The structure is stabilized by a network of hydrogen bonds involving the amino and carboxylate groups of both molecules and the water molecules. Fig. 2 gives a stereoscopic view of the packing of the molecules in the unit cell. The amino groups each take part in three hydrogen bonds, to two water O atoms and O(1) of the carboxyl groups [N(1)*A*···O*W*3, 2·944 (1), H1N(1)···O*W*3, 2·01 Å; N(1)–H1N(1)···O*W*3, 166°; N(1)*A*···O*W*2, 2·764 (1), H2N(1)···O*W*2, 1·94 Å; N(1)–H2N(1)···O*W*2, 145°; N(1)*A*···O(1)*A*, 2·751 (1), H3N(1)···O(1)*A*, 1·74 Å; N(1)–H3N(1)···O(1)*A*, 178°; N(1)*B*···O*W*1, 2·775 (1), H1N(1)···O*W*1, 1·81 Å; N(1)–H1N(1)···O*W*1, 172°; N(1)*B*···O*W*3, 2·860 (1), H2N(1)···O*W*3, 2·05 Å; N(1)–H2N(1)···O*W*3, 151°; N(1)*B*···O(1)*B*, 2·776 (1), H3N(1)···O(1)*B*, 1·78 Å; N(1)–H3N(1)···O(1)*B*, 177°]. Two water molecules, O*W*1 and O*W*2, donate two hydrogen bonds to the carbonyl oxygens and receive one each from the amino N atoms [O*W*1···O(1)*A*, 2·753 (1), H1O*W*1···O(1)*A*, 1·88 Å, O*W*1–H1O*W*1···O(1)*A*, 172°; O*W*1···O(2)*B*, 2·853 (1), H2O*W*1···O(2)*B*, 2·01 Å, O*W*1–H2O*W*1···O(2)*B*, 162°; O*W*2···O(2)*A*, 2·721 (1), H1O*W*2···O(2)*A*, 1·89 Å, O*W*2–H1O*W*2···O(2)*A*, 175°; O*W*2···O(2)*B*, 2·768 (1), H2O*W*2···O(2)*B*, 1·90 Å, O*W*2–H2O*W*2···O(2)*B*, 152°]. The third water oxygen, O*W*3, by contrast receives two hydrogen bonds from each of the amino N atoms of molecules *A* and *B* and donates two hydrogen bonds to the carbonyl oxygens O(2) of *A* and *B* [O*W*3···O(2)*B*, 2·833 (1), H1O*W*3···O(2)*B*, 1·96 Å, O*W*3–H1O*W*3···O(2)*B*, 177°; O*W*3···O(2)*A*, 2·724 (1), H2O*W*3···O(2)*A*, 1·93 Å, O*W*3–H2O*W*3···O(2)*A*, 145°]. The hydrogen-bonding environment of O*W*1 is trigonal non-planar; O*W*2 is trigonal planar and O*W*3 is tetrahedral.

We thank Dr R. Parthasarathy for the use of crystallographic facilities and helpful discussions, and Mr Louis Leone, a summer student, for participating in this project. This work is supported by the New York State Department of Health.

References

CHACKO, K. K., SWAMINATHAN, S. & BHATTACHARJEE, S. K. (1981). *Biomolecular Structure, Conformation, Function and Evolution*, Vol. 1, edited by R. SRINIVASAN, pp. 621–631. Oxford: Pergamon Press.

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

GAUDESTAD, O., MOSTAD, A. & ROMMING, C. (1976). *Acta Chem. Scand. Ser. B*, **30**, 501–504.

GERMAIN, G., MAIN, P. & WOOLFSON, M. M. (1971). *Acta Cryst.* A**27**, 368–376.

JOHNSON, C. K. (1965). *ORTEP*. Report ORNL-3794. Oak Ridge National Laboratory, Tennessee, USA.

NEUMAN, A., GILLIER, H., AVENEL, D. & PERRET, G. (1984). *Acta Cryst.* C**40**, 2124–2126.

SATYSHUR, K. A. & RAO, S. T. (1983). *Acta Cryst.* C**39**, 1672–1673.

Acta Cryst. (1988). C**44**, 850–853

Structure of *N*-Pivaloyl-*N*′-methyl-L-prolinamide*

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(*Received* 1 *September* 1987; *accepted* 16 *December* 1987)

Abstract. $C_{11}H_{20}N_2O_2$ (Piv-L-Pro-NHMe; Piv, pivaloyl and NHMe, methylamino): $M_r = 212{\cdot}30$, orthorhombic, $P2_12_12_1$, $a = 23{\cdot}366$ (2), $b = 7{\cdot}972$ (1), $c = 6{\cdot}445$ (1) Å, $V = 1200{\cdot}5$ (3) Å^3, $Z = 4$, $D_x = 1{\cdot}174$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}76$ cm^{-1}, $F(000) = 464$, $T = 295$ K. The final R value for 897 observed [$I \geq 3\sigma(I)$] reflections is 0·055. The conformation of the two amide bonds is *trans* and the L-Pro residue shows a φ, ψ set of torsion angles falling in region F of the energy map where poly(L-Pro) II and collagen structures are found. The dihedral angle δ between the two amide groups is 79·2 (10)°.

Introduction. The 3 → 1 intramolecularly H-bonded peptide conformation, also termed C_7 form or γ-turn, is a ring structure that is folded by an H bond between the main-chain peptide N–H of residue 3 and the C=O of residue 1 (Némethy & Printz, 1972). The occurrence of this type of folding has been unequivocally demonstrated by X-ray diffraction in crystals of two *cyclic* peptides and a very limited number of *proteins* (thermolysin, ferricytochrome c) (Toniolo, 1980). So

* Linear Oligopeptides. 187. Part 186: Bardi, Piazzesi, Toniolo, Jensen & Senning (1988).

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0108-2701/88/050850-04$03.00

far, no experimental evidence has been found, however, for the existence of the γ-turn conformation in crystalline *linear* peptides.

We considered the terminally blocked amino acid *N*-pivaloyl-*N'*-methyl-L-prolinamide (Piv-L-Pro-NHMe) to be a promising candidate for adopting the γ-turn conformation in the crystal state on the basis of the following properties: (i) In $CDCl_3$ solution at low concentration, where self-association is absent, in addition to the IR absorption band at 3457 cm^{-1} (stretching mode of free N—H groups) a relatively intense band at 3330 cm^{-1} (H-bonded N—H groups) is seen. (ii) Published ^1H and ^{13}C NMR studies are in favour of the occurrence of the γ-turn conformation to a substantial extent in the equilibrium mixtures of this compound in a variety of solvents (Nagaraj, Venkatachalapathi & Balaram, 1980; Giessner-Prettre, Cung & Marraud, 1987). (iii) The solid-state IR absorption spectrum shows an intense band at 1606 cm^{-1}, due to the Piv-Pro amide carbonyl stretching mode, shifted markedly to lower wavenumbers compared with the free amide carbonyl of Piv-L-Pro-OMe (OMe, methoxy) which is seen at 1626 cm^{-1} (Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1982). In addition, the methylamide carbonyl is free (1686 cm^{-1}). The stretching band of H-bonded N—H groups is found at 3323 cm^{-1} under these experimental conditions.

As part of our continuing study on the various types of intramolecularly H-bonded conformations formed by short peptides (Toniolo, 1980), the present paper is concerned with the molecular and crystal structure of Piv-L-Pro-NHMe.

Experimental. Colourless crystals of Piv-L-Pro-NHMe (Nagaraj, Venkatachalapathi & Balaram, 1980) were obtained from an ethyl acetate/petroleum ether solution by slow evaporation. Crystal 0·12×0·12×0·8 mm. Intensities were collected on a Philips PW 1100 four-circle diffractometer operating in the $\theta/2\theta$ scan mode (with scan width 1·2° and scan speed 0·03° s^{-1}) with graphite-monochromatized Mo $K\alpha$ radiation. 1262 reflections up to $2\theta = 50°$ were measured, of which 897 had intensities greater than $3\sigma(I)$. h, k, l range 0–26, 0–9, 0–7. During data collection three standard reflections were measured every 180 min to check stability of the crystal and the electronics. Intensities were corrected for Lorentz and polarization factors; no absorption correction was applied.

The structure was solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined on F by block-diagonal least squares with anisotropic thermal parameters for all non-H atoms ($w = 1$). The H atoms were partially localized on the ΔF map and all refined isotropically. All calculations were performed on the IBM 370/158 computer of the University of Padova, using *SHELX*76 (Sheldrick, 1976). The final R value was 0·055. $S = 0·69$. $(\Delta/\sigma)_{max}$ in final refinement cycle for non-H atoms 0·73. Max. and min. heights in final ΔF synthesis 0·25 and −0·29 e $Å^{-3}$. Atomic scattering factors from *SHELX*. Table 1 gives the final atomic coordinates and isotropic thermal parameters for the non-H atoms.*

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å²) *for the non-*H *atoms of Piv-*L*-Pro-*NH*Me (with e.s.d.'s in parentheses)*

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

	x	y	z	U_{eq}
O(1)	0·6838 (2)	0·1668 (5)	0·8569 (7)	0·0527
O(2)	0·6575 (2)	−0·2322 (5)	0·8622 (7)	0·0625
N(1)	0·6335 (2)	0·0429 (6)	1·1084 (7)	0·0439
N(2)	0·7473 (2)	−0·2557 (6)	0·9897 (8)	0·0519
C(1)	0·5333 (2)	0·1633 (9)	0·8278 (12)	0·0726
C(2)	0·5732 (3)	0·3888 (9)	1·0697 (12)	0·0760
C(3)	0·6047 (3)	0·3712 (9)	0·6964 (11)	0·0703
C(4)	0·5865 (2)	0·2667 (8)	0·8859 (11)	0·0516
C(5)	0·6380 (2)	0·1533 (7)	0·9501 (9)	0·0412
C(6)	0·5835 (3)	−0·0096 (9)	1·2325 (11)	0·0662
C(7)	0·6065 (5)	−0·1376 (22)	1·3757 (28)	0·1125
C(8)	0·6674 (3)	−0·1480 (11)	1·3625 (12)	0·0696
C(9)	0·6841 (3)	−0·0591 (8)	1·1581 (10)	0·0457
C(10)	0·6947 (3)	−0·1887 (8)	0·9863 (10)	0·0457
C(11)	0·7643 (3)	−0·3881 (9)	0·8450 (12)	0·0609

Table 2. *Bond lengths* (Å) *and bond angles* (°) *for Piv-*L*-Pro-*NH*Me (with e.s.d.'s in parentheses)*

O(1)–C(5)	1·232 (7)	C(2)–C(4)	1·564 (10)
O(2)–C(10)	1·231 (8)	C(3)–C(4)	1·538 (10)
N(1)–C(5)	1·352 (7)	C(4)–C(5)	1·561 (8)
N(1)–C(6)	1·476 (8)	C(6)–C(7)	1·477 (19)
N(1)–C(9)	1·470 (8)	C(7)–C(8)	1·428 (14)
N(2)–C(10)	1·340 (8)	C(8)–C(9)	1·546 (10)
N(2)–C(11)	1·463 (9)	C(9)–C(10)	1·535 (9)
C(1)–C(4)	1·538 (8)		

C(5)–N(1)–C(6)	130·9 (5)	O(1)–C(5)–C(4)	119·3 (5)
C(5)–N(1)–C(9)	117·5 (5)	N(1)–C(5)–C(4)	121·2 (5)
C(6)–N(1)–C(9)	111·2 (5)	N(1)–C(6)–C(7)	104·3 (7)
C(10)–N(2)–C(11)	121·7 (5)	C(6)–C(7)–C(8)	111·4 (12)
C(1)–C(4)–C(2)	110·9 (5)	C(7)–C(8)–C(9)	106·0 (9)
C(1)–C(4)–C(3)	108·7 (5)	N(1)–C(9)–C(8)	103·7 (5)
C(1)–C(4)–C(5)	112·2 (5)	N(1)–C(9)–C(10)	110·2 (5)
C(2)–C(4)–C(3)	108·6 (5)	C(8)–C(9)–C(10)	110·3 (6)
C(2)–C(4)–C(5)	108·2 (5)	O(2)–C(10)–N(2)	123·1 (6)
C(3)–C(4)–C(5)	108·1 (5)	O(2)–C(10)–C(9)	123·0 (6)
O(1)–C(5)–N(1)	119·5 (5)	N(2)–C(10)–C(9)	113·9 (6)

Discussion. Bond lengths and bond angles of Piv-L-Pro-NHMe (Table 2) compare well with those found in other tertiary pivalamides (Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1982; Aubry, Cung & Marraud, 1985), proline derivatives (Balasubramanian, Lakshminarayanan, Sabesan, Tegoni, Venkatesan & Ramachandran, 1971; Ashida &

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44622 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Kakudo, 1974; De Tar & Luthra, 1977; Nair & Vijayan, 1981; Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1983; Ashida, Tsunogae, Tanaka & Yamane, 1987), and secondary noncyclic amides (Chakrabarti & Dunitz, 1982). In particular: (i) Bond angles of the Piv-Pro amide bond are perturbed by steric hindrance between the bulky *tert*-butyl group and the C(6) atom, resulting in an extremely large C(5)–N(1)–C(6) angle, 130·9 (5)°, and in a small C(5)–N(1)–C(9) angle, 117·5 (5)°. (ii) Bond lengths involving the C(7) atom are shorter than usual, 1·477 (19) and 1·428 (14) Å. The high anisotropy of the C(7) thermal motion (Fig. 1) is due to static structural disorder.

The dihedral angle δ between the normals to the average planes of the two amide groups of Piv-L-Pro-NHMe is 79·2 (10)° in agreement with the observed preference for this angle in *N*-acyl, *N'*-methyl α-amino acid amides (Chen & Parthasarathy, 1978). The dihedral angle between the normals to the average planes of the pivaloyl group and the pyrrolidine ring is 5·3 (12)°.

The amide torsion angles ω (IUPAC–IUB Commission on Biochemical Nomenclature, 1970) are *trans*: 179·9 (5) [C(9)–N(1)–C(5)–C(4), pivalamide] and 176·6 (6)° [C(11)–N(2)–C(10)–C(9), methylamide]. In the Piv-Pro compounds studied so far, the pivalamide group is frozen in the *trans* conformation (Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1982) since in this arrangement the central C(4) atom of the bulky *tert*-butyl moiety of the pivaloyl group and the disubstituted C^{α} atom of the linked amino acid residue are also *trans* to each other.

The *tert*-butyl moiety of the pivaloylamino group of Piv-L-Pro-NHMe adopts the usual *A* conformation with respect to the amide group (Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1982). In this conformation the C(3) methyl group is eclipsed with respect to the C(5)=O(1) bond [C(3)–C(4)–C(5)–N(1) = $\theta^{1,3}$ = −177·5 (5)°] and the other two methyl groups, C(1) and C(2), are skew [C(1)–C(4)–C(5)–N(1) = $\theta^{1,1}$ = −57·7 (7); C(2)–C(4)–C(5)–N(1) = $\theta^{1,2}$ = 65·0 (7)°]. Consequently, the plane of the amide moiety nearly bisects the C(1)–C(4)–C(2) angle. In this conformation the C(6) atom would have experienced severe steric interactions with both C(1) and C(2) methyls, if not relieved by the aforementioned marked opening of the C(5)–N(1)–C(6) bond angle.

The set of φ, ψ [C(5)–N(1)–C(9)–C(10), N(1)–C(9)–C(10)–N(2)] angles for the L-Pro residue, −70·5 (7) and 163·2 (5)°, falls in region *F* (Zimmerman, Pottle, Némethy & Scheraga, 1977) of the conformational energy map, where poly(L-Pro)$_n$ II and collagen structures are found, at variance with the corresponding sets of values shown by Ac-L-Pro-NHMe (Ac, acetyl) (Matsuzaki & Iitaka, 1971) and Ac-L-Pro-NH$_2$ (Drück, Littke & Main, 1979), the only two *N*-acylated prolinamides whose structures have been solved so far (Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1983), which fall in region *A* where the right-handed α/3$_{10}$-helices are found (−76·3, −15·8, and −80·1, −14·2°, respectively).

The pyrrolidine ring of the L-Pro residue has a conformation described as C_s (envelope) symmetry with C^{β}-*exo* or conformation *B* (Balasubramanian, Lakshminarayanan, Sabesan, Tegoni, Venkatesan & Ramachandran, 1971; Ashida & Kakudo, 1974; De Tar & Luthra, 1977; Nair & Vijayan, 1981; Benedetti, Bavoso, Di Blasio, Pavone, Pedone, Toniolo & Bonora, 1983), the ring torsion angles being C(6)–N(1)–C(9)–C(8) = θ = −14·6 (7), C(7)–C(8)–C(9)–N(1) = χ_1 = 18·5 (9), C(6)–C(7)–C(8)–C(9) = χ_2 = −16·5 (13), N(1)–C(6)–C(7)–C(8) = χ_3 = 7·5 (13) and C(9)–N(1)–C(6)–C(7) = χ_4 = 5·2 (9)°. Ring conformation *B* is also adopted by Ac-L-Pro-NHMe (Matsuzaki & Iitaka, 1971) and Ac-L-Pro-NH$_2$ (Drück, Littke & Main, 1979).

There are no intramolecular hydrogen bonds in Piv-L-Pro-NHMe. Rather, chains of molecules are formed *via* intermolecular N–H···O=C(pivaloyl-amide) hydrogen bonds (Fig. 2). The N(2)···O(1) ($\frac{3}{2}-x$, $-y$, $\frac{1}{2}+z$) distance is 2·949 (10) Å, falling within the most probable range for the length of an

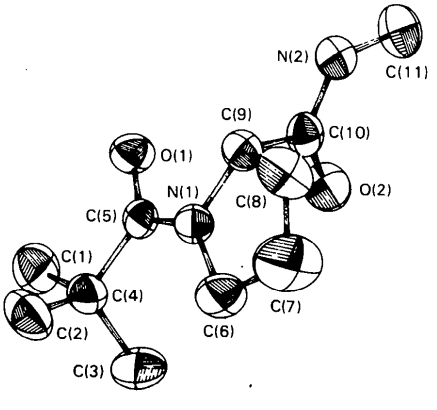

Fig. 1. Molecular structure of Piv-L-Pro-NHMe with the numbering of atoms.

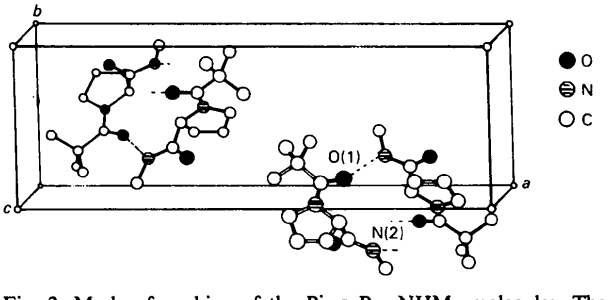

Fig. 2. Mode of packing of the Piv-L-Pro-NHMe molecules. The intermolecular hydrogen bond is indicated as a dashed line.

(amide)N–H···O=C(amide) hydrogen bond (Ramakrishnan & Prasad, 1971; Taylor, Kennard & Versichel, 1984).

To summarize, despite the solution behaviour and solid-state IR absorption spectra, the Piv-L-Pro-NHMe molecules do not fold up in the γ-turn conformation in the crystalline state. Other crystalline amino acid derivatives and linear peptides, promising candidates for adopting such an intramolecularly hydrogen-bonded structure, are currently under scrutiny in our laboratory.

References

ASHIDA, T. & KAKUDO, M. (1974). *Bull. Chem. Soc. Jpn*, **47**, 1129–1133.

ASHIDA, T., TSUNOGAE, Y., TANAKA, I. & YAMANE, T. (1987). *Acta Cryst.* B**43**, 212–218.

AUBRY, A., CUNG, M. T. & MARRAUD, M. (1985). *J. Am. Chem. Soc.* **107**, 7640–7647.

BALASUBRAMANIAN, R., LAKSHMINARAYANAN, A. V., SABESAN, M. N., TEGONI, G., VENKATESAN, K. & RAMACHANDRAN, G. N. (1971). *Int. J. Protein Res.* **3**, 25–33.

BARDI, R., PIAZZESI, A. M., TONIOLO, C., JENSEN, O. E. & SENNING, A. (1988). *Biopolymers*. In the press.

BENEDETTI, E., BAVOSO, A., DI BLASIO, B., PAVONE, V., PEDONE, C., TONIOLO, C. & BONORA, G. M. (1982). *Int. J. Pept. Protein Res.* **20**, 312–319.

BENEDETTI, E., BAVOSO, A., DI BLASIO, B., PAVONE, V., PEDONE, C., TONIOLO, C. & BONORA, G. M. (1983). *Biopolymers*, **22**, 305–317.

CHAKRABARTI, P. & DUNITZ, J. D. (1982). *Helv. Chim. Acta*, **65**, 1555–1562.

CHEN, C. S. & PARTHASARATHY, R. (1978). *Int. J. Pept. Protein Res.* **11**, 9–18.

DE TAR, D. L. F. & LUTHRA, N. P. (1977). *J. Am. Chem. Soc.* **99**, 1232–1244.

DRÜCK, U., LITTKE, W. & MAIN, P. (1979). *Acta Cryst.* B**35**, 253–255.

GIESSNER-PRETTRE, C., CUNG, M. T. & MARRAUD, M. (1987). *Eur. J. Biochem.* **163**, 79–87.

IUPAC–IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE (1970). *J. Mol. Biol.* **52**, 1–17.

MAIN, P., FISKE, S. J., HULL, S. E., LESSINGER, L., GERMAIN, G., DECLERCQ, J.-P. & WOOLFSON, M. M. (1980). *MULTAN80. A System of Computer Programs for the Automatic Solution of Crystal Structures from X-ray Diffraction Data*. Univs. of York, England, and Louvain, Belgium.

MATSUZAKI, T. & IITAKA, Y. (1971). *Acta Cryst.* B**27**, 507–516.

NAGARAJ, R., VENKATACHALAPATHI, Y. V. & BALARAM, P. (1980). *Int. J. Pept. Protein Res.* **16**, 291–298.

NAIR, C. M. K. & VIJAYAN, M. (1981). *J. Indian Inst. Sci. Sect. C*, **63**, 81–103.

NÉMETHY, G. & PRINTZ, M. P. (1972). *Macromolecules*, **5**, 755–758.

RAMAKRISHNAN, C. & PRASAD, N. (1971). *Int. J. Protein Res.* **3**, 209–231.

SHELDRICK, G. M. (1976). *SHELX76*. Program for crystal structure determination. Univ. of Cambridge, England.

TAYLOR, R., KENNARD, O. & VERSICHEL, W. (1984). *Acta Cryst.* B**40**, 280–288.

TONIOLO, C. (1980). *CRC Crit. Rev. Biochem.* **9**, 1–44.

ZIMMERMAN, S. S., POTTLE, M. S., NÉMETHY, G. & SCHERAGA, H. A. (1977). *Macromolecules*, **10**, 1–9.

Acta Cryst. (1988). C**44**, 853–856

Structure and Conformation of a Nucleoside Analog 5-Nitro-1-β-D-arabinofuranosyluracil

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(*Received* 24 *March* 1987; *accepted* 1 *October* 1987)

Abstract. $C_9H_{11}N_3O_8$, $M_r = 271$, orthorhombic, $P2_12_12_1$, $a = 9{\cdot}241$ (2), $b = 20{\cdot}518$ (4), $c = 6{\cdot}187$ (1) Å, $V = 1173{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}29$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 1{\cdot}57$ cm^{-1}, $F(000) = 600$, $T = 288$ K, final $R = 0{\cdot}051$ for 1078 observed reflections. Conformational features of the nucleoside include a glycosidic bond conformation in the *anti* range, a ribose moiety in the C(2′)-*endo* (^2E) form and the C(5′)–O(5′) bond *gauche* to both C(4′)–O(4′) and C(4′)–C(3′).

Introduction. Pyrimidine nucleosides and nucleotides substituted at the 5 position by various functional groups are very interesting for their antiviral, antitumor

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0108-2701/88/050853-04$03.00