

attempts to explain the variation of bond lengths in terms of electronic effects due to the partial double bond character of C(7)–O.

Table 5. *The shorter intermolecular contacts (Å) excluding hydrogen atoms*

Symmetry code			
(i)	$\frac{1}{2}-x,$	$-y,$	$\frac{1}{2}+z$
(ii)	$\frac{1}{2}+x,$	$\frac{1}{2}-y,$	$-z$
(iii)	$\frac{1}{2}+x,$	$-\frac{1}{2}-y,$	$-z$
(iv)	$1-x,$	$\frac{1}{2}+y,$	$-\frac{1}{2}-z$

C(23)···C(17 ^b)	3·50	C(10)···C(23 ⁱⁱⁱ)	3·65
C(9)···C(3 ⁱⁱ)	3·54	C(8)···C(3 ⁱⁱ)	3·66
C(9)···C(2 ⁱⁱ)	3·55	C(10)···C(20 ⁱⁱ)	3·68
C(3)···C(19 ⁱⁱⁱ)	3·57	C(21)···O ^{iv}	3·73
C(3)···C(20 ⁱⁱ)	3·61	C(3)···C(18 ⁱⁱ)	3·74
C(23)···C(18 ^b)	3·64	C(9)···C(20 ⁱⁱ)	3·76
C(8)···C(2 ⁱⁱ)	3·65		

The crystal packing is shown in Fig. 2, and the shorter intermolecular contact distances, excluding those involving H atoms, are in Table 5. None of these is shorter than the sum of the van der Waals radii. Contact distances involving the I⁻ ion are all greater than 4 Å.

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The Crystal Structure of an Orthorhombic Form of Adenosine-5'-monophosphate

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Adenosine-5'-phosphate monohydrate was crystallized in the orthorhombic space group $P2_12_1$, with $a=22.997$ (2), $b=9.406$ (1), $c=6.599$ (1) Å, $Z=4$. The structure was solved by direct methods and refined to a final R_w of 0.0639 for 1320 significant reflexions measured on an automatic diffractometer. The conformation of the molecule differs significantly from that previously reported for the monoclinic monohydrate [Kraut & Jensen, *Acta Cryst.* (1963), **16**, 79–88]. The sugar conformation, for example, is here C(2)-endo, and the glycosidic torsion angle has altered by almost 50°.

Introduction

The structure of adenosine-5'-monophosphate (5'-AMP) was first determined by Kraut & Jensen (1963), who crystallized it in the monoclinic space group $P2_1$.

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The results of this and other nucleotide structure analyses have been instrumental in furthering knowledge of the structures of the nucleic acids (Arnott, 1970). Especially useful and interesting have been the findings that the solid-state conformations of the nucleotides have been found to fall into a small number of discrete classes (Sundaralingam, 1969, 1973). How-

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ever, the degree of conformational flexibility of these molecules has long been a subject of dispute, as has the question of whether their solid-state crystal structures really reflect their solution conformations. Recent NMR studies unfortunately provide conflicting results (Barry, North, Glasel, Williams & Xavier, 1971; Sarma, Mynott, Hruska & Wood, 1973). Conformational energy calculations (Thornton & Bayley, 1975) suggest that 5'-AMP, at least, is relatively flexible, with a small number of preferred conformations. The Kraut & Jensen structure corresponds to a very low-energy (*i.e.* highly favoured) state.

It is therefore of some interest to examine the conformation of 5'-AMP in a different crystallographic environment, possibly providing an indication of the conformational rigidity of the molecule. As part of our programme of studies on nucleic acid constituents we have obtained crystals of an orthorhombic form, which we have subjected to a full single-crystal analysis.

Experimental

Colourless, long thin laths of 5'-AMP (Sigma Chemical Co.) were obtained by slow evaporation from aqueous solution. They showed parallel extinction under the polarizing microscope. Photographs revealed the crystals to have orthorhombic symmetry. Systematic absences $h00$, $0k0$ and $00l$ with h , k and $l=2n+1$ respectively, uniquely identified the space group as $P2_12_12_1$. Cell dimensions were obtained from least-squares refinement of 2θ values measured on a diffractometer.

Crystal data

$C_{10}H_{14}N_5O_7P \cdot H_2O$, F.W. 365.23. Orthorhombic needles, elongated along b . $a=22.997$ (2), $b=9.406$ (1), $c=6.599$ (1) Å, $V=1427.43$ Å³, $D_o=1.73$ (2) (by flotation), $D_c=1.711$ g cm⁻³ for $Z=4$. $F(000)=756$, $\mu=21.17$ cm⁻¹ for Cu $K\alpha$ radiation ($\lambda_{K\alpha}=1.54178$ Å). Space group $P2_12_12_1$ (No. 19).

Intensities were collected on a Siemens automatic four-circle diffractometer. 1549 unique reflexions were measured with a θ - 2θ scan technique, to a limit of 70° in θ , and Ni-filtered Cu $K\alpha$ radiation. Of these 1320 were considered to have counts significantly above background, with $I > 2.5\sigma(I)$. An absorption correction was not applied in view of the small size of the crystal ($0.20 \times 0.05 \times 0.02$ mm).

Structure determination and refinement

The structure was solved by direct methods with a multisolution tangent formula technique programmed by Dr G. M. Sheldrick. The positions of all 24 non-hydrogen atoms (including a water O atom) were clearly revealed in the most consistent E map. Refinement was by full-matrix least squares, $\sum w(F_o^2 - F_c^2/k^2)$ being minimized; weights w were chosen as $1/\sigma^2(F_o^2)$ from counting statistics, and k was a scale factor. The positional coordinates of all H atoms except those attached to the water molecule and to a phosphate O atom, were deduced from difference syntheses calculated during the later stages of refinement. These missing H atoms were not located at any stage of the analysis. Convergence of refinement was achieved with

Table 1. Final positional ($\times 10^4$) and anisotropic (U_{ij}) thermal parameters ($\times 10^3$) for the non-hydrogen atoms

Estimated standard deviations are given in parentheses.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)'	1867 (3)	1117 (8)	7401 (16)	28 (4)	9 (4)	41 (5)	1 (4)	-4 (4)	0 (3)
C(2)	3419 (4)	3729 (10)	7416 (18)	27 (4)	36 (5)	46 (6)	-3 (6)	5 (5)	-2 (3)
C(2)'	1415 (4)	537 (9)	8895 (14)	37 (5)	12 (4)	31 (5)	-7 (4)	1 (4)	1 (4)
C(3)'	1170 (4)	-718 (8)	7704 (14)	31 (4)	13 (4)	29 (5)	1 (4)	-4 (4)	-3 (3)
C(4)	2469 (3)	3341 (6)	7523 (15)	25 (4)	21 (4)	28 (4)	-2 (4)	-4 (4)	-3 (3)
C(4)'	1226 (4)	-279 (9)	5445 (14)	38 (5)	10 (4)	31 (5)	-4 (4)	-3 (4)	-4 (3)
C(5)	2328 (3)	4835 (8)	7554 (15)	30 (4)	9 (4)	32 (5)	3 (4)	1 (4)	-2 (3)
C(5)'	685 (4)	325 (10)	4498 (18)	42 (5)	21 (5)	50 (6)	-15 (5)	-10 (5)	1 (4)
C(6)	2797 (3)	5765 (9)	7551 (14)	33 (4)	29 (5)	19 (4)	-3 (5)	-3 (4)	-15 (4)
C(8)	1516 (3)	3722 (8)	7606 (16)	23 (4)	19 (4)	39 (5)	1 (4)	-2 (4)	-2 (3)
N(1)	3334 (3)	5187 (7)	7520 (14)	24 (4)	24 (4)	47 (5)	2 (4)	-2 (4)	-8 (3)
N(3)	3004 (3)	2793 (7)	7421 (14)	28 (3)	19 (4)	51 (5)	0 (4)	2 (4)	-2 (3)
N(6)	2740 (4)	7199 (7)	7580 (16)	43 (5)	9 (4)	51 (5)	1 (4)	-1 (5)	-10 (3)
N(7)	1738 (3)	5023 (6)	7605 (14)	34 (4)	6 (3)	44 (5)	-2 (4)	-4 (4)	-3 (3)
N(9)	1947 (3)	2685 (6)	7557 (13)	27 (3)	10 (3)	33 (4)	1 (3)	2 (4)	0 (3)
O(1)	185 (3)	4059 (7)	5767 (14)	53 (4)	29 (4)	81 (6)	-22 (5)	2 (5)	5 (3)
O(1)'	1688 (3)	784 (6)	5415 (9)	46 (3)	22 (3)	26 (3)	-3 (3)	4 (3)	-12 (3)
O(2)	770 (3)	3217 (6)	2602 (14)	37 (3)	24 (3)	68 (5)	2 (4)	3 (4)	-10 (3)
O(2)'	1652 (3)	195 (6)	10765 (11)	56 (4)	15 (3)	33 (3)	-2 (3)	-4 (4)	-7 (3)
O(3)	-254 (2)	2464 (7)	3089 (11)	24 (3)	30 (4)	63 (5)	12 (3)	-1 (3)	-8 (3)
O(3)'	1545 (3)	-1928 (6)	8090 (10)	54 (4)	6 (3)	50 (4)	-1 (3)	-7 (3)	5 (3)
O(5)'	523 (3)	1634 (6)	5546 (11)	55 (4)	17 (3)	38 (4)	2 (3)	-7 (4)	8 (3)
P	319 (1)	2953 (2)	4183 (4)	24 (1)	17 (1)	56 (2)	2 (1)	-1 (1)	-3 (1)
O(W)*	5341 (4)	-1851 (8)	4223 (16)	58 (5)	31 (4)	77 (6)	-6 (5)	-8 (6)	0 (4)

* O(W) refers to the water O atom.

non-hydrogen positional and anisotropic thermal parameters, and hydrogen positional and isotropic thermal parameters, all varied simultaneously. The final R_w was 0.0639 ($R_w = \sum w||F_o| - |F_c|| / \sum w|F_o|$); R was 0.0652. The final parameters are listed in Tables 1 and 2.*

Scattering factors and anomalous dispersion corrections were taken from *International Tables for X-ray Crystallography* (1974). The signs of the dispersion corrections were taken by reference to the known D-ribose absolute configuration of the molecule; the positional parameters all correspond to the correct

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31580 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. Final positional ($\times 10^3$) and isotropic (U) thermal parameters ($\times 10^2$) for the hydrogen atoms

Estimated standard deviations are in parentheses. In each case the non-hydrogen atom to which each hydrogen atom is bonded, is shown.

The average X-H distance is 1.00 (14) Å.

	x	y	z	U
H(1) (N1)	373 (4)	538 (10)	766 (18)	5 (3)
H(2) (C2)	379 (4)	322 (9)	734 (16)	4 (2)
H(6) (N6)	233 (3)	753 (8)	750 (16)	2 (2)
H(6)'(N6)	304 (4)	751 (9)	774 (15)	2 (2)
H(8) (C6)	109 (3)	354 (7)	757 (13)	1 (2)
H(1)'(C1')	233 (3)	76 (7)	759 (13)	1 (2)
H(2)'(C2')	109 (3)	120 (9)	900 (15)	3 (2)
H(2)''(O2')	211 (4)	14 (11)	1075 (19)	6 (3)
H(3)'(C3')	70 (3)	-85 (8)	789 (13)	2 (2)
H(3)''(O3')	159 (4)	-183 (9)	680 (16)	6 (4)
H(4)'(C4')	136 (5)	-109 (13)	439 (20)	8 (4)
H(5)'(C5')	23 (4)	-14 (10)	470 (15)	5 (3)
H(5)''(C5')	79 (4)	39 (9)	293 (15)	3 (2)

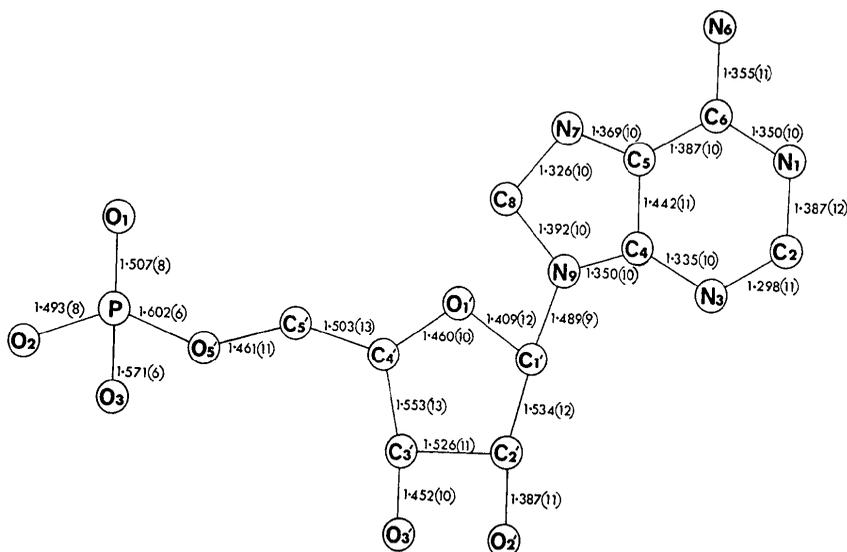


Fig. 1. Intramolecular bonded distances in Å. Estimated standard deviations are given in parentheses.

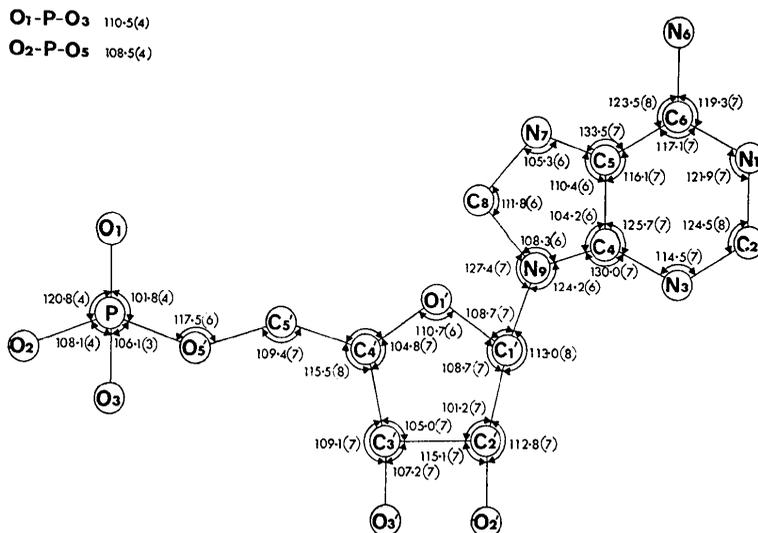


Fig. 2. Valence angles, in degrees, with estimated standard deviations in parentheses.

configuration. The calculations were performed with a set of programs written by Dr G. M. Sheldrick, and implemented on a CDC 7600 computer.

Discussion

The molecular structure – bond lengths and angles

The analysis has shown that 5'-AMP exists in the orthorhombic form as a zwitterion with protonation at N(1); the monoclinic form has the same distribution

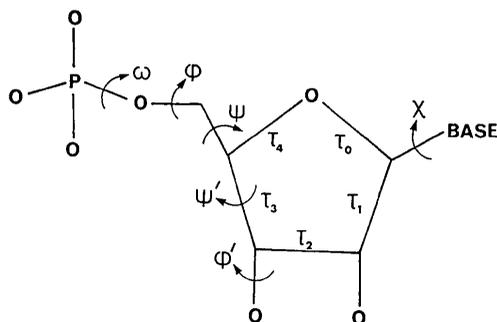


Fig. 3. The conformational angles of a nucleotide unit. These are considered positive for a right-handed clockwise rotation (Sundaralingam, 1969). Angles ω , ϕ' are not applicable to a monomer, *i.e.* a mononucleotide.

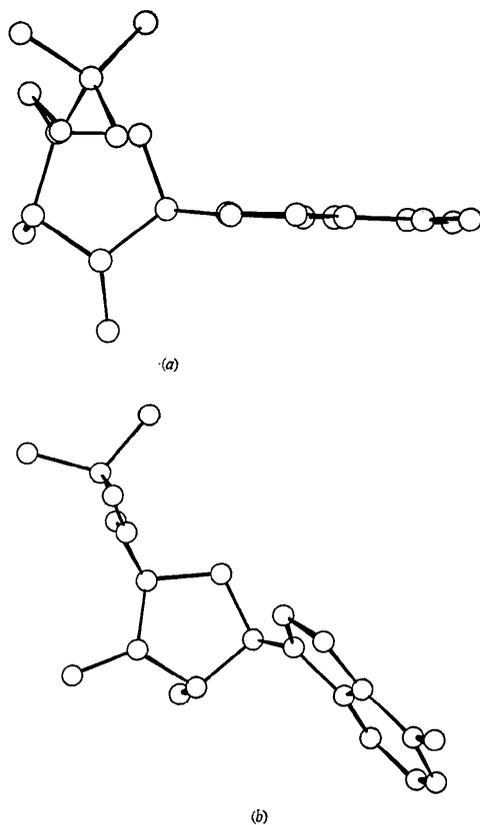


Fig. 4. Views of (a) orthorhombic 5'-AMP and (b) monoclinic 5'-AMP, perpendicular to the C(1)'-O(1)'-C(5)' sugar plane.

of charge, with a negative charge presumably located on a phosphate O atom. Intramolecular bond lengths and angles for orthorhombic 5'-AMP are shown in Figs. 1 and 2. The values found compare well with those reported for monoclinic 5'-AMP, although there are a few significant bond length differences – these are detailed below.

Average bond lengths and angles for the adenine base have been reported in a survey (Voet & Rich, 1970). The geometry of the adenine in orthorhombic 5'-AMP is comparable with these averages; as noted elsewhere (Saenger, 1973) protonation at N(1) has induced slight differences between the zwitterion and neutral molecules. N(1)-C(2), particularly, is lengthened in the ionic form, and the angle at N(1) is slightly widened. The anomalously long C(4)-C(5) recorded here (1.442 Å), compared with averages of 1.365 for neutral and 1.392 Å for protonated molecules, does not fit into this pattern and cannot easily be explained. C(5)-C(6), on the other hand, is much shorter than in monoclinic 5'-AMP (1.387 compared to 1.448 Å) and conforms with the tabulated averages. The adenine ring is planar within experimental error (Table 3).

Table 3. Least-squares planes

Atoms marked (*) have been excluded from the calculation of the plane. Deviations from the planes are in Å.

Adenine ring

N(1) 0.022, C(2) -0.012, N(3) -0.015, C(4) 0.010,
C(5) -0.001, C(6) -0.002, N(6) -0.019, N(7) -0.012,
C(8) 0.001, N(9) 0.015

Sugar ring

C(1)' 0.000, C(2)' 0.359*, C(3)' -0.146*, C(4)' 0.000,
O(1)' 0.000

The equations for the least-squares planes are in the form:

$$px + qy + rz = s.$$

	<i>p</i>	<i>q</i>	<i>r</i>	<i>s</i>
Adenine ring	0.025	-0.022	0.999	5.028
Sugar ring	0.685	-0.727	-0.042	1.974

The geometry of the ribose sugar ring conforms well with expected values (Saenger, 1973), although the two hydroxyl bonds do differ more than might be expected from a reported mean of 1.41 Å. The commonly observed finding of O(1)'-C(4)' longer than O(1)'-C(1)' is seen here.

Although no proton was found on any of the phosphate O atoms, its probable location was readily deduced. P-O(3) is undoubtedly a double bond. Since O(2) has a close contact (2.5 Å) with protonated N(1), it is likely that it carries a negative charge, rather than a proton, which must therefore be attached to O(1).

Molecular conformation

The conformational angles used in this discussion are defined in Fig. 3. These are discussed in some detail by, for example, Sussman, Seeman, Kim & Berman (1972) and Sundaralingam (1969). Table 4 gives the

values found for the angles, both from this analysis and for some other related nucleotides. It is apparent that the two 5'-AMP structures exhibit markedly different conformations in all parts of the molecules. These differences are shown in Figs. 4 and 5, which particularly highlight the nearly 50° difference in the O(1')-C(1')-N(9)-C(8) (χ) glycosidic torsion angle. The monoclinic form has a *syn* conformation, and the orthorhombic may be said to be *anti* (although only just); however, although the χ value for the former falls well within ranges of values for many purine nucleotides, that for the latter does not (Sundaralingam, 1969).

This is probably connected with the C(2')-*endo* sugar conformation observed here, which contrasts with the C(3')-*endo* of the monoclinic form. This difference is shown in Fig. 5. The observed ribose torsion angles and out-of-plane deviations (Table 3) are typical of C(2')-*endo* puckering. The results of the conformational energy calculations of Thornton & Bayley (1975) are given in detail for a C(3')-*endo* sugar only; however, these authors do suggest that a C(2')-*endo* puckering would prefer a χ angle of about 60°, with preference for the *syn* state. This is indeed roughly what we find.

These two sugar conformations are encountered equally commonly among purine and pyrimidine nucleosides and nucleotides. However, a C(2')-*endo* adenylyl sugar is quite rare. Examples of its occurrence illustrate well the supposition that nucleotides are relatively flexible, and can adopt differing conformations without having to overcome a large energy barrier. Thus, of the two independent molecules in the crystal structure of adenosine triphosphate (Kennard *et al.*, 1971), one has a C(2')-*endo* sugar, and the other a C(3')-*endo*. The recently-reported structures of two dinucleoside phosphate-drug complexes show a C(2')-*endo* adenylyl sugar, in contrast to the C(3')-*endo* of the uncomplexed dinucleoside phosphates (Seeman, Day & Rich, 1975; Tsai, Jain & Sobell, 1975). It seems that, for drug interaction to occur, this conformational change is needed.

Intermolecular packing

Figs. 6 and 7 show two views of the crystal structure, which consists of chains of 5'-AMP molecules linked

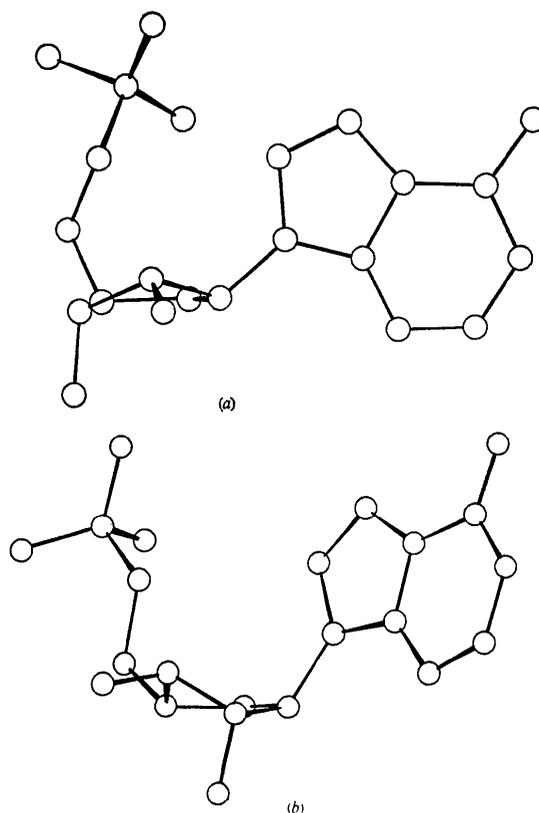


Fig. 5. (a), (b), as in Fig. 4, but now viewed along the C(1')-O(1')-C(5') sugar plane.

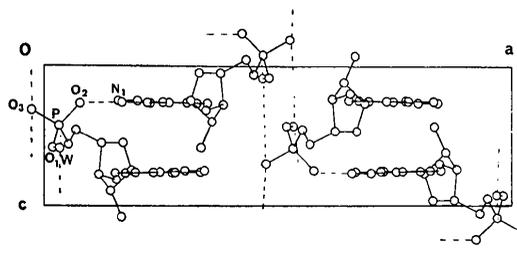


Fig. 6. The *b*-axis projection of the crystal structure; dashed lines represent hydrogen bonds.

Table 4. Some nucleotide and polynucleotide conformations, torsion angles are in degrees

	χ	ϕ	ψ	ψ'	τ_0	τ_1	τ_2	τ_3	τ_4	Sugar pucker
This study	72.5	137.3	62.3	-32.3	-14.2	27.8	-30.2	23.3	-5.8	C(2')- <i>endo</i>
Monoclinic 5'-AMP (a)	25.7	177.2	40.0	74.8	4.8	-29.8	42.3	-40.0	22.8	C(3')- <i>endo</i>
3'-AMP (a)	3.8	149.5	171.2	83.8	-3.4	-19.1	34.6	-37.6	25.6	C(3')- <i>endo</i>
Adenylyl-3',5'-uridine (b) (adenylyl group only)	3.5	173	57	—	—	—	—	—	—	C(3')- <i>endo</i>
Adenylyl-2',5'-uridine (a) (adenylyl group only)	54.6	—	45.3	148.4	-30.5	43.5	-37.8	20.2	6.1	C(2')- <i>endo</i>
B-DNA (c)	66	213	36	156	-4	25	-35	33	-19	C(2')- <i>endo</i>
RNA-11 (d)	14	180	48	83	3	126	37	-36	21	C(3')- <i>endo</i>

(a) Values have been taken from the compilation of Sundaralingam (1969). (b) Day, Seeman, Rosenberg & Rich (1973). The mean values for the two independent molecules are given. The torsion angles for the sugar residues are not reported. (c) Arnott & Hukins (1972). (d) Arnott, Hukins & Dover (1972).

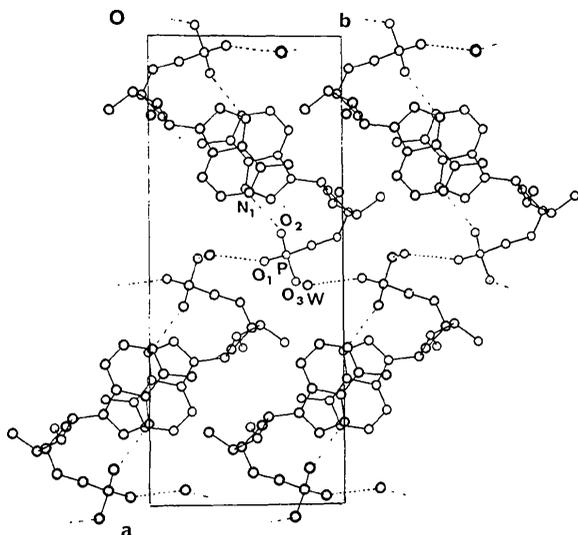


Fig. 7. The *c*-axis projection of the crystal structure.

together by strong hydrogen bonds to water molecules. These chains extend in both the *b* and *c* directions. The hydrogen bonds are from phosphate O atoms to the water O; O(1)···O(W) is 2.651 and O(3)···O(W) 2.623 Å. There is also a very short (Donohue, 1969; Fuller, 1959) N(1)···O(2) interaction of 2.550 Å, involving *c*-axis screw-related molecules (Fig. 7). The adenine bases are nearly parallel both to each other and to *a*, some stacking being evident, and with a mean inter-base spacing of about 3.5 Å. As has been pointed out (Bugg, Thomas, Sundaralingam & Rao, 1971), partial base overlap is usual for this class of compound.

It is not surprising, in view of the conformational differences, that there are considerable differences in the packing modes of orthorhombic and monoclinic 5'-AMP in spite of their both crystallizing with one water molecule per nucleotide. For example, in the latter crystal structure, only two of the three phosphate O atoms participate in hydrogen bonding, whereas the sugar hydroxyl O(2') and O(3') do.

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