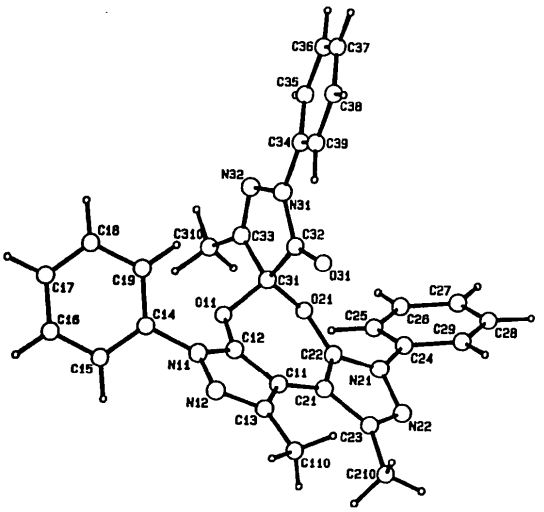

Fig. 1. *PLUTO* plot (Motherwell, 1978) and numbering scheme for furlone yellow.

distortion in the dioxepin ring. The spiro pyrazoline ring lies in nearly perpendicular arrangement with the other pyrazoline rings, at an angle of 101·4 (2)° with ring 1 and 100·1 (2)° with ring 2. The perpendicularity is due to the steric repulsion between the methyl and keto groups attached to the spiro pyrazoline ring and the phenyl rings attached to the other pyrazoline rings. The twist angles between the phenyl and the pyrazoline rings, 47·5 (2), 41·2 (3) and 24·5 (4)° for pyrazoline rings 1, 2 and spiro, respectively, are mainly caused by the packing forces. The packing is maintained by the π-electron overlap between the phenyl rings in adjacent molecules, in such a way that the phenyl rings attached to the adjacent spiro pyrazoline rings overlap each other (spiro↔spiro) and the phenyl rings attached to the pyrazoline rings 1 and 2 overlap in a head-to-tail

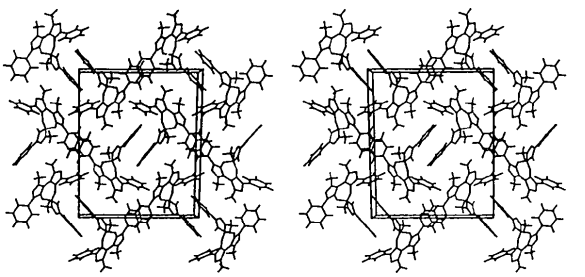

Fig. 2. A stereoscopic view of the packing. The *b* axis is horizontal and the *c* axis vertical.

fashion with those in adjacent molecules (1↔2↔1↔2). There are no intermolecular contacts shorter than the sum of van der Waals radii.

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Conformation of Methylated Amino Acids: Structure of 3,4-Dimethoxy-α-methyl-DL-phenylalanine Sesquihydrate

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Abstract. $C_{12}H_{17}NO_4.1{\cdot}5H_2O$, $M_r = 266{\cdot}3$, triclinic, $P\bar{1}$, $a = 5{\cdot}872$ (1), $b = 11{\cdot}437$ (2), $c = 20{\cdot}434$ (1) Å, $\alpha = 95{\cdot}74$ (1), $\beta = 96{\cdot}91$ (1), $\gamma = 89{\cdot}18$ (1)°, $V = 1355{\cdot}5$ Å^3, $Z = 4$, $D_m = 1{\cdot}29$, $D_x = 1{\cdot}305$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 8{\cdot}3$ cm^{-1}, $F(000) = 572$, $T = 294$ K, $R = 0{\cdot}038$ for 4006 reflections, $I \geq 3\sigma(I)$.

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Both the molecules *A* and *B* in the asymmetric unit exist as zwitterions. With respect to the D enantiomer, the torsion angles ψ_1 and ψ_2 are +47·2 and −134·4° in molecule *A* and +33·3 and −147·5° in molecule *B* respectively. The torsion angles of the α-methyl group, NH_3^+ and COO^- groups with respect to C^ν are in molecules *A* and *B* respectively +67·2, +66·8, −174·3, −175·6, and −59·2 and −59·5°. The hydrogen-bonding environment of water O*W*1 is trigonal non-planar; O*W*2 is trigonal planar and O*W*3 is tetrahedral. The crystal structure is stabilized by a number of hydrogen bonds involving the amino and carboxylate groups of both molecules *A* and *B* and the water molecules.

Introduction. Dihydroxyphenylalanine (DOPA) is an amino acid found in seedlings, pods and beans. 3-*O*-Methyl-DOPA is a metabolite of DOPA in man and animals. Aldomet, the antihypertensive drug, is the α-methyl analog of DOPA. The title compound, a 3,4-dimethoxy analog of DOPA, and the other analogs of DOPA act as antimetabolites and as amino-acid antagonists (Chacko, Swaminathan & Bhattacharjee, 1981). The crystal structure of the title compound was investigated to understand the effect of methylation on the conformation of this amino acid.

Experimental. Crystals of the title compound (Sigma) were grown by slow evaporation of an aqueous methanol solution at room temperature. They are plate-like; D_m by flotation (bromoform/benzene); unit-cell parameters on Enraf–Nonius CAD-4 diffractometer using 25 reflections with $8 \le \theta \le 20°$; crystal of dimensions 0·7 × 0·3 × 0·15 mm; three-dimensional data ($2\theta_{max} = 154°$ for Cu $K\alpha$ radiation), $\omega/2\theta$ scan; ω scan widths $(0{\cdot}75 + 0{\cdot}14 \tan\theta)°$, aperture width $(3{\cdot}0 + 1{\cdot}2 \tan\theta)$ mm; max. time spent on any reflection measurement 100 s; faster scan used for strong reflections; intensities of three reflections monitored after every hour of exposure; variation in intensity ≤3% during complete data collection; orientation matrix checked every 100 reflections; 5472 reflections were measured, 3932 significant $[I \ge 3\sigma(I)]$; h 0→7, k −14→14, l −25→25; Lorentz and polarization corrections; intensities of three reflections at $\chi \sim 90°$ measured for different values of φ from 0 to 360° and resultant curve of transmission as a function of φ used to calculate absorption for all reflections. Max. and min. transmission factors 0·99 and 0·89 with average 0·94. Structure solved using *MULTAN* (Germain, Main & Woolfson, 1971); *E* values ($|E| \ge 1{\cdot}5$) used as input to *MULTAN* and correct set with highest figure of merit of 1·145 and residual value of 0·19 gave all the atoms in both the molecules in the asymmetric unit; refinement with anisotropic thermal factors led to $R = 0{\cdot}089$; difference electron density maps revealed positions of H atoms; final cycles of refinement with anisotropic thermal parameters for non-hydrogen atoms, isotropic for hydrogen atoms and extinction-parameter refinement ($g = 1{\cdot}8 \times 10^{-5}$) led to $R = 0{\cdot}038$ for 3932 reflections; $wR = 0{\cdot}062$, $S = 2{\cdot}07$, $w[|F_o| - (1/k) \times |F_c|]^2$ minimized, $w = 4|F_o|^2/\sigma^2(|F_o|)^2$ and $\sigma^2(|F_o|)^2 = [\sigma^2(I) + p^2I^2]$/LP where $p = 0{\cdot}05$, $\sigma(I)$ is standard deviation of intensity I based on counting statistics; k is scale factor; max. and av. Δ/σ 0·15 and 0·01; final $|\Delta\rho| = 0{\cdot}15$ e Å^{-3}. Program and atomic scattering factors as in Enraf–Nonius (1979) *Structure Determination Package*; Fourier and torsion-angle programs by Dr S. T. Rao and *ORTEP* by Johnson (1965).

Discussion. The final atomic parameters are given in Table 1.* The bond distances are similar to the values found in other methylated amino acids like α-methyl-DOPA (Neuman, Gillier, Avenel & Perret, 1984), DL-α-methyl-*m*-tyrosine (Satyshur & Rao, 1983) and α-methyl-*p*-tyrosine (Gaudestad, Mostad & Romming, 1976). Atom C^β is coplanar with the benzene ring and the two methoxy groups lie in the phenyl plane. The bond angle at the C^β atom (113·7 and 115·3° in molecules *A* and *B*) is significantly larger than 109° 28′ and is similar to the values found in the structures of DL-α-methyl-*m*-tyrosine and α-methyl-DOPA. The remaining bond angles are similar to those found in DL-α-methyl-*m*-tyrosine, α-methyl-DOPA and α-methyl-*p*-tyrosine structures.

Fig. 1 shows the conformation of the D enantiomer of the methylated amino acid in both molecules in the unit cell and gives in addition the atom-numbering scheme. Although both molecules have similar conformations, there are some essential differences. The C(1)–O(1) distance [1·241 (1) and 1·250 (1) Å in molecules *A* and *B* respectively] is shorter than C(1)–O(2) [1·250 (1) and 1·268 (1) Å in *A* and *B* respectively] by 0·009 and 0·018 Å respectively. C(1)–O(2) of *B* is considerably longer than in *A* because O(1) and O(2) of molecule *A* each hydrogen bond twice whereas O(1) and O(2) of molecule *B* hydrogen bond once and thrice respectively. The unsymmetrical intermolecular environment of *B* is consistent with its unsymmetrical C–O bond lengths. The standard deviations of torsion angles are <0·4°. The torsion angle χ'[C(6)C(5)C(4)C(2)] in the two molecules *A* and *B* is −89 and −87° respectively. Of the two possible conformations, the amino nitrogen N(1) takes the *trans* conformation with respect to the C(4)–C(2) bond [torsion angle C(5)C(4)C(2)N(1) −174° in *A* and −176° in *B*]. The carboxylate group adopts the *gauche*$^-$ conformation in both *A* and *B* [C(5)C(4)C(2)C(1) −59° in both *A* and *B*] whereas the

* Lists of structure factors, bond lengths and angles and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44521 (39 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

α-methyl group takes up the *gauche*$^+$ in *A* and *B* [C(5)C(4)C(2)C(3) 67 and 66° respectively]. The torsion angles ψ_1 and ψ_2 are +47·2 and −134·4° in molecule *A* and +33·3 and −147·5° in *B*.

Table 1. *Final positional parameters, equivalent isotropic thermal parameters for non-hydrogen atoms and isotropic thermal parameters for hydrogen atoms with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}\sum_i\sum_j \beta_{ij}\alpha_i\alpha_j.$$

	x	y	z	B(Å²)
Molecule *A*				
O(1)	0·3488 (2)	0·29536 (9)	0·40327 (5)	3·18 (2)
O(2)	0·1900 (2)	0·47260 (9)	0·41799 (7)	4·05 (2)
O(3)	−0·2524 (2)	0·0647 (1)	0·13636 (6)	4·57 (3)
O(4)	0·6046 (2)	0·1985 (1)	0·11175 (6)	5·10 (3)
N(1)	0·2280 (2)	0·3655 (1)	0·43788 (6)	2·74 (2)
C(1)	0·1855 (2)	0·3635 (1)	0·40470 (7)	2·59 (2)
C(2)	0·0455 (2)	0·3114 (1)	0·38647 (7)	2·55 (2)
C(3)	0·0603 (3)	0·1791 (1)	0·38762 (8)	3·18 (3)
C(4)	0·0907 (3)	0·3510 (1)	0·31929 (8)	3·32 (3)
C(5)	0·0931 (3)	0·3139 (1)	0·26335 (7)	3·24 (3)
C(6)	0·0800 (3)	0·2057 (2)	0·22545 (8)	3·39 (3)
C(7)	−0·2525 (3)	0·1693 (2)	0·17552 (7)	3·44 (3)
C(8)	−0·4431 (3)	0·2422 (2)	0·16179 (7)	3·75 (3)
C(9)	−0·4557 (3)	0·3497 (2)	0·19854 (9)	4·20 (4)
C(10)	−0·2819 (3)	0·3852 (2)	0·24878 (8)	3·92 (3)
C(11)	0·0516 (4)	−0·0075 (2)	0·1445 (1)	5·00 (4)
C(12)	−0·7779 (4)	0·2782 (3)	0·0887 (1)	6·03 (5)
H1N(1)	0·209 (3)	0·342 (2)	0·4790 (9)	3·6 (4)*
H2N(1)	0·226 (3)	0·449 (2)	0·4360 (9)	4·3 (4)*
H3N(1)	0·379 (4)	0·337 (2)	0·425 (1)	6·8 (6)*
H1C(3)	0·026 (3)	0·160 (2)	0·4310 (9)	4·1 (4)*
H2C(3)	0·056 (4)	0·136 (2)	0·358 (1)	5·1 (5)*
H3C(3)	0·212 (3)	0·149 (2)	0·381 (1)	4·6 (4)*
H1C(4)	0·241 (3)	0·318 (2)	0·3088 (9)	4·5 (4)*
H2C(4)	0·110 (4)	0·437 (2)	0·325 (1)	5·3 (5)*
HC(6)	0·950 (3)	0·155 (2)	0·7663 (9)	4·5 (4)*
HC(9)	0·586 (3)	0·397 (2)	0·191 (1)	4·8 (5)*
HC(10)	−0·288 (4)	0·466 (2)	0·275 (1)	5·3 (6)*
H1C(11)	−0·028 (4)	0·040 (2)	0·189 (1)	6·2 (5)*
H2C(11)	0·079 (4)	0·040 (2)	0·135 (1)	5·9 (5)*
H3C(11)	0·086 (4)	−0·073 (2)	0·112 (1)	6·1 (5)*
H1C(12)	−0·871 (4)	0·307 (2)	0·123 (1)	7·3 (6)*
H2C(12)	−0·869 (4)	0·240 (2)	0·049 (1)	7·8 (7)*
H3C(12)	0·716 (4)	0·348 (2)	0·074 (1)	6·0 (6)*
Molecule *B*				
O(1)	0·8803 (2)	0·0924 (1)	0·67824 (5)	3·32 (2)
O(2)	0·6892 (2)	0·18248 (9)	0·59651 (5)	3·00 (2)
O(3)	0·7679 (3)	0·2323 (1)	0·95394 (6)	5·51 (3)
O(4)	1·0764 (3)	0·3814 (1)	0·93839 (7)	5·78 (3)
N(1)	0·2860 (2)	0·1020 (1)	0·62268 (5)	2·45 (2)
C(1)	0·7042 (2)	0·1309 (1)	0·64900 (6)	2·35 (2)
C(2)	0·4769 (2)	0·1176 (1)	0·67898 (6)	2·28 (2)
C(3)	0·4777 (3)	0·0109 (1)	0·71771 (7)	2·95 (3)
C(4)	0·4201 (3)	0·2332 (1)	0·72019 (7)	2·88 (3)
C(5)	0·5989 (3)	0·2729 (1)	0·77726 (7)	2·92 (3)
C(6)	0·5949 (3)	0·2324 (2)	0·83922 (7)	3·47 (3)
C(7)	0·7579 (3)	0·2688 (2)	0·89194 (8)	3·76 (3)
C(8)	0·9269 (3)	0·3494 (2)	0·88297 (8)	3·88 (3)
C(9)	0·9311 (3)	0·3893 (2)	0·82206 (9)	4·15 (4)
C(10)	0·7669 (3)	0·3511 (2)	0·76927 (8)	3·72 (3)
C(11)	0·6007 (4)	0·1498 (2)	0·96463 (9)	6·21 (5)
C(12)	1·2364 (4)	0·4720 (2)	0·9334 (1)	6·23 (5)
H1N(1)	0·311 (3)	0·035 (2)	0·5910 (8)	3·3 (4)*
H2N(1)	0·267 (3)	0·163 (2)	0·5983 (9)	4·1 (4)*
H3N(1)	0·146 (3)	0·095 (2)	0·6412 (9)	4·1 (4)*
H1C(3)	0·503 (3)	0·058 (2)	0·6894 (9)	4·6 (4)*
H2C(3)	0·324 (3)	0·006 (2)	0·7336 (9)	4·7 (4)*
H3C(3)	0·595 (3)	0·021 (2)	0·7543 (9)	4·1 (4)*
H1C(4)	0·274 (3)	0·215 (2)	0·7387 (8)	3·2 (3)*
H2C(4)	0·402 (3)	0·296 (1)	0·6874 (8)	3·0 (3)*
HC(6)	0·479 (3)	0·178 (1)	0·8471 (8)	3·1 (3)*
HC(9)	0·050 (4)	0·444 (2)	0·813 (1)	4·9 (5)*
HC(10)	0·766 (3)	0·379 (1)	0·7297 (8)	3·1 (3)*
H1C(11)	0·643 (4)	0·129 (2)	0·009 (1)	7·6 (7)*
H2C(11)	0·439 (5)	0·187 (3)	0·957 (1)	8·3 (7)*
H3C(11)	0·599 (4)	0·077 (2)	0·933 (1)	6·5 (6)*
H1C(12)	0·304 (5)	0·489 (2)	0·977 (1)	7·9 (7)*
H2C(12)	0·353 (4)	0·448 (2)	0·907 (1)	7·3 (6)*
H3C(12)	0·160 (5)	0·542 (2)	0·915 (1)	7·9 (7)*

Table 1 (*cont.*)

	x	y	z	B(Å²)
OW1	0·3982 (2)	0·0910 (1)	0·53927 (5)	4·22 (3)
OW2	0·3972 (2)	0·4168 (1)	0·5794 (1)	6·66 (4)
OW3	0·0744 (2)	0·29573 (9)	0·56030 (5)	3·37 (2)
H1OW1	0·368 (4)	0·157 (2)	0·557 (1)	6·5 (6)*
H2OW1	0·356 (5)	0·103 (3)	0·499 (1)	8·2 (7)*
H1OW2	0·526 (4)	0·448 (2)	0·581 (1)	6·3 (6)*
H2OW2	0·418 (4)	0·337 (2)	0·590 (1)	6·8 (6)*
H1OW3	0·042 (5)	0·262 (2)	0·573 (1)	7·8 (7)*
H2OW3	0·056 (4)	0·374 (2)	0·573 (1)	6·3 (6)*

Starred atoms were refined isotropically. Anisotropically refined atoms are given in the form of the isotropic equivalent thermal parameter defined as: $\frac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab(\cos\gamma)B(1,2) + ac(\cos\beta)B(1,3) + bc(\cos\alpha)B(2,3)]$.

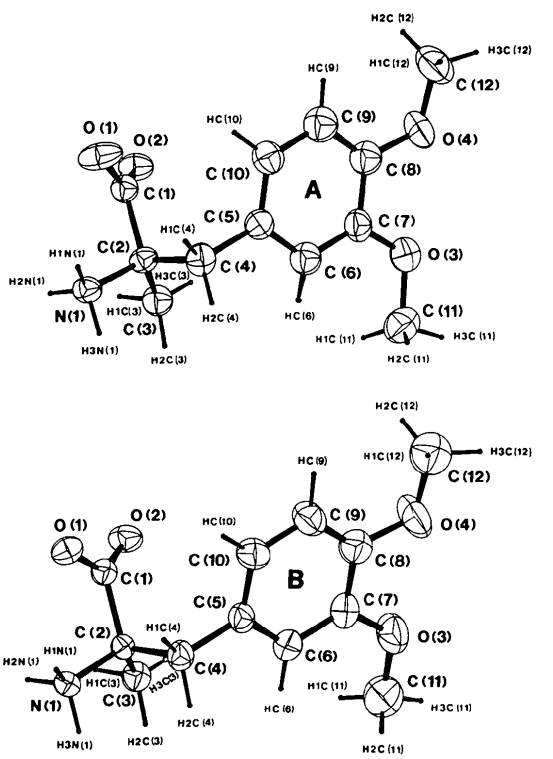

Fig. 1. *ORTEP* (Johnson, 1965) diagrams of both the molecules showing the atom-numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

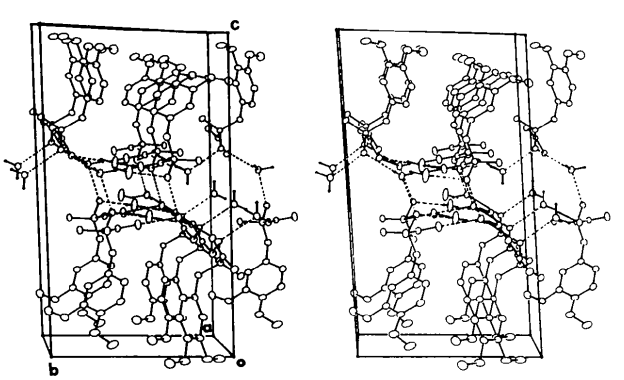

Fig. 2. Stereo packing diagram viewed down the *a* axis. Broken lines indicate hydrogen bonds.

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.

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

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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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