indazole systems. The first twisting is presumably due to a weak hydrogen bond between O(12*A*) and C(20)($1-x$, $-y$, $1-z$); the O---H—C distance is 3·343 (4) Å. The morpholine cation adopts a chair conformation. Bond lengths N(16)—C(17) and N(16)—C(21) (Table 2) due to the protonation of the nitrogen atom are slightly larger than the single N—C bond. Oxygen O(19) participates in the following hydrogen bonds: O(19)---H(71A^i) 2·34 (3), O(19)···C(7A^i) 3·310 (4) Å, O(19)---H(71A^i)—C(7A^i) 156 (2)°; O(19)---H(71B^i) 2·38 (3), O(19)···C(7B^i) 3·327 (4) Å, O(19)---H(71B^i)—C(7B^i) 157 (2)°; symmetry code (i) $1·5-x$, $-0·5+y$, $0·5-z$.

Fig. 3 shows the molecular packing in the unit cell. In the crystal lattice the two independent molecules of 3,5-dinitroindazole are almost parallel and partly overlap. They form layers approximately perpendicular to z and about 3·3 Å distant. The molecules overlap in the following order: molecule *A* overlaps molecule *B* of a complex in the equivalent position $-0·5+x$, $0·5-y$, $0·5+z$.

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Structure of 1-(2-Deoxy-β-D-ribofuranosyl)-5-[(1*S*)-2,2-dibromocyclopropyl]uracil

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Abstract. $C_{12}H_{14}Br_2N_2O_5$, $M_r=426·07$, orthorhombic, $P2_12_12_1$, $a=5·861$ (1), $b=18·609$ (4), $c=13·433$ (3) Å, $V=1465·1$ (3) Å^3, $Z=4$, $D_x=1·931$ g cm^{-3}, λ(Cu $K\alpha_1$) = 1·5405 Å, $\mu=73·1$ cm^{-1}, $F(000)=840$, $T=293$ K, $R=0·037$, GOF = 2·6 for 2145 observed reflections. The absolute configuration about C(7) of the cyclopropane ring is *S*. The 5-substituted pyrimidine is *anti* with respect to the deoxyribose and the 2′-deoxyribose is in the 2′-*endo* pucker mode. The torsion angle about C(4′)—C(5′) is *gauche–gauche*.

Introduction. (*E*)-5-(2-Bromovinyl)-2′-deoxyuridine (BVDU) is a potent and selective antiviral agent against herpes simplex virus type 1 (HSV-1) and varicella-zoster virus (VZV) in cell culture, in animals and in the clinic (Jones, Sayers, Walker & De Clercq, 1988). Its activity is due to selective phosphorylation by HSV-1 encoded thymidine kinase and metabolic trapping within infected cells, but not in uninfected host cells (Cheng, Dutschman, Fox, Watanabe & Machida, 1981; De Clercq, Descamps, De Somer, Barr, Jones & Walker, 1979). Structure–activity correlations (Goodchild, Porter, Raper, Sim, Upton, Vitney & Wadsworth, 1983) for olefinic 5-substituted-2′-deoxyuridines indicate that optimum inhibition of HSV-1 occurs when the C(5) olefinic substituent is conjugated with the pyrimidine ring, is not longer than four carbon atoms in length, has *E* stereochemistry and includes a hydrophobic electronegative atom. Exploitation of differences between virus-specific enzymes and the corresponding host-cell enzymes provides a promising strategy in the design of more effective and less toxic antiherpes drugs. It was thus anticipated that 1-(2-deoxy-β-D-ribofuranosyl)uracil possessing a 5-(2,2-dibromocyclopropyl) substituent could act as a biological isostere of the 5-(2-bromovinyl) substituent present in BVDU. The hybridization of the cyclopropane ring results in a higher electron density along the C—C bonds, making them more like those of

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ethylene than those of ethane. The cyclopropane ring can be viewed as a small ring with 'double-bond character'. Furthermore, a cyclopropyl group can interact with neighboring π-electron systems and p-electron centers in a fashion similar to a vinyl group (De Meijere, 1979; Gassman, 1967). Recently we prepared two diastereomers of the title compound and the crystal structure of one diastereomer was determined to ascertain the absolute configuration about C(7) of the 2,2-dibromocyclopropyl moiety.

Experimental. The title compound recrystallized from MeOH:$CHCl_3$ [9:1(v/v)] as translucent white plates. Space group determined by systematic absences in diffractometer-collected intensity data. Unit-cell parameters determined by least-squares refinement of 25 high-angle reflections ($80 \le 2\theta \le 118°$) constrained to an orthorhombic cell. Data collected on an Enraf–Nonius CAD-4 diffractometer, Cu $K\alpha$ radiation with Ni filter, crystal dimensions $0{\cdot}120 \times 0{\cdot}100 \times 0{\cdot}500$ mm.

A hemisphere of data ($-6 \le h \le 0$, $-20 \le k \le +20$, $-15 \le l \le +15$) corresponding to $1{\cdot}5 \le \theta \le 60°$ was collected. These 4799 measurements were averaged over 222 symmetry to give 2148 reflections ($R_{merge} = 0{\cdot}017$). Three of these reflections, 102, 103, 230, were deleted due to large secondary extinction; all of the remaining 2145 reflections were considered observed and used in the subsequent refinement. Empirical absorption and Lorentz polarization factors were applied. Max. and min. transmission 1·000 and 0·679. Four check reflections, $0\bar{7}\bar{3}$, $\bar{2}5\bar{1}$, $0\bar{7}3$ and $\bar{4}00$, were collected after every four hours of exposure time and no significant variation in intensity was observed. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974, pp. 99–102). All calculations were carried out using *LATCON* (Stewart, Kruger, Ammon, Dickinson & Hall, 1976), *XTAL*2.2 (Hall & Stewart, 1987) and *ORTEP*II (Johnson, 1976) software.

The bromine coordinates were determined from a Patterson map (Patterson, 1935; Stout & Jensen, 1968) and a preliminary electron density map ($R = 0{\cdot}316$) was generated from these coordinates. The remaining non-hydrogen atoms were evident in this initial ΔF map. Least-squares refinement on F of the 21 non-hydrogen-atom coordinates and U's reduced R to 0·180, and at this point non-hydroxyl hydrogen atoms were introduced with idealized geometries. Isotropic H-atom coordinates were fixed for all subsequent refinement. H(O3′) was located on a partially refined difference Fourier map but no peak corresponding to H(O5′) was found. Hence H(O5′) was introduced such that it would form a linear hydrogen bond with O4′ (see Table 3). Subsequent cycles of full-matrix least-squares refinement with scale factor and anisotropic Gaussian parameters for all non-hydrogen atoms resulted in $R = 0{\cdot}037$, $wR = 0{\cdot}030$, $w = \sigma_F^{-2}$, GOF = 2·6 (190 parameters) for the 1S invertomer (Table 1) and $R = 0{\cdot}046$, $wR = 0{\cdot}042$, $w = \sigma_F^{-2}$, GOF = 3·6 for the 1R invertomer. Hence the absolute configuration about C(7) of the cyclopropane ring was deduced to be S. This was confirmed by the correct stereochemistry of the β-(2′)-deoxyribose. The maximum shift/e.s.d. was 0·02 and the average shift/e.s.d. was 0·003 after the final cycle of refinement. The largest peak in the final ΔF map was 0·49 e Å^{-3} and the largest hole was 0·98 e Å^{-3}.

Table 1. *Non-hydrogen-atom coordinates and equivalent isotropic Gaussian parameters* (Å^2 × 10^3)

	x	y	z	U_{eq}†
Br(91)	0·40800 (9)	0·24622 (3)	0·92096 (4)	43·4 (1)
Br(92)	0·13452 (9)	0·12702 (2)	0·80506 (4)	45·0 (1)
C(9)	0·1873 (8)	0·2274 (2)	0·8201 (3)	32·3 (9)
C(8)	−0·0075 (8)	0·2785 (2)	0·8069 (4)	38·5 (9)
C(7)	0·1831 (8)	0·2750 (2)	0·7281 (3)	32·3 (10)
C(6)	0·3505 (7)	0·3922 (2)	0·7729 (3)	25·6 (8)
C(5)	0·3513 (8)	0·3325 (2)	0·7160 (3)	28·5 (9)
C(4)	0·5389 (8)	0·3203 (2)	0·6480 (3)	30·0 (10)
O(4)	0·5645 (6)	0·2678 (2)	0·5949 (3)	50·9 (9)
N(3)	0·6995 (6)	0·3749 (2)	0·6451 (3)	28·7 (8)
C(2)	0·7140 (8)	0·4319 (2)	0·7095 (3)	27·3 (9)
O(2)	0·8808 (5)	0·4721 (1)	0·7114 (2)	34·5 (6)
N(1)	0·5293 (6)	0·4417 (2)	0·7705 (2)	27·0 (7)
C(5′)	0·1458 (10)	0·4579 (3)	1·0310 (3)	38·9 (10)
O(5′)	0·0022 (6)	0·4464 (2)	0·9486 (2)	43·9 (8)
C(4′)	0·3505 (8)	0·5031 (2)	1·0049 (3)	28·5 (8)
O(4′)	0·5082 (5)	0·4638 (1)	0·9414 (2)	26·7 (6)
C(3′)	0·3033 (8)	0·5737 (2)	0·9494 (3)	29·7 (9)
O(3′)	0·4677 (6)	0·6245 (2)	0·9828 (2)	41·6 (7)
C(2′)	0·3414 (8)	0·5526 (2)	0·8412 (3)	29·4 (9)
C(1′)	0·5308 (7)	0·4982 (2)	0·8482 (3)	25·0 (8)

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

Discussion. Atomic coordinates and equivalent isotropic Gaussian parameters (U_{eq}'s) with e.s.d.'s (Schomaker & Marsh, 1983) are given in Table 1.* Bond lengths and angles are given in Table 2. Table 3 contains hydrogen-bonding information and Table 4 lists the important torsion angles for the deoxyribonucleoside. Fig. 1 is an *ORTEP*II (Johnson, 1976) plot with 50% thermal ellipsoids. Fig. 2 is a stereo *ORTEP* representation of the molecule with a proposed hydrogen-bonding scheme.

Bond lengths and angles are similar to those of deoxyuridine (Green, Rosenstein, Shiono, Abraham, Trus & Marsh, 1975) and of the (1,1-dibromocyclopropyl) moiety in other compounds (Lauher & Ibers, 1975; Jason & Ibers, 1977). Similar to most other pyrimidine deoxyribonucleosides, the pyrimidine ring is

*Lists of anisotropic Gaussian parameters, least-squares-plane information, structure factor amplitudes and hydrogen coordinates plus isotropic Gaussian parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51536 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

Br(91)–C(9)	1·905 (4)	C(4)–O(4)	1·218 (5)
Br(92)–C(9)	1·903 (4)	C(2)–O(2)	1·232 (5)
C(8)–C(9)	1·496 (6)	N(1)–C(1′)	1·483 (5)
C(7)–C(9)	1·520 (6)	C(1′)–C(2′)	1·506 (6)
C(7)–C(8)	1·540 (7)	C(2′)–C(3′)	1·521 (6)
C(5)–C(7)	1·464 (6)	C(3′)–C(4′)	1·535 (6)
C(5)–C(6)	1·350 (5)	C(4′)–C(5′)	1·507 (7)
C(4)–C(5)	1·447 (6)	C(3′)–O(3′)	1·422 (5)
N(3)–C(4)	1·385 (6)	C(5′)–O(5′)	1·407 (6)
C(2)–N(3)	1·371 (5)	C(1′)–O(4′)	1·412 (5)
N(1)–C(2)	1·370 (6)	C(4′)–O(4′)	1·454 (5)
N(1)–C(6)	1·394 (5)		

Br(91)–C(9)–Br(92)	111·5 (2)	O(2)–C(2)–N(1)	122·2 (4)
Br(91)–C(9)–C(8)	119·0 (3)	C(2)–N(1)–C(1′)	120·7 (4)
Br(91)–C(9)–C(7)	118·8 (3)	C(2)–N(1)–C(6)	121·4 (3)
Br(92)–C(9)–C(8)	119·1 (3)	C(1′)–N(1)–C(6)	117·1 (3)
Br(92)–C(9)–C(7)	118·9 (3)	N(1)–C(1′)–O(4′)	107·6 (3)
C(8)–C(9)–C(7)	61·4 (3)	N(1)–C(1′)–C(2′)	115·4 (3)
C(9)–C(8)–C(7)	60·1 (3)	O(4′)–C(1′)–C(2′)	106·9 (3)
C(8)–C(7)–C(9)	58·5 (3)	C(5)–C(6)–N(1)	121·8 (4)
C(7)–C(5)–C(6)	122·5 (4)	C(1′)–O(4′)–C(4′)	110·6 (3)
C(7)–C(5)–C(4)	117·9 (3)	O(4′)–C(4′)–C(3′)	105·0 (3)
C(4)–C(5)–C(6)	119·3 (4)	O(4′)–C(4′)–C(5′)	111·2 (3)
C(5)–C(4)–O(4)	126·0 (4)	C(3′)–C(4′)–C(5′)	116·5 (4)
C(5)–C(4)–N(3)	114·8 (3)	C(4′)–C(3′)–O(3′)	107·0 (3)
C(4)–C(4)–N(3)	119·2 (4)	C(4′)–C(3′)–C(2′)	102·5 (3)
C(4)–N(3)–C(2)	126·3 (4)	O(3′)–C(3′)–C(2′)	111·9 (3)
N(3)–C(2)–O(2)	122·3 (4)	C(1′)–C(2′)–C(3′)	102·8 (3)
N(3)–C(2)–N(1)	115·6 (4)	C(4′)–C(5′)–O(5′)	112·2 (3)

Table 3. *Hydrogen-bond lengths* (Å) *and angles* (°)

*D*H	*A*′	*D*H···*A*′	∠(*D*–H···*A*)	Symmetry operator on *A*
N(3)	O(3′)	2·92	164	$\frac{3}{2}-x, 1-y, z-\frac{1}{2}$
O(3′)	O(4)	2·87	177	$1-x, y+\frac{1}{2}, \frac{3}{2}-z$
O(5′)	O(4′)	2·92	180*	$x-1, y, z$
C(9)	O(5′)	3·28	172	x, y, z

*H(O5′) coordinates calculated to fit a linear hydrogen bond to O(4′).

Table 4. *Characteristic torsion angles* (°)

χ	O(4′)–C(1′)–N(1)–C(2)	−118·4 (4)
γ	O(5′)–C(5′)–C(4′)–C(3′)	50·4 (5)
δ	C(5′)–C(4′)–C(3′)–O(3′)	145·6 (3)
ν_0	C(4′)–O(4′)–C(1′)–C(2′)	−13·1 (4)
ν_1	O(4′)–C(1′)–C(2′)–C(3′)	29·9 (4)
ν_2	C(1′)–C(2′)–C(3′)–C(4′)	−34·3 (4)
ν_3	C(2′)–C(3′)–C(4′)–O(4′)	27·1 (4)
ν_4	C(3′)–C(4′)–O(4′)–C(1′)	−9·2 (4)

anti with respect to the furanose [$\chi = -118{\cdot}4\ (4)°$, see Table 4 for definitions of torsion angles], and the deoxyribose is in the 2′-*endo* conformation. For 2′-*endo* pyrimidines, $-144 \le \chi \le -115°$ (Saenger, 1984). The deoxyribose puckering mode is described by *P*, the pseudorotation phase angle (Altona & Sundaralingam, 1972; Saenger, 1984). Here, $P = 176{\cdot}3°$ which designates the deoxyribose ring as being $^2T_3$, a variant of the 2′-*endo* mode, in agreement with least-squares-plane calculations for the deoxyribose moiety. The ring pucker amplitude $\tau_m = 35{\cdot}5°$, which is in agreement with $\langle\tau_m\rangle = 38 \pm 3°$ that is observed for nucleosides.

The glycosidic C(1′)–N(1) bond length is 1·483 (5) Å, again indicating the *anti* conformer as the value of the C(1′)–N(1) bond length is linearly correlated to the C(1′)–N(1) torsion angle (Hung-Yin Lin, Sundaralingam & Arora, 1971; Saenger, 1984). As the torsion angle goes from 180 to −140°, the glycosidic bond length in pyrimidines falls nearly monotonically from 1·51 to 1·48 Å.

Another important stereochemical feature of deoxyribonucleosides is the orientation of the (5′)-methoxyl group with respect to the furanose ring which is specified by γ, the C(4′)–C(5′) torsion angle (Shefter

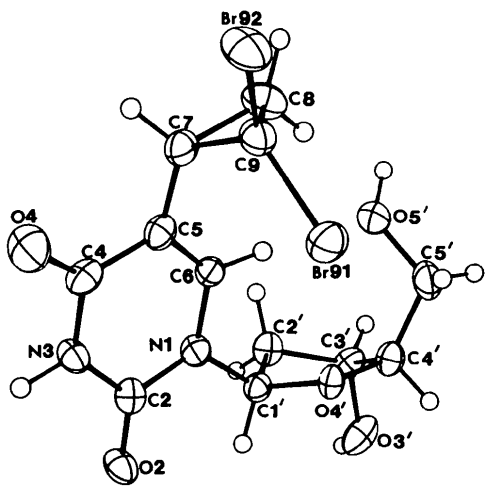

Fig. 1. An *ORTEP*II (Johnson, 1976) drawing of the title compound including the atomic numbering scheme. Thermal ellipsoids are at the 50% probability level and hydrogen atoms are spheres of arbitrary size.

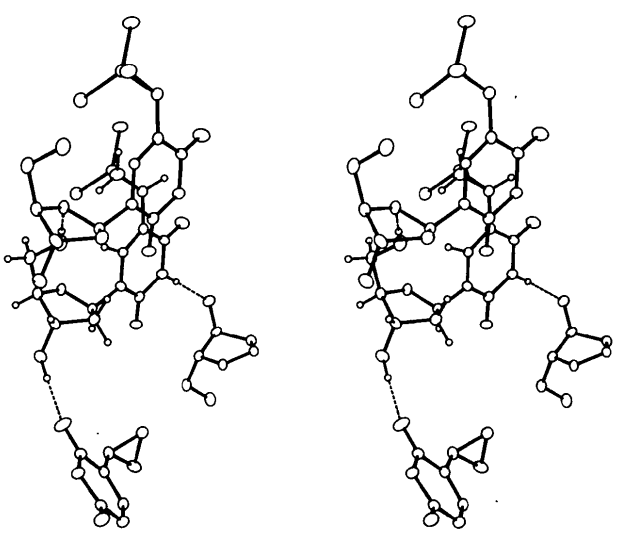

Fig. 2. A stereo *ORTEP*II drawing illustrating the hydrogen-bonding scheme. Bonds shown (dashed lines) are N(3) to O(3′), O(3′) to O(4) and O(5′) to O(4′).

& Trueblood, 1965). The preferred mode γ in pyrimidine nucleoside crystal structures is *gauche–gauche* (Saenger, 1984) and in accord with this $\gamma = 50{\cdot}4\ (4)°$.

The pyrimidine ring is approximately planar, with the greatest deviation from the six-atom least-squares plane being 0·05 Å. The molecular packing is characterized by herringbone stacking of the uridine bases with an interplanar spacing of 3·1 Å. There are three hydrogen bonds and they are listed with their corresponding symmetry operations in Table 3. The O(5′) donates a hydrogen bond to the deoxyribose ether oxygen and the pyrimidine H(6) is also situated in an ideal geometry to donate a hydrogen bond to O(5′) although C(6)–H(6) is not a classical hydrogen-bond donor. The C(6)–O(5′) contact distance is 3·28 Å and the C–H···O angle is 172°.

Both bromine atoms exhibit large U_{eq}'s, presumably due to the inability of the applied absorption correction adequately to account for the high absorption coefficient of bromine. The Br–C bond distance is 1·904 Å, giving a bromine covalent radius of 1·1 Å and a bromine van der Waals radius of 1·8 Å. Indeed, the closest Br–Br contact observed has a contact distance of 3·62 Å, twice the calculated van der Waals radius for bromine. In addition, note the 2·89 Å contact between Br(92) and O(4) which is 0·3 Å shorter than the sum of the van der Waals radii of bromine and oxygen.

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Structure of Droperidol–Ethanol (1/1)

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Abstract. 1-{1-[4-(4-Fluorophenyl)-4-oxobutyl]-1,2,-3,6-tetrahydro-4-pyridyl}-1,3-dihydro-2*H*-benzimidazol-2-one ethanol solvate, $C_{22}H_{22}FN_3O_2.C_2H_6O$, $M_r = 426{\cdot}3$, triclinic, $P\bar{1}$, $a = 6{\cdot}083\ (3)$, $b = 10{\cdot}296\ (1)$, $c = 16{\cdot}018\ (2)$ Å, $\alpha = 100{\cdot}93\ (1)$, $\beta = 92{\cdot}72\ (2)$, $\gamma = 96{\cdot}27\ (2)°$, $V = 976{\cdot}7$ Å^3, $Z = 2$, $D_x = 1{\cdot}45$ g cm^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71073$ Å, $\mu = 0{\cdot}97$ cm^{-1}, $F(000) = 452$, $T = 90\ (2)$ K, final $R = 0{\cdot}046$ for 2261

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