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X-ray Determination of the Molecular Structure of an Analogue of Tubercidin: Deaza-1-isotubercidin

By Arnaud Ducruix, Claude Riche and Claudine Pascard

Institut de Chimie des Substances Naturelles, CNRS, 91190-*Gif/Yvette, France*

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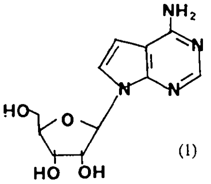
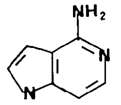
Crystals of deaza-1-isotubercidin picrate, $C_{12}H_{16}N_3O_4.C_6H_2N_3O_7$, are monoclinic, space group $P2_1$, with $a=7{\cdot}814$, $b=7{\cdot}557$, $c=16{\cdot}966$ Å, $\beta=91{\cdot}63°$, and $Z=2$. 1981 three-dimensional data were measured on a four-circle diffractometer. The crystal structure was solved by direct methods and refined to an R value of 5·5%. The structure is that of the picrate salt of an azaindole linked to carbon C(1′) of a ribose through the nitrogen N(5). N(1) is protonated. The planes of the aromatic picrate ring and of the base of the nucleoside are stacked alternately along **a**. There is no complex formation.

Introduction

Tubercidin (1) shows antitumour activity (Bloch & Nichol, 1964). It differs from adenosine by substitution of a C atom on position 7. This nucleoside has a certain toxicity and Bisagni and collaborators, at Orsay, have attempted to synthesize model substances, in particular a dideazaadenosine, by condensation of a suitably protected azaindole derivative with a haloribofuranosyl moiety (2) (Ducrocq, Bisagni, Lhoste, Mispelter & Defaye, 1976).



(1)



(2)

Since chemical transformations and NMR spectra could not identify the N atom to which the sugar was linked, and in order to determine the configuration of the anomeric C atom of the ribose, an X-ray analysis was undertaken. The free nucleoside could not be crystallized and so the structure of the picrate was investigated. A preliminary account of the X-ray results has already been published (Ducruix, Riche & Pascard, 1976).

Experimental

Crystal data

Deaza-1-isotubercidin picrate, monoclinic, $P2_1$, $C_{12}H_{16}N_3O_4.C_6H_2N_3O_7$, $M=494$. Yellow prisms: 0·35 × 0·35 × 0·12 mm, $a=7{\cdot}814$, $b=7{\cdot}557$, $c=16{\cdot}966$ Å, $\beta=91{\cdot}63°$, $V=1001{\cdot}4$ Å^3, $D_c=1{\cdot}64$ g cm^{-3}, $Z=2$, λ(Cu $K\alpha$) = 1·5418 Å.

Data collection

Automatic four-circle diffractometer PW 1100. θ–2θ scan at 3° min^{-1}, two background measurements per reflexion up to $2\theta=136°$. Graphite monochromator. Number of observed reflexions: 1981. No correction was made for absorption.

Structure determination

The structure was solved by direct methods, with symbolic addition (Karle & Karle, 1966) and the phase function (Riche, 1973). The first maximum of the phase function gave an E map in which 23 atoms were identified. By recycling, the 35 non-hydrogen atoms were located. All the H atoms appeared on subsequent difference maps.

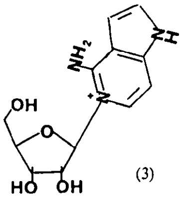
Refinement

The atomic parameters were refined by full-matrix least squares. The thermal parameters were anisotropic for heavy atoms, isotropic for H atoms. The final R value for 1981 observed reflexions is 5·5%.* The mean δ/σ for the last cycle is 0·3.

The f curves were, for C, N and O, those of Doyle & Turner (1968), and for H, the values given by Stewart, Davidson & Simpson (1965).

Results

The molecule proved to be the N(5)-substituted 5-azaindole. The configuration of the anomeric C atom is β.



(3)

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* A list of structure factors has been deposited with the Library Lending Division as Supplementary Publication No. SUP 31738 (12 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

The parameters and their estimated standard deviations are listed in Table 1 for the heavy atoms and Table 2 for the H atoms. The atoms belonging to the picrate anion are labelled *P* and those belonging to the base, *B*. The different ions are shown in Fig. 1.

Bond lengths of the picrate moiety and of the nucleoside analogue are given in Table 3 and valency angles in Table 4. The nomenclature of the base is that of an indole.

Picrate

No H atom was observed around O*P*(1), thus establishing a picrate anion: C*P*(1)–O*P*(1) 1·240 Å.

The interatomic angles and bond values are in perfect agreement with those found in other picrates: serotonine picrate monohydrate (Thewalt & Bugg, 1972), 1-methylnicotinamide iodide picrate (Freeman & Bugg, 1974).

Deviations from the least-squares plane through the aromatic picrate ring are given Table 5. As expected, the ring is planar within experimental error. The NO_2 groups on each side of O*P*(1) are twisted symmetrically, the dihedral angles being 26·6 [N*P*(2)–O*P*(2)–O*P*(3)] and 34·6° [N*P*(6)–O*P*(6)–O*P*(7)]. The third nitro group is in the plane of the picrate ring.

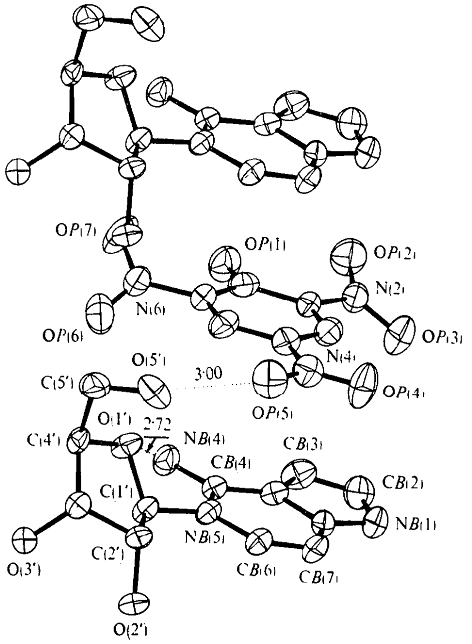

Fig. 1. Perspective drawing of the ions stacked along a.

Table 1. *Final atomic coordinates* (× 10⁴) *for heavy atoms*

The thermal parameters are defined in the expression: $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$.

	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}	B
C*P*(1)	4663 (6)	3875 (9)	2758 (3)	92 (9)	167 (13)	32 (2)	−1 (9)	−1 (4)	−2 (5)	3·3
C*P*(2)	5281 (6)	3552 (3)	3563 (3)	96 (8)	180 (13)	20 (2)	4 (9)	−5 (3)	−11 (4)	2·9
C*P*(3)	6042 (6)	2002 (8)	3806 (3)	120 (9)	152 (12)	26 (2)	−14 (9)	−5 (3)	7 (4)	3·2
C*P*(4)	6251 (6)	651 (7)	3272 (3)	117 (10)	109 (20)	26 (2)	1 (8)	0 (4)	3 (4)	2·8
C*P*(5)	5716 (6)	807 (6)	2499 (3)	115 (9)	142 (11)	30 (2)	−23 (9)	−11 (4)	−2 (4)	3·2
C*P*(6)	4958 (6)	2359 (8)	2251 (3)	106 (9)	173 (12)	22 (2)	−5 (10)	−7 (3)	0 (5)	3·0
N*P*(2)	5147 (5)	4977 (7)	4147 (2)	142 (8)	161 (10)	23 (2)	−10 (9)	−4 (3)	1 (4)	3·3
N*P*(4)	7079 (6)	−971 (7)	3540 (3)	157 (9)	147 (10)	32 (2)	−1 (9)	1 (3)	4 (4)	3·6
N*P*(6)	4433 (6)	2476 (7)	1424 (2)	136 (8)	207 (11)	24 (2)	−16 (9)	−10 (3)	8 (4)	3·6
O*P*(1)	4078 (5)	5317 (6)	2526 (2)	192 (8)	199 (10)	33 (2)	70 (8)	−11 (3)	7 (4)	4·4
O*P*(2)	6229 (5)	4990 (6)	4694 (2)	227 (8)	209 (10)	32 (1)	9 (8)	−29 (3)	−11 (4)	4·7
O*P*(3)	4042 (5)	6074 (6)	4076 (2)	203 (8)	251 (11)	43 (2)	109 (9)	−7 (3)	−9 (4)	5·2
O*P*(4)	7268 (5)	−2159 (6)	3064 (2)	238 (9)	168 (9)	40 (2)	47 (8)	4 (3)	−2 (4)	4·7
O*P*(5)	7557 (6)	−1065 (6)	4222 (2)	315 (10)	197 (9)	29 (2)	57 (9)	−33 (3)	9 (4)	5·2
O*P*(6)	5283 (5)	1671 (7)	950 (2)	251 (9)	380 (14)	26 (1)	68 (10)	3 (3)	−3 (3)	5·9
O*P*(7)	3166 (5)	3295 (7)	1224 (2)	198 (8)	316 (12)	42 (2)	85 (9)	−49 (3)	−11 (4)	5·7
C(1′)	639 (6)	−972 (7)	1476 (3)	97 (9)	114 (10)	22 (2)	12 (8)	−13 (3)	−6 (4)	2·5
C(2′)	1383 (5)	−2812 (7)	1386 (3)	81 (8)	134 (10)	24 (2)	25 (9)	−3 (3)	5 (4)	2·6
C(3′)	452 (6)	−3435 (7)	638 (3)	105 (9)	159 (12)	21 (2)	16 (8)	−4 (3)	7 (4)	2·9
C(4′)	−1282 (6)	−2485 (7)	654 (2)	105 (8)	124 (11)	17 (2)	−20 (8)	−10 (3)	−10 (4)	2·4
C(5′)	−2768 (6)	−3638 (8)	870 (3)	110 (9)	201 (13)	31 (2)	−17 (10)	2 (3)	−19 (5)	3·6
O(1′)	−1092 (4)	−1128 (5)	1256 (2)	91 (6)	127 (7)	33 (1)	18 (6)	−14 (2)	−10 (3)	3·0
O(2′)	3189 (4)	−2747 (6)	1308 (2)	70 (5)	206 (8)	30 (1)	17 (6)	−4 (2)	2 (3)	3·3
O(3′)	1344 (4)	−2896 (6)	−47 (2)	104 (6)	256 (9)	20 (1)	9 (1)	2 (2)	3 (3)	3·6
O(5′)	−2533 (5)	−4428 (6)	1612 (2)	192 (8)	160 (8)	35 (2)	19 (7)	33 (3)	9 (3)	4·1
N*B*(1)	1262 (5)	2468 (8)	4341 (2)	152 (8)	243 (13)	21 (2)	−19 (10)	−10 (3)	−13 (4)	3·9
C*B*(2)	441 (7)	4065 (9)	4145 (3)	164 (12)	220 (15)	31 (2)	−8 (12)	1 (4)	−22 (5)	4·2
C*B*(3)	−116 (7)	4010 (8)	3401 (3)	136 (11)	128 (12)	41 (3)	19 (10)	−9 (4)	−5 (5)	3·7
C*B*(4)	139 (6)	1494 (8)	2342 (3)	85 (8)	150 (11)	21 (2)	0 (8)	−3 (3)	4 (4)	2·7
N*B*(5)	782 (5)	−177 (6)	2262 (2)	87 (7)	146 (9)	22 (2)	7 (7)	−10 (3)	−4 (3)	2·7
C*B*(6)	1644 (6)	−1021 (8)	2887 (3)	109 (9)	195 (13)	24 (2)	21 (10)	−9 (3)	3 (5)	3·3
C*B*(7)	1900 (6)	−331 (8)	3590 (3)	116 (9)	176 (13)	23 (2)	10 (9)	−16 (3)	8 (4)	3·2
C*B*(8)	1224 (6)	1399 (8)	3691 (3)	109 (9)	183 (12)	17 (2)	−26 (9)	0 (3)	−4 (4)	2·9
C*B*(9)	355 (6)	2303 (9)	3093 (3)	81 (8)	199 (13)	25 (2)	1 (10)	−4 (3)	5 (5)	3·2
N*B*(4)	−656 (6)	2275 (7)	1745 (2)	132 (8)	176 (10)	24 (2)	60 (8)	−10 (3)	−9 (4)	3·3

Table 2. *Fractional coordinates* ($\times 10^3$) *and B values* (Å^2) *for hydrogen atoms*

	x	*y*	*z*	*B*
H(*P*3)	663	192	437	3·5
H(*P*5)	569	−1	223	3·0
H(1′)	108	−14	113	2·4
H(2′)	103	−357	190	2·6
H(3′)	23	−491	70	2·8
H(4′)	−164	−205	13	2·6
H*a*(5′)	−403	−319	74	3·5
H*b*(5′)	−269	−431	43	3·5
H(O2′)	432	−305	170	3·4
H(O3′)	244	−302	20	3·5
H(O5′)	−279	−393	198	3·9
H(N*B*1)	169	245	479	3·9
H(*B*2)	10	475	461	4·1
H(*B*3)	−59	480	321	3·4
H(*B*6)	197	−194	274	3·4
H(*B*7)	258	−93	399	3·2
H*a*(N*B*4)	−110	197	127	3·2
H*b*(N*B*4)	−100	318	179	3·2

Table 3. *Bond distances* (Å)

C*P*(1)–C*P*(2)	1·456 (7)	C(1′)—N*B*(5)	1·464 (6)
C*P*(1)–C*P*(6)	1·456 (8)	C(2′)—C(3′)	1·520 (6)
C*P*(1)–O*P*(1)	1·241 (8)	C(2′)—O(2′)	1·421 (5)
C*P*(2)–C*P*(3)	1·371 (8)	C(3′)—C(4′)	1·535 (7)
C*P*(2)–N*P*(2)	1·469 (7)	C(3′)—O(3′)	1·430 (6)
C*P*(3)–C*P*(4)	1·377 (8)	C(4′)—C(5′)	1·506 (7)
C*P*(4)–C*P*(5)	1·370 (7)	C(4′)—O(1′)	1·453 (6)
C*P*(4)–N*P*(4)	1·453 (7)	C(5′)—O(5′)	1·401 (6)
C*P*(5)–C*P*(6)	1·375 (8)	N*B*(1)–C*B*(2)	1·402 (9)
C*P*(6)–N*P*(6)	1·453 (6)	N*B*(1)–C*B*(8)	1·366 (7)
N*P*(2)–O*P*(2)	1·238 (5)	C*B*(2)–C*B*(3)	1·325 (8)
N*P*(2)–O*P*(3)	1·200 (6)	C*B*(3)–C*B*(9)	1·444 (9)
N*P*(4)–O*P*(4)	1·220 (6)	C*B*(4)–N*B*(5)	1·368 (7)
N*P*(4)–O*P*(5)	1·209 (6)	C*B*(4)–C*B*(9)	1·418 (7)
N*P*(6)–O*P*(6)	1·220 (6)	N*B*(5)–C*B*(6)	1·394 (6)
N*P*(6)–O*P*(7)	1·208 (6)	C*B*(6)–C*B*(7)	1·313 (7)
C(1′)—C(2′)	1·517 (8)	C*B*(7)–C*B*(8)	1·423 (9)
C(1′)—O(1′)	1·398 (5)	C*B*(8)–C*B*(9)	1·385 (7)

Table 4. *Bond angles* (°)

C*P*(2)–C*P*(1)–C*P*(6)	111·6 (5)	C*P*(4)–N*P*(4)–O*P*(5)	118·1 (4)	C(4′)—C(5′)—O(5′)	112·6 (4)
C*P*(2)–C*P*(1)–O*P*(1)	123·7 (5)	O*P*(4)–N*P*(4)–O*P*(5)	123·5 (5)	C(1′)—O(1′)—C(4′)	109·0 (4)
C*P*(6)–C*P*(1)–O*P*(1)	124·5 (5)	C*P*(6)–N*P*(6)–O*P*(6)	117·6 (5)	C*B*(2)–N*B*(1)–C*B*(8)	108·6 (5)
C*P*(1)–C*P*(2)–C*P*(3)	123·7 (5)	C*P*(6)–N*P*(6)–O*P*(7)	120·6 (5)	N*B*(1)–C*B*(2)–C*B*(3)	109·6 (5)
C*P*(1)–C*P*(2)–N*P*(2)	118·8 (4)	O*P*(6)–N*P*(6)–O*P*(7)	121·8 (5)	C*B*(2)–C*B*(3)–C*B*(9)	107·0 (5)
C*P*(3)–C*P*(2)–N*P*(2)	117·5 (4)	C(2′)—C(1′)—O(1′)	105·5 (4)	N*B*(5)–C*B*(4)–C*B*(9)	116·9 (4)
C*P*(2)–C*P*(3)–C*P*(4)	119·6 (5)	C(2′)—C(1′)—N*B*(5)	116·6 (4)	C(1′)—N*B*(5)–C*B*(4)	116·8 (4)
C*P*(3)–C*P*(4)–C*P*(5)	121·8 (5)	O(1)′—C(1′)—N*B*(5)	109·0 (4)	C(1′)—N*B*(5)–C*B*(6)	121·8 (4)
C*P*(3)–C*P*(4)–N*P*(4)	118·7 (4)	C(1′)—C(2′)—C(3′)	101·1 (4)	C*B*(4)–N*B*(5)–C*B*(6)	121·2 (4)
C*P*(5)–C*P*(4)–N*P*(4)	119·5 (5)	C(1′)—C(2′)—O(2′)	111·2 (4)	N*B*(5)–C*B*(6)–C*B*(7)	124·6 (5)
C*P*(4)–C*P*(5)–C*P*(6)	118·9 (5)	C(3′)—C(2′)—O(2′)	112·7 (4)	C*B*(6)–C*B*(7)–C*B*(8)	115·3 (5)
C*P*(1)–C*P*(6)–C*P*(5)	124·3 (5)	C(2′)—C(3′)—C(4′)	104·0 (4)	N*B*(1)–C*B*(8)–C*B*(7)	129·9 (5)
C*P*(1)–C*P*(6)–N*P*(6)	118·6 (4)	C(2′)—C(3′)—O(3′)	110·9 (4)	N*B*(1)–C*B*(8)–C*B*(9)	107·4 (5)
C*P*(5)–C*P*(6)–N*P*(6)	117·1 (5)	C(4′)—C(3′)—O(3′)	109·3 (4)	C*B*(7)–C*B*(8)–C*B*(9)	122·7 (5)
C*P*(2)–N*P*(2)–O*P*(2)	116·8 (4)	C(3′)—C(4′)—C(5′)	114·9 (4)	C*B*(3)–C*B*(9)–C*B*(4)	133·2 (5)
C*P*(2)–N*P*(2)–O*P*(3)	120·2 (4)	C(3′)—C(4′)—O(1′)	105·6 (4)	C*B*(3)–C*B*(9)–C*B*(8)	107·5 (5)
O*P*(2)–N*P*(2)–O*P*(3)	122·9 (5)	C(5′)—C(4′)—O(1′)	107·5 (4)	C*B*(4)–C*B*(9)–C*B*(8)	119·3 (5)
C*P*(4)–N*P*(4)–O*P*(4)	118·4 (4)				

Table 5. *Mean planes and atomic deviations* (Å)

Picrate	I	Base	II	Sugar	III	IV
C*P*(1)*	0·001	N*B*(1)*	−0·007	C(1′)	0·496	0·054*
C*P*(2)*	0·000	C*B*(2)*	0·006	C(2′)	−0·053*	−0·559
C*P*(3)*	0·000	C*B*(3)*	0·006	C(3′)	0·087*	−0·048*
C*P*(4)*	0·000	C*B*(4)*	0·005	C(4′)	−0·082*	0·072*
C*P*(5)*	−0·002	N*B*(5)*	−0·004	O(1′)	0·027*	−0·039*
C*P*(6)*	0·002	C*B*(6)*	0·003	C(5′)	−1·409	−1·005
N*P*(2)	0·051	C*B*(7)*	0·007	O(2′)	0·708	−0·113
N*P*(4)	0·018	C*B*(8)*	0·000	O(3′)	1·387	1·242
N*P*(6)	0·019	C*B*(9)*	−0·009			
O*P*(1)	0·087	N*B*(4)	0·009			
O*P*(2)	0·582	H*a*(N*B*4)	−0·133			
O*P*(3)	−0·391	H*b*(N*B*4)	0·013			
O*P*(4)	0·025	O(1′)	−1·029			
O*P*(5)	0·036	C(1′)	0·084			
O*P*(6)	0·597	C(5′)	−2·700			
O*P*(7)	−0·560					

$\bar{\sigma}=0{\cdot}005$ Å

Plane		Plane	
I	$0{\cdot}9016X+0{\cdot}3681Y-0{\cdot}2270Z-3{\cdot}1825=0$	III	$0{\cdot}4585X+0{\cdot}6535Y-0{\cdot}6022Z+2{\cdot}2868=0$
II	$0{\cdot}8746X+0{\cdot}3891Y-0{\cdot}2894Z+0{\cdot}7189=0$	IV	$0{\cdot}2237X+0{\cdot}6174Y-0{\cdot}7541Z+2{\cdot}2988=0$

* Atoms defining the planes.

Base

It is interesting to compare this deazaadenosine (azaindole) with the results obtained previously on purines and analogues.

The molecular dimensions of the pyrrole ring are in good agreement with those of tubercidin (Abola & Sundaralingam, 1973). C(2)–C(3) is shorter (1·325 Å) than the corresponding bond in tubercidin (1·359 Å). The difference series showed the presence of a H atom bonded to N*B*(1).

In the pyridine ring, the largest bond difference occurs in C(7)–C(8) (1·423 Å), and is due to the replacement of N(3) (in purine nomenclature) by a C atom [C(7)]. C(6)–C(7) is short (1·313 Å) and exhibits marked bouble-bond character [see neutral adenine (Lai & Marsh, 1972) and N(1)-protonated adenine (Kistenmacher & Shigematsu, 1975)].

The base is essentially planar (see Table 5). The amino group lies this in plane; C(1′) undergoes a large displacement (0·084 Å) from this plane.

Sugar

The ribose ring can be described as follows: $\Delta=0$, $\varphi_m=39°$ (Altona & Sundaralingam, 1972): C(2′)-*endo*, C(1′)-*exo*, with C(2′) at +0·34 and C(1′) at −0·26 Å from the C(3′)–C(4′)–O(1′) plane. The C(5′)–O(5′) bond is *gauche–gauche*: $\varphi_{OO}=58{\cdot}8$, $\varphi_{OC}=58{\cdot}5°$. The endocyclic torsion angles are shown in Fig. 2.

The H atom bonded to O(3′) was located at 1·97 Å from O(2′), thus indicating an internal hydrogen bond. The existence of such internal bonds has been corroborated by studies on acidities of ribosides in solution (Darzynkiewicz, Sierakowski & Shugar, 1975).

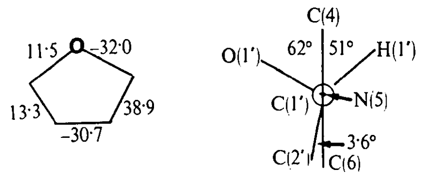

Fig. 2. Endocyclic torsion angles for the ribose ring and Newman projection around N*B*(5)–C(1′).

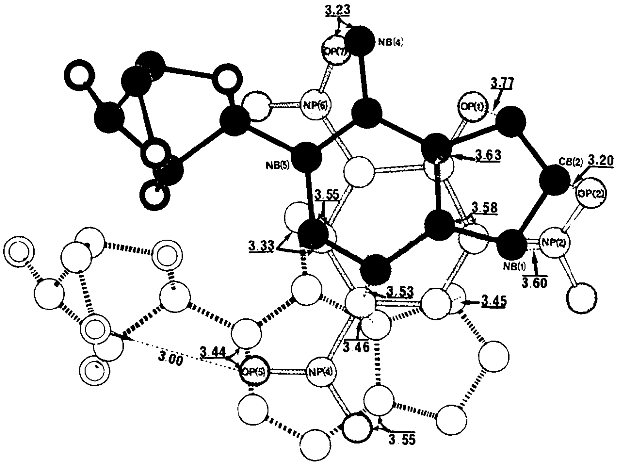

Fig. 3. Same molecules as in Fig. 1 projected on the benzene plane of the intercalated picrate ion. The shortest distances between the atoms of the different layers are indicated. ◎ and **O** represent O atoms.

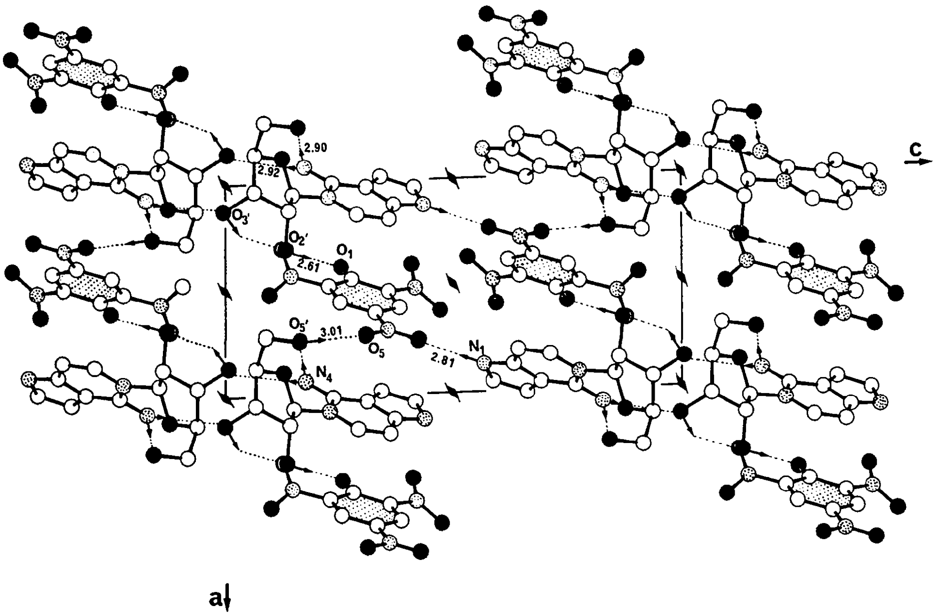

Fig. 4. Molecular packing. O atoms are represented by black circles, and N atoms by dotted circles. The arrows and dotted lines indicate the H atoms and the directions of the hydrogen bonds.

Glycosidic bond

The distance between C(1′) and N*B*(5) is 1·464 Å [CN bond in adenosine: 1·466 Å (Lai & Marsh, 1972)]. The external angle C(2′)–C(1′)–N*B*(5) is greater (116·6°) than O(1′)–C(1′)–N*B*(5) (109°). The angle C(1′)–N*B*(5)–C*B*(6) is, in the same way, greater (121·8°) than C(1′)–N*B*(5)–C*B*(4) (116·8°). This brings one H of the amino group closer to the ribose endocyclic O atom: O(1′)–N*B*(4) 2·74 Å, O(1′)–H*a*(N*B*4) 2·34 Å.

The Newman projection around N*B*(5)–C(1′) is given in Fig. 2.

The base is in the *anti* position. C(2′), C(1′), N*B*(5), C*B*(6) are nearly in the same plane, and this disposition causes the H atom bonded to C*B*(6) to lie 2·02 Å from H(2′), and 3·11 Å from H(1′).

This favoured conformation of the nucleoside analogue in the crystalline state is probably due to intermolecular forces – the presence of a picrate anion in a parallel plane to that of the base, giving rise to a short distance O*P*(7)···N*B*(4) (3·23 Å) – along with the existence of a hydrogen bond O(5′)···O*P*(5) (3·00 Å).

Stacking and hydrogen bonds

The molecules are stacked along **a** with the planes of the picrate ion and of the base ring practically parallel (the angle between the planes is 4·1°). Fig. 3 shows a picrate anion sandwiched between two azaindoles. The maximum overlap is between the picrate anion and the base of the same asymmetric unit (shortest distance is between C*B*(7) and the picrate plane: 3·47 Å). Between the same picrate ion and the plane of the base translated along **a**, the distance does not differ (shortest distance between N*P*(4) and the base plane is 3·45 Å).

The two nitro groups N*P*(2)–O*P*(2)–O*P*(3) and N*P*(6)–O*P*(6)–O*P*(7) are rotated symmetrically towards the base belonging to the same asymmetric unit, thus bringing O*P*(2) to 3·20 Å from C*B*(2), and O*P*(7) 3·23 Å from N*B*(4).

There is a hydrogen bond (3·00 Å) between O(5′) of the sugar of the nucleoside translated along **a**, to the oxygen O*P*(5) of the picrate.

The formation of a complex pair does not occur, and the relation between the nucleoside analogue and the picrate is that of a salt.

The other hydrogen bonds are:

Atoms at *x,y,z*	Distance to				Atoms situated at
O*P*(1)	H(2′)	1·88	O(2′)	2·61	*x*, *y*−1, *z*
O*P*(4)	H(N*B*1)	2·09	N*B*(1)	2·81	1−*x*, *y*−½, 1−*z*
O(3′)	H*a*	2·08	N*B*(4)	2·92	−*x*, *y*−½, −*z*
O(5′)	H*b*	2·18	N*B*(4)	2·90	*x*, *y*−1, *z*

The packing (Fig. 4) indicates the hydrogen-bonding scheme.

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