refined by full-matrix least squares. The locations of H atoms were calculated stereochemically, except for those of the water molecule. Non-H atoms refined with anisotropic thermal parameters, and

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H atoms with isotropic thermal parameters (fixed at $B = 5{\cdot}0$ Å^2). $\sum w(|F_o| - |F_c|)^2$ minimized; $w = 1{\cdot}0$ for $F_o < 385{\cdot}0$, $w = (385{\cdot}0/F_o)^2$ for $F_o \geq 385{\cdot}0$. Final $R = 0{\cdot}059$, $wR = 0{\cdot}059$, $S = 2{\cdot}88$ for 359 variables, secondary-extinction factor (g) $7{\cdot}1\,(2) \times 10^{-7}$ [$|F_o| = |F_c|/(1 + gI_c)$]; $\Delta/\sigma < 0{\cdot}52$, largest peak in final ΔF map $+0{\cdot}37$ e Å^{-3}; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs: Enraf–Nonius *SDP* (Frenz, 1984), *ORTEP*II (Johnson, 1976). The structure of the SGB1534 molecule is shown in Fig. 1, and a packing diagram is given in Fig. 2; positional parameters and equivalent values of the anisotropic temperature factors are given in Table 1, bond distances and angles are listed in Table 2.*

Related literature. Title compound has hypotensive activity (Nabata, Aono, Ishizuka & Sakai, 1985). For the preparation see Nagano, Takagi, Kubodera, Matsunaga, Nabata & Ohba (1983).

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, least-squares planes and torsion angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44313 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square Chester CH1 2HU, England.

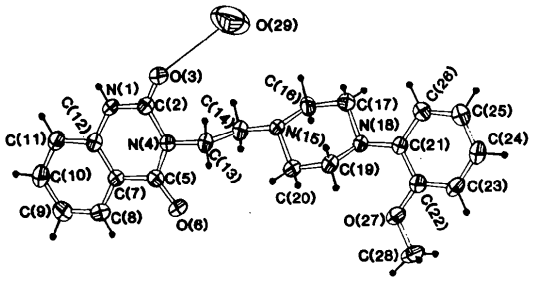

Fig. 1. A perspective view of the molecule with the numbering scheme.

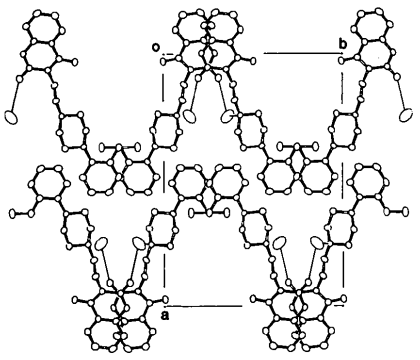

Fig. 2. Crystal structure projected along the c axis. Hydrogen bonds are indicated by single lines.

Table 1. *Final fractional coordinates and equivalent isotropic temperature factors for non-*H *atoms with e.s.d.'s in parentheses*

$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}(Å^2)
N(1)	−0·0050 (3)	0·2861 (4)	0·2754 (9)	3·9 (1)
C(2)	0·0519 (3)	0·2529 (5)	0·380 (1)	3·6 (2)
O(3)	0·0940 (2)	0·3061 (3)	0·4659 (7)	4·7 (1)
N(4)	0·0599 (3)	0·1502 (4)	0·3878 (8)	3·5 (1)
C(5)	0·0151 (3)	0·0850 (5)	0·290 (1)	3·5 (2)
O(6)	0·0285 (2)	−0·0039 (3)	0·2990 (7)	4·7 (1)
C(7)	−0·0472 (3)	0·1267 (5)	0·187 (1)	3·3 (2)
C(8)	−0·0978 (4)	0·0675 (5)	0·094 (1)	4·2 (2)
C(9)	−0·1568 (4)	0·1082 (6)	0·003 (1)	5·0 (2)
C(10)	−0·1655 (3)	0·2091 (6)	0·004 (1)	4·5 (2)
C(11)	−0·1158 (3)	0·2696 (5)	0·092 (1)	4·0 (2)
C(12)	−0·0564 (3)	0·2271 (5)	0·184 (1)	3·4 (2)
C(13)	0·1202 (3)	0·1125 (5)	0·509 (1)	4·0 (2)
C(14)	0·1844 (3)	0·1034 (5)	0·409 (1)	4·0 (2)
N(15)	0·2454 (3)	0·0722 (4)	0·5336 (9)	4·1 (1)
C(16)	0·3097 (3)	0·0848 (5)	0·448 (1)	4·6 (2)
C(17)	0·3737 (3)	0·0540 (5)	0·573 (1)	5·0 (2)
N(18)	0·3669 (3)	−0·0502 (4)	0·6159 (8)	3·8 (1)
C(19)	0·3034 (3)	−0·0620 (5)	0·705 (1)	4·3 (2)
C(20)	0·2399 (3)	−0·0329 (5)	0·577 (1)	4·0 (2)
C(21)	0·4280 (3)	−0·0954 (5)	0·705 (1)	4·4 (2)
C(22)	0·4296 (4)	−0·1983 (5)	0·723 (1)	4·2 (2)
C(23)	0·4878 (4)	−0·2440 (5)	0·808 (1)	5·3 (2)
C(24)	0·5472 (4)	−0·1917 (6)	0·873 (1)	5·3 (2)
C(25)	0·5480 (4)	−0·0920 (6)	0·853 (1)	5·2 (2)
C(26)	0·4880 (4)	−0·0446 (5)	0·771 (1)	5·3 (2)
O(27)	0·3706 (3)	−0·2461 (3)	0·6470 (8)	5·7 (1)
C(28)	0·3694 (4)	−0·3502 (6)	0·667 (1)	5·9 (2)
O(29)	0·2490 (4)	0·3559 (6)	0·429 (1)	14·0 (3)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

N(1)–C(2)	1·348 (8)	N(15)–C(16)	1·472 (9)
N(1)–C(12)	1·391 (8)	N(15)–C(20)	1·478 (8)
C(2)–O(3)	1·214 (8)	C(16)–C(17)	1·514 (10)
C(2)–N(4)	1·413 (8)	C(17)–N(18)	1·469 (9)
N(4)–C(5)	1·386 (8)	N(18)–C(19)	1·473 (9)
N(4)–C(13)	1·479 (8)	N(18)–C(21)	1·422 (8)
C(5)–O(6)	1·242 (8)	C(19)–C(20)	1·518 (9)
C(5)–C(7)	1·461 (9)	C(21)–C(22)	1·414 (10)
C(7)–C(8)	1·388 (9)	C(21)–C(26)	1·385 (10)
C(7)–C(12)	1·384 (9)	C(22)–C(23)	1·370 (10)
C(8)–C(9)	1·369 (10)	C(22)–O(27)	1·371 (8)
C(9)–C(10)	1·388 (11)	C(23)–C(24)	1·384 (10)
C(10)–C(11)	1·373 (10)	C(24)–C(25)	1·372 (11)
C(11)–C(12)	1·385 (9)	C(25)–C(26)	1·398 (10)
C(13)–C(14)	1·532 (10)	O(27)–C(28)	1·431 (9)
C(14)–N(15)	1·475 (8)		

C(2)–N(1)–C(12)	124·9 (5)	C(14)–N(15)–C(16)	109·1 (6)
N(1)–C(2)–O(3)	123·4 (6)	C(14)–N(15)–C(20)	110·4 (5)
N(1)–C(2)–N(4)	115·8 (5)	C(16)–N(15)–C(20)	107·2 (5)
O(3)–C(2)–N(4)	120·8 (6)	N(15)–C(16)–C(17)	110·8 (7)
C(2)–N(4)–C(5)	124·1 (5)	C(16)–C(17)–N(18)	108·6 (5)
C(2)–N(4)–C(13)	116·4 (5)	C(17)–N(18)–C(19)	108·0 (5)
C(5)–N(4)–C(13)	119·6 (5)	C(17)–N(18)–C(21)	115·8 (5)
N(4)–C(5)–O(6)	119·3 (6)	C(19)–N(18)–C(21)	114·5 (6)
N(4)–C(5)–C(7)	116·6 (6)	N(18)–C(19)–C(20)	108·7 (6)
O(6)–C(5)–C(7)	124·1 (6)	N(15)–C(20)–C(19)	108·8 (5)
C(5)–C(7)–C(8)	121·3 (6)	N(18)–C(21)–C(22)	119·0 (6)
C(5)–C(7)–C(12)	119·4 (6)	N(18)–C(21)–C(26)	123·8 (6)
C(8)–C(7)–C(12)	119·3 (6)	C(22)–C(21)–C(26)	117·2 (6)
C(7)–C(8)–C(9)	120·1 (6)	C(21)–C(22)–C(23)	120·3 (6)
C(8)–C(9)–C(10)	119·6 (7)	C(21)–C(22)–O(27)	115·3 (6)
C(9)–C(10)–C(11)	121·6 (6)	C(23)–C(22)–O(27)	124·3 (6)
C(10)–C(11)–C(12)	118·1 (6)	C(22)–C(23)–C(24)	121·4 (7)
N(1)–C(12)–C(7)	119·0 (5)	C(23)–C(24)–C(25)	119·6 (7)
N(1)–C(12)–C(11)	119·7 (6)	C(24)–C(25)–C(26)	119·3 (7)
C(7)–C(12)–C(11)	121·3 (6)	C(21)–C(26)–C(25)	122·1 (7)
N(4)–C(13)–C(14)	109·7 (6)	C(22)–O(27)–C(28)	116·8 (6)
C(13)–C(14)–N(15)	109·2 (6)		

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Structure of 2′,3′,5′-Tri-*O*-acetyl-8-bromoguanosine

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Abstract. $C_{16}H_{18}BrN_5O_8$, $M_r = 488{\cdot}2$, triclinic, $P1$, $a = 8{\cdot}201\ (5)$, $b = 8{\cdot}761\ (5)$, $c = 15{\cdot}392\ (13)$ Å, $\alpha = 95{\cdot}38\ (6)$, $\beta = 103{\cdot}11\ (6)$, $\gamma = 110{\cdot}25\ (6)°$, $U = 992$ Å^3, $Z = 2$, $D_x = 1{\cdot}63$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 20{\cdot}5$ cm^{-1}, $F(000) = 496$, $T = 293$ K, $R = 0{\cdot}071$ for 4066 unique observed $[F > 3\sigma(F)]$ reflections. The *N*-glycosidic torsion angles χ have values 98·1 (1) and 85·6 (1)°, in the high *anti* range, which are unusual for ribose nucleosides. (Molecule I values are given first throughout.) The sugar puckers are ${}_2E$ (C2′-*exo*), with $P = -19\ (1)°$ and $\psi_m = 22\ (1)°$, which is unusual, and ${}^3_2T$ (C2′-*exo*/C3′-*endo*), with $P = 5\ (1)°$ and $\psi_m = 8\ (1)°$. The C4–C5 conformations, with $\gamma = 41{\cdot}7\ (3)$ and $51{\cdot}3\ (3)°$, are +*sc* (*gauche–gauche*).

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 had dimensions 0·5 × 0·46 × 0·08 mm. Cell parameters were measured on the diffractometer using 14 reflections in the 2θ

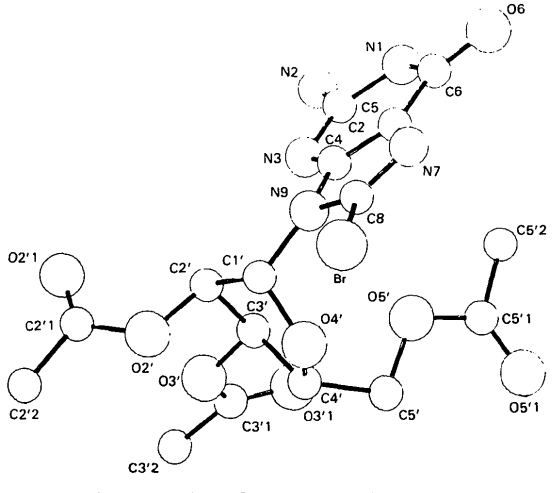

Fig. 1. Atomic numbering of molecule I viewed perpendicular to N7, C1′ and O4′.

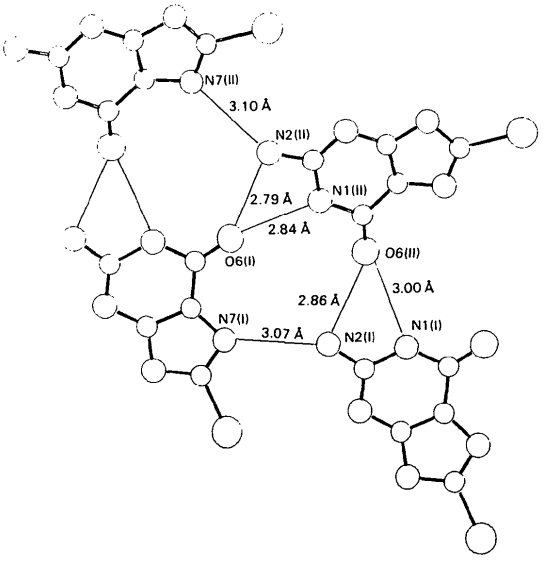

Fig. 2. Packing of bases viewed down **c**. Ribose rings omitted for clarity.

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