stable than (Ib), while structure (IIa) is 3·0 kcal-mol^{-1} (12·6 kJ mol^{-1}) more stable than (IIb). For (I), the presence of an intermolecular hydrogen bond can easily explain that (Ib), while higher in energy, is the preferred structure in the crystalline state. For compound (II), (IIa), which is lower in energy, corresponds to the X-ray structure. No major interactions are found in the crystal of (II).

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Structures of the 1-(2-Deoxy-2-fluoro-β-D-arabinopyranosyl)thymine–Water Complex and 1-(2-Deoxy-2-fluoro-β-D-arabinopyranosyl)-5-ethyluracil*

BY H. L. DE WINTER, N. M. BLATON, O. M. PEETERS AND C. J. DE RANTER†

Laboratorium voor Analytische Chemie en Medicinale Fysicochemie, Instituut voor Farmaceutische Wetenschappen, Katholieke Universiteit Leuven, Van Evenstraat 4, B-3000 Leuven, Belgium

AND A. VAN AERSCHOT AND P. HERDEWIJN

Laboratorium voor Farmaceutische Chemie, Rega Institute for Medical Research, Katholieke Universiteit Leuven, B-3000 Leuven, Belgium

Abstract. (I) 1-(2-Deoxy-2-fluoro-β-D-arabinopyranosyl)thymine–water complex, $C_{10}H_{13}FN_2O_5.H_2O$, $M_r = 278·24$, monoclinic, $P2_1$, $a = 8·669$ (4), $b = 6·395$ (3), $c = 10·713$ (7) Å, $\beta = 103·73$ (5)°, $V = 576·9$ (6) Å^3, $Z = 2$, $D_m = 1·60$, $D_x = 1·602$ Mg m^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, $\mu = 0·134$ mm^{-1}, $F(000) = 292$, room temperature, final $R = 0·030$ for 1307 unique observed $[F \geq 4\sigma(F)]$ reflections. (II) 1-(2-Deoxy-2-fluoro-β-D-arabinopyranosyl)-5-ethyluracil, $C_{11}H_{15}FN_2O_5$, $M_r = 274·25$, hexagonal, $P6_5$, $a = 10·108$ (7), $c = 19·48$ (1) Å, $V = 1724$ (2) Å^3, $Z = 6$, $D_m = 1·54$, $D_x = 1·585$ Mg m^{-3}, graphite-monochromated Mo $K\alpha$ radiation, $\lambda = 0·71069$ Å, $\mu = 0·127$ mm^{-1}, $F(000) = 864$, room temperature, final $R = 0·026$ for 694 unique observed $[F \geq 4\sigma(F)]$ reflections. The geometries of molecules (I) and (II) show a close similarity. In both structures the sugar ring adopts a slightly distorted chair conformation and for both molecules the fluorine and one of the hydroxyl substituents are placed in an axial position on the ring. The N-glycosidic torsion angle χ between the pyranose ring and the pyrimidine base is oriented $-ac$ for both molecules. The terminal C of the ethyl group in (II) deviates from the base least-squares plane. The packing in both crystals is determined by intermolecular hydrogen bonds and base-stacking forces. In (I) the solvent water is kept from being disordered by a dense network of strong hydrogen bonds. In (II) the molecules are packed in such a way that a single stranded left-handed helix is formed which resembles the structure of the 6_1 poly(2'-O-methylcytidine) single stranded helix. No intramolecular hydrogen bonds are present. The conformational parameters are in accordance with the IUPAC–IUB Joint Commission on Biochemical Nomenclature (1983) guidelines.

Introduction. The crystal structures of the title compounds have been determined as part of a continuing program of investigation of potentially anti-viral


Table 1. *Experimental data*

	(I)	(II)
Space group	$P2_1$	$P6_5$
Crystal dimensions (mm)	$0.1 \times 0.4 \times 0.6$	$0.3 \times 0.3 \times 0.5$
Lattice parameters		
No. of reflections	34	24
2θ range (°)	$20 \le 2\theta \le 30$	$20 \le 2\theta \le 26$
Scan technique	$\omega/2\theta$	$\omega/2\theta$
Maximum 2θ (°)	55	50
hkl range	$-11 \le h \le 11$	$-12 \le h \le 12$
	$0 \le k \le 8$	$0 \le k \le 12$
	$-14 \le l \le 14$	$0 \le l \le 23$
Standard reflections	005, 040	$451, 5\bar{1}1$
No. of measured reflections	2890	3306
No. of unique reflections	1445	1055
No. of unique observed reflections $[F \ge 4\sigma(F)]$	1307	694
R_{int} on F for equivalent observed reflections	0.015	0.025
R, wR	0.030, 0.037	0.026, 0.030
Goodness-of-fit S	1.41	0.90
Weighting scheme	$w = 1/[\sigma(F_o)]^2$	$w = 1/[\sigma(F_o)]^2$
Max. shift/e.s.d.	0.01	0.01
Min. and max residual electron density (e Å^{-3})	$-0.25, +0.20$	$-0.16, +0.12$
No. of refined parameters	215	170
No. of reflections per refined parameter	6.1	4.1
Absorption coefficient μ (mm^{-1})	0.134	0.127

modified nucleosides. The synthesis of (I) and (II) will be described elsewhere.

Experimental. Transparent colourless crystals obtained at room temperature, (I) from methanol–water and (II) from methanol. 1-(2-Deoxy-2-fluoro-β-D-arabinopyranosyl)thymine, (I), crystallized with one water molecule per asymmetric unit. Density measured by flotation in n-heptane/CCl$_4$. Space group determined from systematic absences. X-ray diffraction data collected on a Stoe Stadi-4 four-circle diffractometer, cell constants by least-squares refinement of the setting angles of 34 (I) and 24 (II) reflections respectively. Experimental details are set out in Table 1. Standard reflections measured every two hours show only statistical fluctuations. Data reduction with a locally modified version of Stoe & Co. (1985) *REDU*4 program, Lorentz and polarization corrections were applied, absorption corrections were unnecessary owing to the small absorption coefficients. Scattering factors were taken from Cromer & Waber (*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). Both structures solved with *MULTAN*82 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) which revealed all the non-H atoms of the pyrimidine ring for (I) and 17 of the 19 non-H atoms of molecule (II). Positions of the remaining non-H atoms were located stepwise by subsequent Fourier syntheses. Refinement on F by full-matrix least squares, first with isotropic temperature factors and

then anisotropically. Reflection 100 of (I), badly affected by extinction, was eliminated from the refinement. For both structures all H atoms were found in a difference synthesis. For (I) they were included in the refinement with fixed temperature factors B, $1.3 \times B_{eq}$ (of parent atoms). For (II) most of the H atoms were placed at their calculated positions with a riding distance of 0.95 Å, in order to keep the number of reflections per refined parameter sufficiently high; only H(4), H(6), H(12), H(13) and H(14) (these are the H atoms for which the positions could not be calculated theoretically) were placed at their experimental positions and kept riding. For all H atoms the temperature factor B was kept fixed at $1.3 \times B_{eq}$ (of parent atoms).

All calculations were performed on a Digital PDP-11/73 and MicroVAX 2000 microcomputer using *SDP* (Enraf–Nonius, 1985) and *PARST* (Nardelli, 1983).

$R = $ Me (I), Et (II)
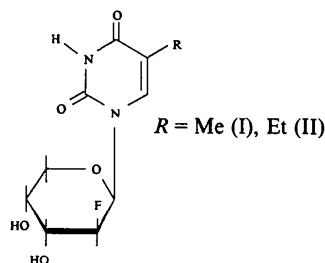
Discussion. The structural formulas of the title compounds are shown in the scheme. *PLUTO* (Motherwell & Clegg, 1978) views of the title compounds with the atomic numbering schemes are shown in Fig. 1. The final atomic coordinates and equivalent isotropic thermal parameters are given in Table 2.* Bond lengths, bond angles and selected torsion angles are given in Table 3. All bond lengths and bond angles of both nucleosides are within the normal range (Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The O(5′)—C(1′) bond lengths in both molecules are 0.020 (3) (I) and 0.028 (7) Å (II) shorter than the C(5′)—O(5′) distances.

A least-squares fit procedure with the program *BMFIT* (Nyburg, 1974) on all the non-H atoms of both molecules [except the water molecule in (I) and C(8) in (II)] showed a close similarity in geometry between molecules (I) and (II) (r.m.s. deviation = 0.16 Å).

Using the method of Cremer & Pople (1975), we calculated as phase angles $\varphi_2 = 82$ (5) (I) and 109 (3)° (II) and $\theta_2 = 177 \cdot 3$ (3) (I) and $172 \cdot 6$ (4)° (II), with total puckering amplitudes $Q = 0 \cdot 570$ (3) (I) and $0 \cdot 571$ (3) Å (II) for the sequences C(1')—C(2')—C(3')—C(4')—C(5')—O(5'). These puckering parameters describe slightly distorted chair conformations, with the total puckering amplitudes Q almost equal for both molecules and similar to comparable pyranosyl rings such as in 4-amino-1-[4-amino-2-oxo-1(2*H*)-pyrimidinyl]-1,4-dideoxy-β-D-glucopyranuronic acid (*C*-Substance) (Swaminathan, McAlister & Sundaralingam, 1980) and in 1-(2,3-dideoxy-*erythro*-β-D-hexopyranosyl)thymine (De Winter, Blaton, Peeters, De Ranter, Van Aerschot & Herdewijn, 1991).

Of the four ring substituents in the two molecules, F(22') and O(33') are placed in axial positions while N(1) and O(44') are in equatorial positions. The relative orientation of the base with respect to the sugar ring is given by the *N*-glycosidic torsion angle
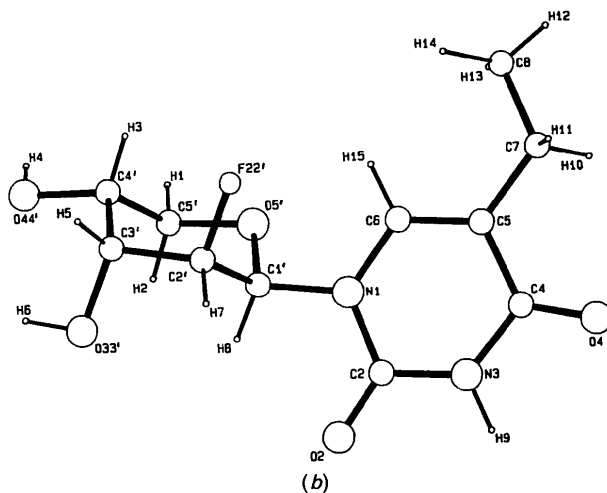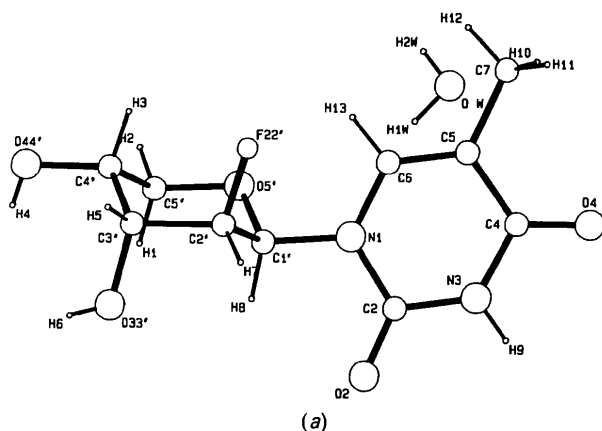

(a)

(b)

Fig. 1. *PLUTO* (Motherwell & Clegg, 1978) plot (a) of (I) and (b) of (II) with atom-numbering schemes.

Table 2. *Fractional atomic coordinates and equivalent isotropic temperature factors* (Å² × 10⁴) *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}
(I)				
N(1)	0·6036 (2)	0·7948 (3)	0·7367 (1)	229 (4)
C(2)	0·4492 (2)	0·7827 (3)	0·6685 (2)	228 (4)
O(2)	0·3373 (2)	0·7932 (3)	0·7178 (1)	316 (4)
N(3)	0·4309 (2)	0·7599 (3)	0·5397 (1)	250 (4)
C(4)	0·5487 (2)	0·7539 (3)	0·4736 (2)	252 (4)
O(4)	0·5126 (2)	0·7469 (3)	0·3567 (1)	362 (4)
C(5)	0·7084 (2)	0·7536 (4)	0·5519 (2)	261 (4)
C(6)	0·7277 (2)	0·7763 (4)	0·6778 (2)	253 (4)
C(7)	0·8440 (3)	0·7362 (5)	0·4900 (2)	392 (5)
C(1')	0·6348 (2)	0·8571 (3)	0·8705 (2)	211 (4)
C(2')	0·6900 (2)	0·6769 (3)	0·9614 (2)	229 (4)
F(22')	0·8249 (1)	0·589*	0·9334 (1)	324 (3)
C(3')	0·7341 (2)	0·7531 (3)	1·0993 (2)	236 (4)
O(33')	0·5910 (1)	0·8182 (3)	1·1277 (1)	308 (4)
C(4')	0·8500 (2)	0·9334 (3)	1·1088 (2)	225 (4)
O(44')	0·8934 (2)	1·0196 (3)	1·2332 (1)	304 (4)
C(5')	0·7834 (2)	1·1004 (3)	1·0120 (2)	257 (4)
O(5')	0·7498 (2)	1·0151 (3)	0·8857 (1)	265 (3)
O(*W*)	0·8523 (2)	0·2413 (3)	0·6543 (1)	445 (4)
(II)				
N(1)	0·0498 (3)	0·7713 (2)	0·7477 (2)	270 (8)
C(2)	0·1332 (3)	0·9230 (3)	0·7624 (2)	249 (9)
O(2)	0·2644 (2)	0·9834 (2)	0·7825 (2)	336 (5)
N(3)	0·0595 (2)	1·0015 (3)	0·7524 (2)	272 (8)
C(4)	−0·0890 (3)	0·9445 (3)	0·7310 (2)	274 (9)
O(4)	−0·1365 (2)	1·0322 (2)	0·7218 (2)	417 (8)
C(5)	−0·1748 (3)	0·7820 (3)	0·7202 (2)	272 (9)
C(6)	−0·1020 (3)	0·7042 (3)	0·7282 (2)	304 (10)
C(7)	−0·3369 (4)	0·7152 (3)	0·6988 (2)	389 (10)
C(8)	−0·4069 (4)	0·5608 (4)	0·6679 (3)	348 (13)
C(1')	0·1257 (3)	0·6812 (3)	0·7516 (2)	270 (9)
C(2')	0·0859 (4)	0·5843 (3)	0·8143 (3)	234 (10)
F(22')	−0·0702 (2)	0·4889 (2)	0·818*	522 (6)
C(3')	0·1611 (3)	0·4867 (3)	0·8135 (2)	353 (10)
O(33')	0·3186 (3)	0·5893 (2)	0·8246 (2)	477 (8)
C(4')	0·1332 (3)	0·4065 (3)	0·7461 (2)	309 (9)
O(44')	0·2264 (2)	0·3369 (2)	0·7448 (2)	364 (6)
C(5')	0·1732 (3)	0·5167 (3)	0·6872 (2)	353 (10)
O(5')	0·0850 (2)	0·5915 (2)	0·6919 (2)	349 (6)

* Parameters kept fixed during refinement.

χ[O(5')—C(1')—N(1)—C(2)], which is $229 \cdot 2$ (2) $(-ac)$ for (I) and $226 \cdot 3$ (3)° $(-ac)$ for (II). The sugar–base C(1')—N(1) glycosyl bond lengths of $1 \cdot 450$ (2) (I) and $1 \cdot 457$ (5) Å (II) are significantly shortened compared with the mean value of $1 \cdot 491$ (4) Å found in the corresponding pyrimidine furanosyl nucleosides (Lin, Sundaralingam & Arora, 1971).

The pyrimidine heterocycles are essentially planar [maximum deviation $0 \cdot 036$ (2) and $0 \cdot 021$ (4) Å for C(4') of (I) and (II) respectively]. However, the heterocyclic substituents deviate more pronouncedly, with C(1') lying $0 \cdot 277$ (2) (I) and $0 \cdot 118$ (4) Å (II) above the plane. The C(4)—C(5)—C(7)—C(8) torsion angle in compound (II) is $161 \cdot 9$ (4)°, leading to a C(8) out-of-plane deviation of $0 \cdot 341$ (5) Å.

The crystal packing of both molecules is determined by intermolecular hydrogen bonds

Table 3. *Bond lengths (Å), bond angles (°) and selected torsion angles (°) with e.s.d.'s in parentheses*

(I)

N(1)	C(2)	1·367 (3)	C(1')	C(2')	1·512 (3)	
N(1)	C(6)	1·376 (2)	C(1')	O(5')	1·403 (2)	
N(1)	C(1')	1·450 (2)	C(2')	F(22')	1·392 (2)	
C(2)	O(2)	1·212 (2)	C(2')	C(3')	1·516 (2)	
C(2)	N(3)	1·359 (2)	C(3')	O(33')	1·409 (2)	
N(3)	C(4)	1·375 (3)	C(3')	C(4')	1·518 (3)	
C(4)	O(4)	1·217 (2)	C(4')	O(44')	1·408 (2)	
C(4)	C(5)	1·438 (2)	C(4')	C(5')	1·505 (3)	
C(5)	C(6)	1·326 (2)	C(5')	O(5')	1·423 (2)	
C(5)	C(7)	1·485 (4)				

N(1)	C(2)	O(2)	123·2 (1)	C(6)	N(1)	C(1')	119·7 (1)
N(1)	C(2)	N(3)	114·4 (2)	C(6)	C(5)	C(7)	122·8 (2)
N(1)	C(6)	C(5)	123·6 (1)	C(1')	C(2')	F(22')	108·8 (1)
N(1)	C(1')	C(2')	112·6 (2)	C(1')	C(2')	C(3')	110·6 (2)
N(1)	C(1')	O(5')	105·9 (1)	C(1')	O(5')	C(5')	111·5 (1)
C(2)	N(1)	C(6)	121·5 (1)	C(2')	C(1')	O(5')	111·5 (1)
C(2)	N(1)	C(1')	118·2 (2)	C(2')	C(3')	O(33')	105·9 (1)
C(2)	N(3)	C(4)	127·2 (1)	C(2')	C(3')	C(4')	108·6 (2)
O(2)	C(2)	N(3)	122·4 (1)	F(22')	C(2')	C(3')	108·0 (1)
N(3)	C(4)	O(4)	119·4 (2)	C(3')	C(4')	O(44')	112·6 (2)
N(3)	C(4)	C(5)	115·5 (1)	C(3')	C(4')	C(5')	110·7 (1)
C(4)	C(5)	C(6)	117·7 (2)	O(33')	C(3')	C(4')	111·3 (2)
C(4)	C(5)	C(7)	119·6 (2)	C(4')	C(5')	O(5')	110·0 (2)
O(4)	C(4)	C(5)	125·3 (2)	O(4')	C(4')	C(5')	110·3 (2)

C(2')	C(1')	O(5')	C(5')	−61·2 (2)	C(4')	C(3')	C(2')	F(22')	66·8 (2)
O(5')	C(1')	C(2')	C(3')	56·4 (3)	C(4')	C(3')	O(33')	H(6)	−93 (2)
O(5')	C(1')	C(2')	F(22')	−62·0 (3)	C(3')	C(4')	C(5')	O(5')	−58·6 (3)
C(1')	C(2')	C(3')	C(4')	−52·1 (3)	C(3')	C(4')	O(44')	H(4)	−69 (2)
C(2')	C(3')	C(4')	O(44')	177·8 (2)	O(44')	C(4')	C(5')	O(5')	176·1 (2)
C(2')	C(3')	C(4')	C(5')	53·8 (3)	C(5')	C(4')	O(44')	H(4)	55 (2)
C(2')	C(3')	O(33')	H(6)	149 (2)	C(4')	C(5')	O(5')	C(1')	62·0 (3)

(II)

N(1)	C(2)	1·360 (3)	C(7)	C(8)	1·482 (6)	
N(1)	C(6)	1·384 (4)	C(1')	C(2')	1·490 (5)	
N(1)	C(1')	1·457 (5)	C(1')	O(5')	1·403 (5)	
C(2)	O(2)	1·215 (4)	C(2')	F(22')	1·379 (3)	
C(2)	N(3)	1·347 (5)	C(2')	C(3')	1·517 (6)	
N(3)	C(4)	1·377 (4)	C(3')	O(33')	1·416 (5)	
C(4)	O(4)	1·214 (5)	C(3')	C(4')	1·494 (6)	
C(4)	C(5)	1·440 (5)	C(4')	O(44')	1·431 (5)	
C(5)	C(6)	1·328 (6)	C(4')	C(5')	1·507 (5)	
C(5)	C(7)	1·486 (5)	C(5')	O(5')	1·431 (5)	

N(1)	C(2)	O(2)	122·7 (3)	C(6)	N(1)	C(1')	120·7 (2)
N(1)	C(2)	N(3)	114·8 (3)	C(6)	C(5)	C(7)	125·2 (3)
N(1)	C(6)	C(5)	123·3 (3)	C(1')	C(2')	F(22')	109·7 (3)
N(1)	C(1')	C(2')	113·6 (3)	C(1')	C(2')	C(3')	111·1 (3)
N(1)	C(1')	O(5')	106·6 (3)	C(1')	O(5')	C(5')	109·6 (3)
C(2)	N(1)	C(1')	118·0 (2)	C(2')	C(1')	O(5')	111·0 (2)
C(2)	N(1)	C(6)	121·3 (3)	C(2')	C(3')	O(33')	105·5 (2)
C(2)	N(3)	C(4)	127·3 (3)	C(2')	C(3')	C(4')	110·0 (3)
O(2)	C(2)	N(3)	122·4 (3)	F(22')	C(2')	C(3')	108·5 (2)
N(3)	C(4)	O(4)	119·0 (3)	C(3')	C(4')	O(44')	107·0 (3)
N(3)	C(4)	C(5)	115·5 (3)	C(3')	C(4')	C(5')	111·1 (3)
C(4)	C(5)	C(6)	117·5 (3)	O(33')	C(3')	C(4')	111·7 (4)
C(4)	C(5)	C(7)	117·2 (3)	C(4')	C(5')	O(5')	109·5 (3)
O(4)	C(4)	C(5)	125·5 (3)	O(44')	C(4')	C(5')	110·5 (4)
C(5)	C(7)	C(8)	115·5 (4)				

C(2')	C(1')	O(5')	C(5')	−64·4 (4)	C(4')	C(3')	C(2')	F(22')	71·3 (4)
O(5')	C(1')	C(2')	C(3')	56·8 (4)	C(4')	C(3')	O(33')	H(6)	−54·6 (4)
O(5')	C(1')	C(2')	F(22')	−63·1 (4)	C(3')	C(4')	C(5')	O(5')	−58·1 (4)
C(1')	C(2')	C(3')	C(4')	−49·3 (4)	C(3')	C(4')	O(44')	H(4)	−171·8 (3)
C(2')	C(3')	C(4')	O(44')	171·0 (4)	O(44')	C(4')	C(5')	O(5')	−176·6 (3)
C(2')	C(3')	C(4')	C(5')	50·4 (4)	C(5')	C(4')	O(44')	H(4)	−50·7 (4)
C(2')	C(3')	O(33')	H(6)	−174·1 (3)	C(4')	C(5')	O(5')	C(1')	64·6 (4)

Table 4. *Geometry of intermolecular hydrogen bonds with e.s.d.'s in parentheses (distances in Å, angles in °)*

(I)

X—H···Y		d(H···Y)	d(X···Y)	X—H···Y
O(33')—H(6)···O(4)	(1)	2·03 (3)	2·735 (3)	160 (3)
N(3)—H(9)···O(W)	(2)	1·99 (2)	2·817 (3)	165 (2)
C(7)—H(10)···O(44')	(3)	2·47 (3)	3·405 (3)	159 (3)
O(W)—H(1W)···O(5')	(4)	2·50 (3)	3·173 (3)	140 (3)
O(44')—H(4)···O(2)	(5)	2·04 (3)	2·799 (2)	165 (3)
C(2')—H(7)···O(33')	(6)	2·40 (2)	3·317 (3)	169 (2)
O(W)—H(2W)···O(44')	(7)	2·01 (3)	2·867 (3)	175 (3)

Symmetry code: (1) x, y, $z + 1$; (2) $1 - x$, $y + \frac{1}{2}$, $1 - z$; (3) x, y, $z - 1$; (4) x, $y - 1$, z; (5) $1 - x$, $y + \frac{1}{2}$, $2 - z$; (6) $1 - x$, $y - \frac{1}{2}$, $2 - z$; (7) $2 - x$, $y - \frac{1}{2}$, $2 - z$.

(II)

X—H···Y		d(H···Y)	d(X···Y)	X—H···Y
O(33')—H(6)···O(5')	(1)	2·494 (3)	3·326 (4)	140·3 (2)
C(3')—H(5)···O(4)	(2)	2·273 (3)	3·159 (5)	154·8 (2)
O(44')—H(4)···O(2)	(3)	1·843 (3)	2·748 (4)	158·0 (2)
N(3)—H(9)···O(44')	(4)	2·029 (2)	2·940 (4)	159·9 (2)

Symmetry code: (1) y, $y - x$, $z + \frac{1}{6}$; (2) $y - 1$, $y - x - 1$, $z + \frac{1}{6}$; (3) $x - y + 1$, x, $z - \frac{1}{6}$; (4) x, $y + 1$, z.
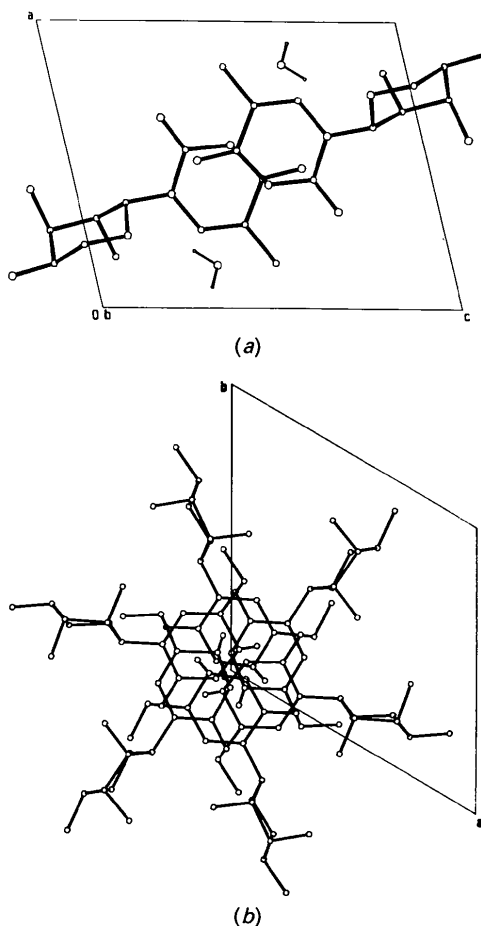

(a)

(b)

Fig. 2. *PLUTO* (Motherwell & Clegg, 1978) plot of the packing in crystals of (a) (I) and (b) (II), along **b** and **c** respectively. Hydrogen bonds are not marked for clarity.

(summarized in Table 4) and base stacking forces. The bases are stacked almost parallel with average interplanar spacings of 3·2 (3) (I) and 3·4 (4) Å (II), respectively, and with the normals to their planes

nearly parallel to the 2_1 or 6_5 axis [dihedral angle between adjacent base least-squares planes is 11·59 (7) (I) and 16·8 (1)° (II) respectively]. It thus appears that the base-stacking properties of nucleosides as described earlier by Bugg & Thomas (1971) are not only found in furanosyl nucleosides but also in pyranosyl nucleosides, although the latter consists of a larger and more rigid six-membered sugar ring instead of the smaller and more flexible five-membered ring. In both compounds only partial base overlap is found with a polar substituent like O(4) (I) or O(2) (II) positioned above the adjacent base (see Fig. 2). The result is that (II) is packed as a single stranded left-handed helix with six molecules per complete turn, an axial rise of 3·2 Å and a pitch of 19·48 (1) Å (for nomenclature see Saenger, 1984). This resembles more or less the structure of the 6_1 poly(2′-O-methylcytidine) single stranded helix (Leslie & Arnott, 1978), the latter with an axial rise of 3·2 Å and a pitch height of 18·9 Å. In contrast, however, the poly(2′-O-methylcytidine) helix is right-handed and the nucleosides are covalently bonded to each other by a sugar–phosphate backbone.

Many crystal structures in which solvent molecules are included are characterized by larger thermal parameters for those solvent molecules. The small thermal vibrations of the water molecule in (I) are a consequence of a dense hydrogen-bond network involving the water molecule and which consists of two extremely strong hydrogen bonds between N(3)—H(9) and the water O atom and from H(2W) towards O(44′), and a third somewhat weaker hydrogen bond between H(1W) and O(5′). The result is a neatly ordered water molecule with small thermal vibrations and normal geometry [mean O(W)—H(W) distance = 0·84 (4) Å and H(1W)—O(W)—H(2W) angle = 101 (3)°]. No intramolecular hydrogen bonds are present.

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N-[(1-Butyl-2-pyrrolidinyl)methyl]-2-methyl-5-sulfamoyl-2,3-dihydrobenzofuran-7-carboxamide

BY I. UEDA, N. MARUBAYASHI, S. HAYANO, S. MURAKAMI AND T. TAHARA

Research Laboratories, Yoshitomi Pharmaceutical Ind. Ltd, 955 Koiwai, Yoshitomi-cho, Fukuoka 871, Japan

Abstract. $C_{19}H_{27}N_3O_4S$, $M_r = 393\cdot5$, monoclinic, $P2_1$, $a = 12\cdot955$ (2), $b = 35\cdot050$ (8), $c = 9\cdot3196$ (7) Å, $\beta = 94\cdot548$ (8)°, $V = 4218$ (1) Å^3, $Z = 8$, $D_m = 1\cdot235$, $D_x = 1\cdot239$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1\cdot5418$ Å, $\mu = 1\cdot58$ mm^{-1}, $F(000) = 1680$, $T = 298$ K, $R = 0\cdot067$ for 4899 observed reflections. An intramolecular N$\cdots$O hydrogen bond between the amide group and benzofuran ring makes these two parts of the molecule flat. These two parts and the sulfamoyl groups of the four unique molecules form a layer by two kinds of