We thank the Fonds der Chemischen Industrie for financial support.

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Acta Cryst. (1990). C**46**, 81–84

Structure of Benzyloxycarbonyl-L-alanyl-L-proline

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(*Received* 23 *February* 1989; *accepted* 24 *April* 1989)

Abstract. $C_{16}H_{20}N_2O_5$, $M_r = 320{\cdot}34$, orthorhombic, $P2_12_12_1$, $a = 8{\cdot}503\ (3)$, $b = 22{\cdot}156\ (6)$, $c = 8{\cdot}588\ (3)$ Å, $V = 1617{\cdot}9$ Å^3, $Z = 4$, $D_m = 1{\cdot}30$, $D_x = 1{\cdot}315$ g cm^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}7107$ Å, $\mu = 0{\cdot}9$ cm^{-1}, $F(000) = 680$, room temperature, $R = 0{\cdot}057$, $wR = 0{\cdot}058$ for 1511 unique reflections [$I > 3\sigma(I)$]. The peptide linkage is in the *trans* conformation. The pyrrolidine ring exists in the envelope conformation. The crystal structure is stabilized by a three-dimensional network of N—H···O and O—H···O hydrogen bonds. There is a stacking interaction between the phenyl group of the benzyloxycarbonyl moiety and the pyrrolidine ring system of the prolyl residue.

Introduction. Proline, a unique imino acid, is an important constituent of many proteins. The five-membered pyrrolidine ring system of proline is formed when the side chain curls back to the protein main chain. This imposes certain restrictions on the conformation of proteins (Balasubramanian, Lakshminarayanan, Sabesan, Tegoni, Venkatesan & Ramachandran, 1971; Ashida & Kakudo, 1974). The conformational aspects of the pyrrolidine ring system are of particular interest as they reveal different modes of puckering in the five-membered ring system (Chacko, Swaminathan & Veena, 1983). In this context the crystal structures of several dipeptides of the type L-Pro-L-*X*, where *X* is one of Gly, Val, Ile, Tyr (reported from this laboratory), Ala, Met and Leu have been found to have similar unit-cell packing, hydrogen bonding and conformation. It seems as though the presence of proline at the N-terminal in these dipeptides dictates the overall conformation irrespective of the second residue. This prompted us to find out whether proline is capable of playing a similar role if it is present at the C-terminal of dipeptides; therefore we have launched a study of dipeptides of the type L-*X*-L-Pro and the structure of L-Phe-L-Pro has already been reported (Panneerselvam & Chacko, 1989). Here we present the crystal structure of benzyloxycarbonyl-L-alanyl-L-proline (Z-LALP).

Experimental. The dipeptide (Z-LALP) was crystallized in water at room temperature. Colourless chunky crystals, dimensions $0{\cdot}3 \times 0{\cdot}2 \times 0{\cdot}2$ mm. Density measured by the flotation method in carbon tetrachloride and benzene. Three-dimensional intensity data were collected on a Nonius CAD-4 diffractometer. The cell constants were determined by least-squares fit of 20 reflections with 2θ range 20–40°, max. $2\theta = 55°$, ω–2θ scan, data collected for the range $0 \le h \le 11$, $0 \le k \le 28$ and $0 \le l \le 11$. Three standard reflections, 3% variation in intensity. A total of 2213 observations were reduced (Lp^{-1}) to a set of 1511 unique reflections with $I > 3\sigma(I)$ used in the structure determination. The structure was solved using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refinement carried out by full-matrix least-squares method using *SHELX*76 (Sheldrick, 1976).

During the initial isotropic refinement, the C^γ atom of the prolyl residue showed a large temperature factor and the bond lengths involving C^γ had abnormal values. The above features indicated a disorder in the position of the C^γ atom. A difference Fourier map, computed after excluding the C^γ atom from the structure-factor calculation, revealed an

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† DCB contribution No. 741.

0108-2701/90/010081-04$03.00

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elongated and dumbbell-shaped peak for the C^{γ} atom suggesting a conformational disorder for the pyrrolidine ring system involving the C^{γ} atom. Similar features have been observed in the structures of the dipeptides L-Pro-L-Val.H_2O (Narasimhan, Chacko & Swaminathan, 1982), L-Pro-Gly.H_2O (Narasimhan & Chacko, 1982), L-Pro-L-Tyr (Veena, Chacko & Aoki, 1988) and L-Pro-L-Ile.H_2O (Panneerselvam, Chacko & Veena, 1989).

We carried out a least-squares refinement (based on F) after constraining the positional parameter of the pyrrolidine ring system including the two disordered positions for the C^{γ} atom. The occupancy factors for the two alternate positions of the C^{γ} atom were given the same value (0·5). All the H atoms, except those of the methylene C^{β}, C^{γ} and C^{δ} atoms of the pyrrolidine ring system, were located from a difference Fourier map. In the final stages of the refinement, the non-H atoms were refined with anisotropic thermal parameters (except the C^{γ} atom) and the H atoms with isotropic thermal parameters. Convergence was reached at final $R = 0{\cdot}057$, $wR = 0{\cdot}058$ $\{w = 3{\cdot}2394/[\sigma(F)^2 + 0{\cdot}000706F^2]\}$ and $S = 2{\cdot}37$. Ratio of max. least-squares shift to e.s.d.'s in the final cycle 0·084. Max. and min. heights in last difference Fourier synthesis 0·21 and $-0{\cdot}18$ e Å^{-3} respectively. The atomic scattering factors for C, N, O and H are from *International Tables for X-ray Crystallography* (1974).

Discussion. The final positional parameters of the atoms are listed in Table 1.* The stereoscopic diagram of the molecule is shown in Fig. 1. The bond lengths, bond angles, torsion angles and hydrogen-bonding scheme are given in Table 2. The dimensions of the peptide group are in good agreement with the average values of peptide dimensions reported in the literature (Ramanadham & Chidambaram, 1978). The N-terminal, blocked with the Z group, is uncharged. At the carboxyl terminal, the bond length C(16)—O(5) [1·316 (5) Å] is significantly longer than C(16)—O(4) [1·201 (5) Å] and the angle C(12)—C(16)—O(5) [113·9 (3)°] is significantly smaller than the commonly observed mean value of 121·6° for ionized carboxyl groups. These values indicate that the carboxyl group is un-ionized, as is expected in an end-protected dipeptide.

The peptide group is slightly non-planar. The best four-atom plane passing through the C(9), O(3), C(11) and C(12) atoms has individual deviations of within ± 0·032 Å with N(2) displaced from the above mean plane by −0·096 Å. The alternate positions C(14) and C(14)′ of the disordered C^{γ} atom deviate on either side of the best four-atom plane through C(12), C(13), C(15) and N(2) of the pyrrolidine ring by 0·44 and −0·44 Å respectively. The conformation of the pyrrolidine ring corresponds to the envelope type, with C(14) and C(14)′ oriented *endo* ($^{\gamma}E$) and *exo* ($_{\gamma}E$) with respect to the C′[C(16)] atom respectively according to the abbreviated nomenclature reported using the pseudorotational concept of the five-membered pyrrolidine ring system (Chacko *et al.*, 1983). A similar feature has been observed in

Table 1. *Atomic coordinates* ($\times 10^4$) *and equivalent isotropic thermal vibrational parameters* ($\times 10^3$) *for non-H atoms with e.s.d.'s in parentheses*

$U_{eq} = (U_{11} + U_{22} + U_{33})/3$.

	x	y	z	U_{eq} (Å^2)
C(1)	11644 (5)	1058 (2)	8681 (5)	57 (3)
C(2)	12936 (6)	1414 (3)	8547 (6)	79 (4)
C(3)	12763 (8)	2046 (4)	8555 (7)	96 (6)
C(4)	11275 (10)	2303 (3)	8709 (8)	99 (5)
C(5)	9977 (6)	1935 (2)	8818 (6)	70 (3)
C(6)	10134 (5)	1316 (2)	8802 (4)	46 (2)
C(7)	8740 (5)	910 (2)	8883 (5)	58 (2)
C(8)	7188 (4)	1018 (2)	6579 (5)	44 (2)
C(9)	5819 (4)	1069 (2)	4132 (5)	43 (2)
C(10)	6131 (6)	882 (2)	2451 (5)	62 (3)
C(11)	4162 (4)	870 (2)	4584 (4)	36 (2)
C(12)	1352 (4)	1039 (2)	4454 (5)	40 (2)
C(13)	377 (5)	1597 (2)	4053 (8)	73 (3)
C(14)	1420 (7)	1989 (4)	3073 (10)	60 (2)*
C(14)′	1478 (7)	2132 (3)	4021 (12)	60 (2)*
C(15)	3077 (5)	1862 (2)	3618 (6)	61 (2)
C(16)	911 (4)	514 (2)	3420 (5)	41 (2)
N(1)	6982 (4)	803 (2)	5134 (4)	49 (2)
N(2)	2974 (4)	1233 (1)	4256 (4)	38 (2)
O(1)	8327 (3)	705 (1)	7323 (1)	52 (2)
O(2)	6463 (4)	1431 (1)	7133 (4)	60 (2)
O(3)	3950 (3)	363 (1)	5137 (3)	49 (2)
O(4)	−213 (4)	201 (2)	3678 (5)	80 (2)
O(5)	1843 (4)	444 (1)	2210 (3)	56 (2)

* Isotropic thermal vibrational parameter.

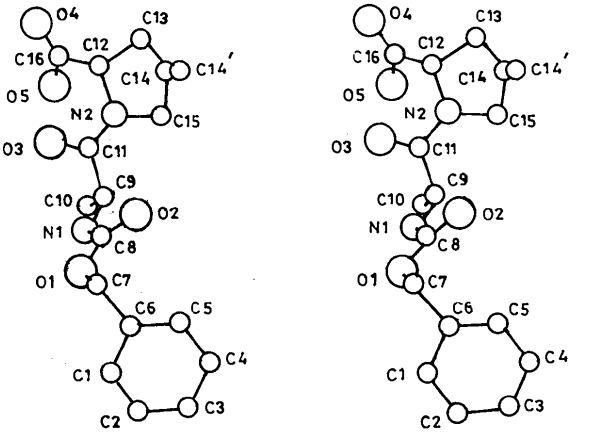

Fig. 1. Stereoscopic diagram of Z-LALP.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond lengths and angles involving H atoms and details of least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52166 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond lengths* (Å), *bond angles* (°), *torsion angles* (°) *and hydrogen-bonding details*

C(1)—C(2)	1·357 (7)	C(9)—C(11)	1·527 (5)
C(2)—C(3)	1·408 (11)	C(11)—O(3)	1·233 (5)
C(3)—C(4)	1·394 (11)	C(11)—N(2)	1·322 (5)
C(4)—C(5)	1·375 (9)	C(12)—N(2)	1·455 (5)
C(5)—C(6)	1·378 (6)	C(12)—C(13)	1·528 (6)
C(1)—C(6)	1·409 (6)	C(13)—C(14)	1·500 (10)
C(6)—C(7)	1·490 (6)	C(13)—C(14)′	1·511 (8)
C(7)—O(1)	1·458 (5)	C(15)—C(14)	1·511 (8)
O(1)—C(8)	1·352 (5)	C(15)—C(14)′	1·525 (8)
C(8)—O(2)	1·202 (5)	C(15)—N(2)	1·500 (5)
C(8)—N(1)	1·341 (6)	C(12)—C(16)	1·511 (6)
N(1)—C(9)	1·437 (5)	C(16)—O(4)	1·201 (5)
C(9)—C(10)	1·525 (6)	C(16)—O(5)	1·316 (5)

C(2)—C(1)—C(6)	120·5 (4)	C(9)—C(11)—N(2)	118·4 (3)
C(1)—C(2)—C(3)	119·5 (5)	C(9)—C(11)—O(3)	119·7 (3)
C(2)—C(3)—C(4)	120·1 (6)	N(2)—C(11)—O(3)	121·7 (3)
C(3)—C(4)—C(5)	119·5 (6)	C(11)—N(2)—C(12)	121·3 (3)
C(4)—C(5)—C(6)	120·8 (4)	C(11)—N(2)—C(15)	126·8 (3)
C(1)—C(6)—C(5)	119·5 (4)	C(12)—N(2)—C(15)	111·9 (3)
C(1)—C(6)—C(7)	118·9 (4)	N(2)—C(12)—C(16)	113·2 (3)
C(5)—C(6)—C(7)	121·6 (4)	N(2)—C(12)—C(13)	104·4 (3)
C(6)—C(7)—O(1)	109·7 (3)	C(13)—C(12)—C(16)	110·9 (3)
C(7)—O(1)—C(8)	116·6 (3)	C(12)—C(13)—C(14)	105·9 (4)
O(1)—C(8)—N(1)	110·4 (3)	C(13)—C(14)—C(15)	105·7 (5)
O(1)—C(8)—O(2)	124·8 (3)	C(14)—C(15)—N(2)	103·4 (4)
N(1)—C(8)—O(2)	124·8 (3)	C(12)—C(13)—C(14)′	107·6 (4)
C(8)—N(1)—C(9)	119·9 (3)	C(13)—C(14)′—C(15)	104·4 (5)
C(10)—C(9)—N(1)	109·6 (3)	C(14)′—C(15)—N(2)	103·3 (4)
C(10)—C(9)—C(11)	108·8 (3)	C(12)—C(16)—O(4)	122·2 (3)
C(11)—C(9)—N(1)	111·4 (3)	C(12)—C(16)—O(5)	113·9 (3)
		O(4)—C(16)—O(5)	123·8 (3)

C(2)—C(1)—C(6)—C(7)		177·6 (4)	C(11)—N(2)—C(12)—C(16)	φ	−62·8 (5)
C(4)—C(5)—C(6)—C(7)		−178·6 (5)	N(2)—C(12)—C(16)—O(4)	ψ_1	161·3 (4)
C(1)—C(6)—C(7)—O(1)	θ_3	−80·4 (5)	N(2)—C(12)—C(16)—O(5)	ψ_2	−20·2 (5)
C(5)—C(6)—C(7)—O(1)	θ_3'	98·6 (5)	N(2)—C(12)—C(13)—C(14)	χ_1	21·6 (5)
C(6)—C(7)—O(1)—C(8)	θ_2	−96·0 (4)	C(12)—C(13)—C(14)—C(15)	χ_2	−30·2 (6)
C(7)—O(1)—C(8)—O(2)		−3·1 (6)	C(13)—C(14)—C(15)—N(2)	χ_3	26·3 (6)
C(7)—O(1)—C(8)—N(1)	θ_1	176·8 (3)	C(14)—C(15)—N(2)—C(12)	χ_4	−13·1 (5)
O(1)—C(8)—N(1)—C(9)	ω_0	179·8 (4)	C(15)—N(2)—C(12)—C(13)	θ_0	−5·1 (4)
C(8)—N(1)—C(9)—C(10)		163·4 (4)	N(2)—C(12)—C(13)—C(14)′	χ_1'	−13·7 (5)
C(8)—N(1)—C(9)—C(11)	φ_0	−76·1 (5)	C(12)—C(13)—C(14)′—C(15)	χ_2'	26·6 (6)
N(1)—C(9)—C(11)—N(2)	ψ	153·0 (4)	C(13)—C(14)′—C(15)—N(2)	χ_3'	−28·4 (6)
N(1)—C(9)—C(11)—O(3)		−32·2 (5)	C(14)′—C(15)—N(2)—C(12)	χ_4'	21·3 (5)
C(9)—C(11)—N(2)—C(12)	ω	171·4 (3)			

D—H···*A*	Symmetry code	*D*···*A*	H···*A*	*D*—H···*A*
N(1)—H1N1···O(4)	(i)	3·005 (5) Å	2·09 (4) Å	148 (3)°
O(5)—H1O5···O(3)	(ii)	2·612 (4)	1·86 (5)	161 (4)

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

other dipeptides, namely L-Pro-L-Val.H_2O, L-Pro-Gly.H_2O, L-Pro-L-Ala.H_2O (Yadava & Padmanabhan, 1978), L-Pro-L-Met.H_2O (Yadava & Padmanabhan, 1981), L-Pro-L-Tyr and L-Pro-L-Ile.H_2O.

The peptide linkage exists in the *trans* conformation [$\omega = 171{\cdot}4\ (3)°$, C(9)—C(11)—N(2)—C(12)]. The rotations about the N—C^α and C^α—C′ bond of the peptide linkage are denoted by φ and ψ respectively (Edsall, Flory, Kendrew, Liquori, Nemethy, Ramachandran & Scheraga, 1966). In this case, the ψ angle for the N-terminal residue is 153·0 (4)° [N(1)—C(9)—C(11)—N(2)]. The φ angle for the C-terminal residue is −62·8 (5)° [C(11)—N(2)—C(12)—C(16)] and ψ_1 and ψ_2 have values 161·3 (4) [N(2)—C(12)—C(16)—O(4)] and −20·2 (5)° [N(2)—C(12)—C(16)—O(5)] respectively. The normal value for the C—C bonds in the aromatic ring of Z-LALP is 1·388 (8) Å. The bond angles C(7)—O(1)—C(8) = 116·6 (3) and O(1)—C(8)—O(2) = 124·8 (3)° are close to the mean values 116·1 and 123·5° respectively. The urethane moiety is planar and the atoms N(1), C(8), O(1) and O(2) are nearly coplanar. The conformation of the Z group, characterized by the torsion angles $\omega_0 = 179{\cdot}8\ (4)$ [O(1)—C(8)—N(1)—C(9)] and $\theta_1 = 176{\cdot}8\ (3)°$ [(C(7)—O(1)—C(8)—N(1)], is thus *trans–trans* as is generally observed (Benedetti Pedone, Toniolo, Dudek, Nemethy & Scheraga, 1983). The values of θ_2, θ_3 and θ_3' are −96·0 (4) [C(6)—C(7)—O(1)—C(8)], −80·4 (5) [C(1)—C(6)—C(7)—O(1)] and 98·6 (5)° [C(5)—C(6)—C(7)—O(1)] respectively.

The molecular packing viewed down the *c* axis is shown in Fig. 2. The hydrogen (N1H1) of the alanyl residue is hydrogen bonded to a translated carboxylate oxygen O(4). The N···O distance is 3·005 (5) Å. The carboxylate oxygen O(5) of the prolyl residue is bonded to a symmetry-related O(3) atom. The O···O hydrogen-bond distance is 2·612 (5) Å and it indicates a strong hydrogen-bonded interaction. These features are similar to the Z-Gly-L-Pro (Tanaka, Kozima, Ashida, Tanaka & Kakudo, 1977) and Z-Gly-DL-Pro (Kojima, Yamane & Ashida, 1978) crystal structures. It is interesting to note that there is also a stacking interaction between the pyrrolidine ring system of the prolyl residue and the phenyl ring of the benzyloxycarbonyl moiety, translated along the *a* axis. The distance of the above interaction is nearly 3·5 Å.

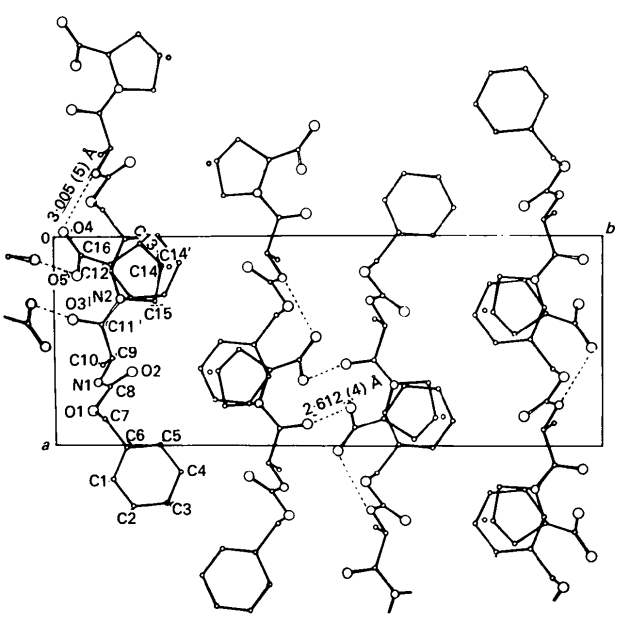

Fig. 2. Molecular packing viewed down the *c* axis.

Thanks are due to the Department of Science and Technology (DST), New Delhi, for the award of a Junior Research Fellowship to KP. This study comes under the financial support of a DST project on 'structure and conformation of peptides'.

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Acta Cryst. (1990). C**46**, 84–86

Structure of 3-(3-Azido-2,3-dideoxy-β-D-*erythro*-pentofuranosyl)cytosine Hydrogen Chloride

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(*Received* 22 *March* 1989; *accepted* 11 *May* 1989)

Abstract. $C_9H_{13}N_6O_3^+.Cl^-$, $M_r = 288{\cdot}7$, monoclinic, $P2_1$, $a = 6{\cdot}308$ (3), $b = 9{\cdot}336$ (5), $c = 10{\cdot}945$ (6) Å, $\beta = 97{\cdot}40$ (4)°, $V = 639$ Å^3, $Z = 2$, $D_x = 1{\cdot}500$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 3{\cdot}1$ cm^{-1}, $F(000) = 300$, $T = 293$ K. $R = 0{\cdot}068$ for 931 unique observed $[F > 4\sigma(F)]$ reflections. The N-glycosidic torsion angle χ has a value of -130 (1)°, in the *anti* range. The sugar pucker is ${}_1T^2$ with $P = 135$ (1)° and $\psi = 38$ (1)°. The C4′–C5′ conformation is *sc* with $\gamma = 48$ (1)°. There are two hydrogen bonds in the structure: O5′···Cl1($-1-x$, $0{\cdot}5+y$, $-1-z$), 3·03 (2) Å and N3···O5′(x, $-0{\cdot}5-y$, z), 2·79 (2) Å. In each case the first atom is the donor.

Introduction. This structure was determined as part of an ongoing investigation of potentially anti-viral nucleoside analogues, with particular reference to possible anti-AIDS compounds.

Experimental. The compound was kindly supplied by Dr J. Rideout of Burroughs Wellcome Co., Research Triangle Park, NC 27709, USA. Crystals were obtained from aqueous solution. Space group and initial cell dimensions were obtained from Weissenberg photographs. Data were collected on a Nicolet *P*3 (four-circle) diffractometer in Aberdeen by RAH.

The crystal had dimensions $0{\cdot}4 \times 0{\cdot}2 \times 0{\cdot}2$ mm. Cell parameters were measured on the diffractometer using the $22\bar{2}$, 004, $20\bar{3}$ and 220 and symmetry-related reflections which have 2θ in the range 15 to 17°. Range of indices: $0 \le h \le 9$; $0 \le k \le 13$; $-15 \le l \le 15$. Data measured using $\omega/2\theta$ scans in the range

0108-2701/90/010084-03$03.00

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