(1974) for hydrogen bonds involving ureido groups. The latter investigators point out that the ureido groups are hydrogen-bond acids and that they therefore form long hydrogen bonds when used as acceptors. The second amino hydrogen H(N4A) does not form any hydrogen bonds. Cases where a potential hydrogen donor is not involved in any close contacts are very rare. H(N4A) appears to be directed towards the center of the phenyl ring of the molecule related by the transformation $\frac{1}{2} - x$, $-\frac{1}{2} + y$, $\frac{3}{2} - z$. The closest atoms are C(5) and C(6): N(4)···C(5)　3·508 (2), H(N4A)···C(5)　2·66 (2); N(4)···C(6)　3·480 (2), H(N4A)···C(6)　2·69 (2) Å. If this interaction between the amino group and the π cloud of the phenyl ring is energetically favorable, it may also contribute to the weakening of the hydrogen bond involving H(N4B). The only other short intermolecular contact is the 3·240 (2) Å contact between C(5) and O(10) ($\frac{1}{2} - x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$).

References

BANTING, L., SMITH, H. J., JAMES, M., JONES, G., NAZARETH, W., NICHOLLS, P. J., HEWLINS, M. J. E. & ROWLANDS, M. G. (1988). *J. Enzyme Inhib.* **2**, 215–229.

BLESSING, R. H. (1987). *Crystallogr. Rev.* **1**, 3–57.

CAMACHO, A. M., BROUGH, A. J., CASH, R. & WILROY, R. (1966). *J. Pediatr.* **68**, 852–853.

Enraf–Nonius (1979). *Structure Determination Package*. Enraf–Nonius, Delft, The Netherlands.

FINCH, N., DZIEMIAN, R., COHEN, J. & STEINETZ, B. G. (1975). *Experientia*, **31**, 1002–1003.

GARTLAND, G. L. & CRAVEN, B. M. (1974). *Acta Cryst.* **B30**, 980–987.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* **A27**, 368–376.

JOHNSON, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

KIM, S.-H. & RICH, A. (1968). *Proc. Natl Acad. Sci. USA*, **60**, 402–408.

SANTEN, R. J., WORGUL, T. J., SAMOJLIK, E., BOUCHER, A. E., LIPTON, A. & HARVEY, H. (1982). *Cancer Res. Suppl.* **42**, 3397s.

SHAW, M. A., NICHOLLS, P. J. & SMITH, H. J. (1988). *J. Steroid Biochem.* **31**, 137–146.

STOUT, G. H. & JENSEN, L. H. (1968). *X-ray Structure Determination*. New York: Macmillan.

VOET, D. (1972). *J. Am. Chem. Soc.* **94**, 8213–8222.

WILLIAMS, P. P. (1973). *Acta Cryst.* **B29**, 1572–1579.

WILLIAMS, P. P. (1974). *Acta Cryst.* **B30**, 12–17.

Structure of the Modified Nucleoside 2',3'-Dideoxy-3'-fluorocytidine*

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Abstract. 1-(2,3-Dideoxy-3-fluoro-β-D-*erythro*-pentofuranosyl)cytosine, $C_9H_{12}FN_3O_3$, $M_r = 229\cdot21$, triclinic, $P1$, $a = 6\cdot997$ (4), $b = 7\cdot396$ (4), $c = 10\cdot639$ (5) Å, $\alpha = 94\cdot48$ (4), $\beta = 107\cdot74$ (4), $\gamma = 104\cdot40$ (4)°, $V = 500\cdot8$ (5) Å^3, $Z = 2$, $D_m = 1\cdot52$, $D_x = 1\cdot520$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0\cdot71069$ Å, $\mu = 0\cdot1198$ mm^{-1}, $F(000) = 240$, $T = 293$ K, final $R = 0\cdot033$ for 2321 unique observed [$F \geq 4\sigma(F)$] reflections. The asymmetric unit contains two molecules A and B. For molecule A, the N-glycosidic torsion angle χ has a value of $-143\cdot5$ (3)°, the sugar pucker is mixed $^2T_1/^2E$ with $P = 154$ (1) (C2' *endo*) and $\psi_m = 40$ (1)°, and the O5'A—C5'A—C4'A—C3'A torsion angle $\gamma = 63\cdot4$ (4)°. For molecule B, $\chi = -153\cdot0$ (3), $\gamma = -71\cdot4$ (4)° and the sugar pucker is ^2E with $P = 164$ (1) (C2' *endo*) and $\psi_m = 36$ (1)°. The packing of the crystal is determined by a network of hydrogen bonds. Base pairing between A and B occurs, and in this way a pseudo-inversion centre is formed between the two bases. The conformational parameters are in accordance with the IUPAC–IUB Joint Commission on Biochemical Nomenclature [*Pure Appl. Chem.* (1983), **55**, 1273–1280] guidelines.

Experimental. The crystal structure of the title compound has been determined as part of a continuing program of investigation of potentially antiviral modified nucleosides, with particular reference to possible anti-AIDS compounds. The method of preparation of the product has been described by Herdewijn, Balzarini, De Clercq, Pauwels, Baba, Broder & Vanderhaeghe (1987). Colourless prismatic crystals from a methanol–amyl acetate solution, $0.3 \times 0.4 \times 0.5$ mm. Density measured by flotation in *n*-heptane/CCl_4. Weissenberg photographs show no systematically absent reflections. Stoe STADI-4 diffractometer, cell constants by least-squares refinement of the setting angles of 24 reflections with $20 \leq 2\theta \leq 30^\circ$, $\omega/2\theta$ scan, $[(\sin\theta)/\lambda]_{max} = 0.7035$ Å^{-1}, $0 \leq h \leq 10$, $-10 \leq k \leq 10$, $-15 \leq l \leq 15$. Intensities of three standard reflections (200, 020, 002) monitored every hour showed no significant decrease in intensity, 3143 reflections measured, 2920 unique reflections of which 2321 were considered observed with $F \geq 4\sigma(F)$. Data reduction with *REDU*4 (Stoe & Co., 1985), Lorentz and polarization corrections, no absorption corrections ($\mu = 0.1198$ mm^{-1}). Scattering factors were taken from *International Tables for X-ray Crystallography* (1974, Vol. IV, Table 2.2B) and for H atoms from Stewart, Davidson & Simpson (1965). Anomalous-dispersion corrections were included for all non-H atoms (Ibers & Hamilton, 1964). Initial attempts to solve the structure with *MULTAN*82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) resulted always in the well known 'chicken-wire' *E* maps. Modification of the default input parameters did not resolve this problem. Comparison of the averaged powers of the normalized structure factors *E* with comparable theoretical values suggested a pseudo-centrosymmetric symmetry for the crystal. Therefore, as an alternative approach to solving the phase problem, the vector-search method was tried. In space group *P*1, only the orientation of the molecules with respect to the crystallographic axes has to be determined. For this purpose, the 1-methylcytosine skeleton was used as an input model for the vector-search rotation-function program *ORIENT* (Beurskens, Beurskens, Strumpel & Nordman, 1987). A default run, with an initial average step scan of 10° and a 0.3 Å grid for the Patterson map did not reveal the correct orientation of the fragment. A second run, with an initial average step scan of 5°, was more successful, and the correctly oriented fragment was subsequently used as input for *DIRDIF* (Beurskens, Bosman, Doesburg, Van den Hark, Prick, Noordik, Beurskens, Gould & Parthasarathi, 1983), which revealed 26 of the 32 non-H atoms. The remaining atoms were located in a subsequent difference map. Refinement on *F* by full-matrix least squares, first with isotropic temperature factors and finally anisotropically. All H atoms were

found in a difference synthesis and they were included in the refinement with a fixed temperature factor $B = 4.0$ Å^2. Final $R = 0.033$, $wR = 0.041$, with $w = 1/[\sigma^2(F_o) + 0.0004F_o^2]$, $S = 1.43$. Largest parameter shift/e.s.d $= 0.02$. Minimum and maximum residual electron density -0.21 and 0.20 e Å^{-3}. The number of reflections per refined parameter 2321/358 $= 6.5$. All calculations were performed on a Digital PDP-11/73 and MicroVAX 2000 microcomputer using *SDP* (Enraf–Nonius, 1985) and *PARST* (Nardelli, 1983).

Discussion. A *PLUTO* view (Motherwell & Clegg, 1978) of the title compound with the atomic numbering scheme is shown in Fig. 1.* The final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1. Bond lengths, bond angles and selected torsion angles are given in Table 2. Table 3 gives the geometry of all hydrogen bonds.

A least-squares fit procedure with the program *BMFIT* (Nyburg, 1974) on the atoms of the cytosine base showed a close geometrical similarity between the cytosine bases of *A* and *B* (r.m.s. deviation $= 0.039$ Å). Except for the C2—O2 bond length of molecule *A* [1.253 (3) Å], which is longer than the standard C=O distance of 1.215 Å, all other bond

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* Lists of structure factors, anisotropic thermal parameters, bond lengths and angles involving H atoms, least-squares planes and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53460 (29 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.
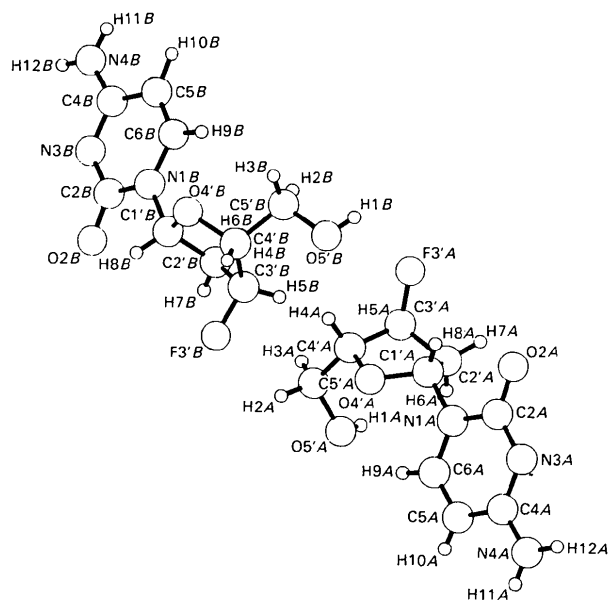

Fig. 1. *PLUTO* plot (Motherwell & Clegg, 1978) of the title compound with atomic numbering scheme.

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* ($\text{Å}^2 \times 10^4$) *with e.s.d.'s in parentheses*

$$U_{eq} = (1/3)\Sigma_i \Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
N1A	−0·0907 (2)	0·6872 (2)	0·0697 (2)	304 (4)
C2A	−0·1364 (3)	0·8329 (3)	0·0009 (2)	306 (5)
O2A	−0·2949 (2)	0·8824 (2)	0·0014 (2)	449 (4)
N3A	−0·0068 (3)	0·9188 (3)	−0·0622 (2)	330 (4)
C4A	0·1642 (3)	0·8657 (3)	−0·0568 (2)	283 (5)
N4A	0·2897 (3)	0·9594 (3)	−0·1180 (2)	360 (4)
C5A	0·2115 (3)	0·7147 (3)	0·0099 (2)	346 (5)
C6A	0·0806 (3)	0·6277 (3)	0·0705 (2)	341 (5)
C1'A	−0·2368 (3)	0·6916 (3)	0·1334 (2)	307 (5)
C2'A	−0·3856 (3)	0·4048 (3)	0·0534 (2)	379 (5)
C3'A	−0·4499 (3)	0·2130 (3)	0·1609 (2)	357 (5)
F3'A*	−0·602	0·392	0·185	355 (4)
C4'A	−0·2522 (3)	0·3796 (3)	0·2829 (2)	303 (5)
O4'A	−0·1211 (2)	0·5464 (2)	0·2563 (2)	345 (4)
C5'A	−0·1318 (4)	0·2354 (3)	0·3153 (3)	406 (5)
O5'A	−0·0538 (3)	0·1866 (3)	0·2129 (2)	545 (5)
N1B	−0·7225 (2)	−0·4424 (2)	0·6593 (2)	286 (4)
C2B	−0·6810 (3)	−0·6004 (3)	0·7154 (2)	278 (4)
O2B	−0·5138 (2)	−0·6331 (2)	0·7223 (2)	412 (4)
N3B	−0·8257 (3)	−0·7096 (2)	0·7599 (2)	300 (4)
C4B	−1·0079 (3)	−0·6712 (3)	0·7444 (2)	269 (4)
N4B	−1·1416 (3)	−0·7760 (3)	0·7951 (2)	363 (5)
C5B	−1·0602 (3)	−0·5221 (3)	0·6764 (2)	332 (5)
C6B	−0·9127 (3)	−0·4101 (3)	0·6374 (2)	316 (5)
C1'B	−0·5594 (3)	−0·3229 (3)	0·6160 (2)	307 (5)
C2'B	−0·5812 (3)	−0·3859 (3)	0·4717 (2)	385 (5)
C3'B	−0·4811 (3)	−0·2022 (3)	0·4341 (2)	409 (5)
F3'B	−0·2621 (2)	−0·1686 (2)	0·4801 (2)	704 (5)
C4'B	−0·5387 (3)	−0·0558 (3)	0·5112 (2)	341 (5)
O4'B	−0·5806 (3)	−0·1371 (2)	0·6230 (2)	373 (4)
C5'B	−0·7321 (3)	−0·0070 (3)	0·4296 (2)	421 (5)
O5'B	−0·6731 (3)	0·0992 (3)	0·3350 (2)	663 (5)

* Positional parameters kept fixed during the refinement.

lengths and bond angles are normal (for tables, see Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The O2's of modified cytidine nucleosides with a similar elongated C2—O2 bond length are always involved in strong hydrogen bonding (Lalitha, Ramakumar & Viswamitra, 1989).

The pyrimidine heterocycles of both bases are almost planar, with only minor deviations from the weighted least-squares planes [max. deviation for molecule *A*: −0·014 (3) Å C4*A*; for molecule *B*: 0·033 (3) Å C2*B*].

Since the geometry of both bases is almost identical, a least-squares fit [*BMFIT*; Nyburgh (1974)] on the atoms of the bases reveals some conformational differences in the sugar rings and their substituents: an r.m.s. deviation of 0·742 Å between the atoms of the sugar rings and substituents (atoms C1' through O5') was calculated. A minor deviation is found in the orientation of the base relative to the sugar moiety, which globally is *anti* for both molecules, but $\chi = -143\cdot5$ (3) for *A* and $-153\cdot0$ (3)° for *B*. The $^2T_1/^2E$ and ^2E puckers of *A* and *B*, respectively, together with the puckering amplitudes of 40 (1) and 36 (1)°, respectively, are all normal (Saenger, 1988) and almost equal. The orientation of O5' with respect to the sugar moiety, described by the O5' —C5'—C4'—C3' torsion angle γ, is different for molecules *A* and *B*. In the first we find a $+sc$

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

N1A—C2A	1·397 (3)	N1B—C2B	1·407 (3)
N1A—C6A	1·373 (4)	N1B—C6B	1·364 (3)
N1A—C1'A	1·463 (3)	N1B—C1'B	1·475 (3)
C2A—O2A	1·253 (3)	C2B—O2B	1·235 (3)
C2A—N3A	1·352 (4)	C2B—N3B	1·359 (3)
N3A—C4A	1·336 (4)	N3B—C4B	1·338 (3)
C4A—N4A	1·338 (4)	C4B—N4B	1·333 (3)
C4A—C5A	1·423 (3)	C4B—C5B	1·428 (3)
C5A—C6A	1·342 (3)	C5B—C6B	1·347 (3)
C1'A—C2'A	1·509 (3)	C1'B—C2'B	1·519 (3)
C1'A—O4'A	1·426 (3)	C1'B—O4'B	1·417 (3)
C2'A—C3'A	1·501 (4)	C2'B—C3'B	1·509 (3)
C3'A—F3'A	1·413 (3)	C3'B—F3'B	1·408 (3)
C3'A—C4'A	1·520 (3)	C3'B—C4'B	1·512 (4)
C4'A—O4'A	1·447 (3)	C4'B—O4'B	1·449 (4)
C4'A—C5'A	1·514 (4)	C4'B—C5'B	1·514 (3)
C5'A—O5'A	1·418 (4)	C5'B—O5'B	1·419 (4)

C2A—N1A—C6A	120·7 (2)	C2B—N1B—C6B	120·7 (2)
C2A—N1A—C1'A	118·4 (2)	C2B—N1B—C1'B	117·5 (2)
C6A—N1A—C1'A	120·9 (2)	C6B—N1B—C1'B	121·7 (2)
N1A—C2A—O2A	118·9 (3)	N1B—C2B—O2B	118·3 (2)
N1A—C2A—N3A	119·3 (3)	N1B—C2B—N3B	118·8 (2)
O2A—C2A—N3A	121·8 (3)	O2B—C2B—N3B	122·9 (3)
C2A—N3A—C4A	119·9 (2)	C2B—N3B—C4B	120·0 (2)
N3A—C4A—N4A	117·3 (3)	N3B—C4B—N4B	118·3 (2)
N3A—C4A—C5A	121·8 (3)	N3B—C4B—C5B	121·8 (2)
N4A—C4A—C5A	120·9 (3)	N4B—C4B—C5B	120·0 (2)
C4A—C5A—C6A	118·0 (2)	C4B—C5B—C6B	117·6 (3)
N1A—C6A—C5A	120·3 (2)	N1B—C6B—C5B	120·8 (3)
N1A—C1'A—C2'A	114·3 (2)	N1B—C1'B—C2'B	113·3 (1)
N1A—C1'A—O4'A	109·1 (2)	N1B—C1'B—O4'B	108·2 (2)
C2'A—C1'A—O4'A	105·1 (2)	C2'B—C1'B—O4'B	106·0 (2)
C1'A—C2'A—C3'A	100·9 (2)	C1'B—C2'B—C3'B	101·7 (2)
C2'A—C3'A—F3'A	107·2 (2)	C2'B—C3'B—F3'B	109·0 (2)
C2'A—C3'A—C4'A	103·7 (2)	C2'B—C3'B—C4'B	103·5 (2)
F3'A—C3'A—C4'A	108·4 (2)	F3'B—C3'B—C4'B	109·6 (2)
C3'A—C4'A—O4'A	106·2 (2)	C3'B—C4'B—O4'B	106·4 (2)
C3'A—C4'A—C5'A	114·9 (2)	C3'B—C4'B—C5'B	113·4 (2)
O4'A—C4'A—C5'A	109·6 (2)	O4'B—C4'B—C5'B	108·4 (3)
C1'A—O4'A—C4'A	108·1 (2)	C1'B—O4'B—C4'B	109·4 (2)
C4'A—C5'A—O5'A	112·8 (2)	C4'B—C5'B—O5'B	106·3 (2)
C2'A—C1'A—O4'A—C4'A	−28·6 (2)	C2'B—C1'B—O4'B—C4'B	−20·4 (2)
O4'A—C1'A—C2'A—C3'A	39·9 (2)	O4'B—C1'B—C2'B—C3'B	34·2 (2)
C1'A—C2'A—C3'A—C4'A	−35·5 (2)	C1'B—C2'B—C3'B—C4'B	−34·3 (2)
C2'A—C3'A—C4'A—O4'A	19·7 (2)	C2'B—C3'B—C4'B—O4'B	23·4 (2)
C3'A—C4'A—O4'A—C1'A	5·4 (2)	C3'B—C4'B—O4'B—C1'B	−1·9 (2)

Table 3. *Geometry of intra- and intermolecular hydrogen bonds* (Å, °) *with e.s.d.'s in parentheses*

X—H···Y	d(H···Y)	d(X···Y)	X—H···Y
O5'A—H1A···O2A^i	2·06 (3)	2·825 (3)	162 (3)
N4A—H11A···O2A^ii	2·25 (3)	3·012 (3)	153 (3)
N4A—H12A···N3B^iii	2·09 (3)	3·029 (3)	172 (3)
N4B—H11B···O2B^iv	2·12 (4)	2·961 (3)	164 (3)
O5'B—H1B···O5'A^iv	2·06 (3)	2·843 (3)	162 (3)
N4B—H12B···N3A^v	2·09 (3)	3·002 (3)	172 (3)

Symmetry code: (i) $x, y - 1, z$; (ii) $x + 1, y, z$; (iii) $x + 1, y + 2, z - 1$; (iv) $x - 1, y, z$; (v) $x - 1, y - 2, z + 1$.

orientation [$\gamma = 63\cdot4$ (4)°], while in molecule *B* [$\gamma = -71\cdot4$ (4)°], we find the unusual $-sc$ conformation.

The packing of the crystal is totally determined by a network of hydrogen bonds, as shown in Fig. 2 and summarized in Table 3. Base pairing between molecules *A* and *B* occurs, since every H12 is hydrogen bonded to N3 of the opposite molecule. In this way, a pseudo ring between the bases of *A* and *B* is formed. The centre of this pseudo ring coincides with a pseudo-inversion centre between both bases, which explains the pseudo-centrosymmetric nature of the crystal. A strong
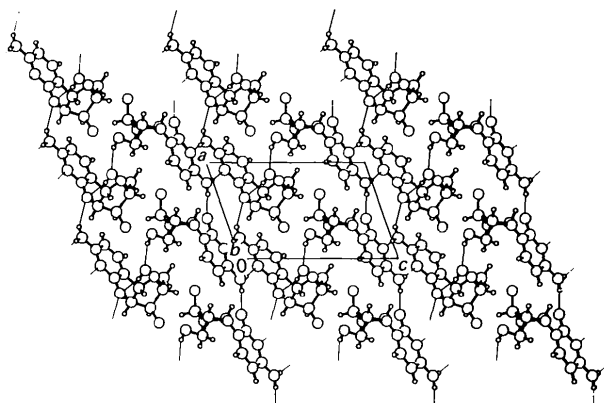
Fig. 2. *PLUTO* plot (Motherwell & Clegg, 1978) of the crystal packing along **b**. Thin lines indicate hydrogen bonds.

hydrogen-bond network along the crystallographic *a* axis is formed by O2*B* and H11*B*—N4*B*, while the packing along **b** is determined by hydrogen bonds between O5'*A*—H1*A* and O2*A*.

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References

ALLEN, F. H., KENNARD, O., WATSON, D. G., BRAMMER, L., ORPEN, A. G. & TAYLOR, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–S19.

BEURSKENS, P. T., BEURSKENS, G., STRUMPEL, M. & NORDMAN, C. E. (1987). *Patterson and Pattersons*, edited by J. P. GLUSKER, B. K. PATTERSON & M. ROSSI, pp. 356–367. Oxford Univ. Press.

BEURSKENS, P. T., BOSMAN, W. P., DOESBURG, H. M., VAN DEN HARK, T. E. M., PRICK, P. A. J., NOORDIK, J. H., BEURSKENS, G., GOULD, R. O. & PARTHASARATHI, V. (1983). *DIRDIF. Applications of Direct Methods to Difference Structure Factors.* Univ. of Nijmegen, The Netherlands.

Enraf–Nonius (1985). *Structure Determination Package.* Enraf–Nonius, Delft, The Netherlands.

EVERAERT, D. H., PEETERS, O. M., BLATON, N. M., DE RANTER, C. J., VAN AERSCHOT, A. & HERDEWIJN, P. (1991). *Acta Cryst.* C47, 678–680.

HERDEWIJN, P., BALZARINI, J., DE CLERCQ, E., PAUWELS, R., BABA, M., BRODER, S. & VANDERHAEGHE, H. (1987). *J. Med. Chem.* 30, 1270–1278.

IBERS, J. A. & HAMILTON, W. C. (1964). *Acta Cryst.* 17, 781–782.

IUPAC-IUB JOINT COMMISSION ON BIOCHEMICAL NOMENCLATURE (1983). *Pure Appl. Chem.* 55, 1273–1280.

LALITHA, H. N., RAMAKUMAR, S. & VISWAMITRA, M. A. (1989). *Acta Cryst.* C45, 1652–1655.

MAIN, P., FISKE, S., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1982). *MULTAN82. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data.* Univs. of York, England, and Louvain, Belgium.

MOTHERWELL, W. D. S. & CLEGG, W. (1978). *PLUTO.* Program for plotting molecular and crystal structures. Univ. of Cambridge, England.

NARDELLI, M. (1983). *Comput. Chem.* 7, 95–98.

NYBURG, S. C. (1974). *Acta Cryst.* B30, 253–254.

SAENGER, W. (1988). *Principles of Nucleic Acid Structure.* New York: Springer Verlag.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* 42, 3175–3187.

Stoe & Co. (1985). *REDU4. Data Reduction Program.* Stoe & Co., Darmstadt, Germany.

Structure of 1-(2-Deoxy-β-D-ribopyranosyl)-5-iodouracil*

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Abstract. 1-(2-Deoxy-β-D-ribopyranosyl)-5-iodo-uracil, $C_9H_{11}IN_2O_5$, $M_r = 354.10$, monoclinic, $P2_1$, a = 5.458 (3), b = 8.237 (4), c = 12.812 (6) Å, β = 98.42 (4)°, V = 569.8 (5) Å³, Z = 2, D_m = 2.05, D_x = 2.063 Mg m⁻³, λ(Mo $K\alpha$) = 0.71069 Å, μ = 2.789 mm⁻¹, $F(000)$ = 344, T = 293 K, final R = 0.039 for 1701 unique observed $[F \geq 4\sigma(F)]$ reflections. The sugar ring adopts a slightly flattened chair conformation. The heterocyclic base is placed in an

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