compared with 0·245 for the whole molecule, suggesting that the thermal parameters of Cl(24) represent a librational motion of the whole ring wagging about C(8) and not a disordered structure. This was confirmed by least-squares refinement of a model with the Cl atom divided between two sites. This model refined to $R = 0{\cdot}058$ but gave very unsatisfactory positional and thermal parameters for Cl(24).

Final refinement (minimizing $\sum w|F_o - |F_c||^2$): 231 refined parameters in two blocks, $R = 0{\cdot}060$, $wR = 0{\cdot}098$, $w = 0{\cdot}1950/[\sigma^2(F) + 0{\cdot}0299F^2]$, mean shift/e.s.d. = 0·064, max. shift/e.s.d. = 0·297, max. difference peak = 0·33 e Å^{-3}, max. negative peak = 0·38 e Å^{-3}.

Discussion. Atomic coordinates for the molecule of (I) are given in Table 1,* with bond lengths and angles in Table 2. The molecule is shown in Fig. 1.

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43970 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

The five-membered ring of the indandione system is twisted so that C(7), C(8) and C(9) are 0·069 (3), 0·253 (3) and 0·146 (2) Å from the plane of the benzene ring. O(11) is raised 0·200 (2) Å above the plane of the benzene ring whereas O(10) is 0·007 (3) Å below the plane. The normals to the planes of the phenyl groups C(12)–C(17) and C(18)–C(23) make angles of 127·5 (1) and 67·4 (1)° to the normal to the plane of C(1)–C(6). These features avoid approaches of the ring protons to O(10) and O(11).

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Structure of (3*R*,6*R*)-3-Isobutyl-1,4-diazabicyclo[4.2.0]octane-2,5-dione and (3*S*,6*R*)-3-Isobutyl-1,4-diazabicyclo[4.4.0]decane-2,5-dione

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Abstract. (I): $C_{10}H_{16}N_2O_2$, $M_r = 196{\cdot}25$, orthorhombic, $P2_12_12_1$, $a = 9{\cdot}097$ (4), $b = 17{\cdot}682$ (6), $c = 6{\cdot}559$ (5) Å, $V = 1055$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}24$ (1) Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}081$ mm^{-1}, $F(000) = 424$, $T = 295$ K. Final $R = 0{\cdot}046$ for 1575 unique observed reflections. (II): $C_{12}H_{20}N_2O_2$, $M_r = 224{\cdot}30$, orthorhombic, $P2_12_12_1$, $a = 10{\cdot}04$ (3), $b = 20{\cdot}22$ (6), $c = 6{\cdot}35$ (1) Å, $V = 1290$ (6) Å^3, $Z = 4$, $D_x = 1{\cdot}16$ (1) Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0{\cdot}074$ mm^{-1}, $F(000) = 488$, $T = 295$ K. Final $R = 0{\cdot}054$ for 1317 unique observed reflections. The 2,5-piperazinedione ring in a twist-boat conformation becomes more puckered as the side-ring size decreases. There is a pronounced non-planarity of bonds at N(7) as a consequence of the side-ring constraints.

Introduction. 2,5-Piperazinediones can serve as model compounds for an investigation of mutual spatial relations between two homoconjugated peptide groups

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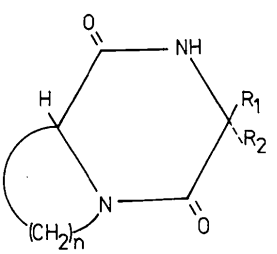
The inherent chirality of the non-planar peptide group is a basis for an interpretation of the CD spectra of compounds containing these groups (Bláha & Maloň, 1980). Some rigid lactams, dilactams and lactones were investigated by CD spectrometry. Results were compared with IR and NMR measurements in solution and with the crystal structure determination (Bláha, Maloň, Tichý, Fričˇ, Usha, Ramakumar & Venkatesan, 1978; Bláha, Buděšinský, Koblicová, Maloň, Tichý, Baker, Hossain & van der Helm, 1982; Bláha, Farag, van der Helm, Hossain, Buděšinský, Maloň, Smolíková & Tichý, 1984; Tichý, Farag, Maloň & Bláha, 1984). The aim of the structure determinations of (I) and (II) was to confirm the influence of the side-ring size on the geometry of the 2,5-piperazinedione ring. The following proline analogues ($n = 3$) were found in the Cambridge Structural Database: 5-bromo-12*S*-tetrahydroaustamide, ACBCAR 29 685 (the *Chemical Abstracts* coden); *cyclo*(-L-methionyl-D-prolyl-), ACACBN 40 C70; pyroergotamine, HCACAV 68 724; *cyclo*(-L-prolyl-D-phenylalanyl-), ACBCAR 32 1051; *cyclo*(-L-prolyl-L-4-hydroxyprolyl-), JACSAT 102 1827; *cyclo*(-L-prolyl-glycyl-), ACBCAR 31 966; *cyclo*(-L-prolyl-L-leucyl-), JACSAT 94 81; *cyclo*(-L-*N*-acetyltryptophanyl-L-prolyl-), TELAY 22 2565; verruculogen, JACSAT 96 6785; 3,4-dehydroproline anhydride, JACSAT 96 539; *N*-(*N*-phenylacetyl-L-alanyl)-*cyclo*(-L-phenylalanyl-D-prolyl-) (Cerrini, Fedeli, Lucente, Mazza, Pinnen & Zanotti, 1984); *cyclo*(-L-prolyl-α-aminoisobutyryl-) (Gdaniec, 1981); *cyclo*(-L-phenylalanyl-L-prolyl-) (Mazza, Lucente, Pinnen & Zanotti, 1984); *cyclo*(-L-prolyl-L-alanyl-) (Cotrait & Leroy, 1979); *cyclo*(-L-prolyl-L-prolyl-) (Benedetti, Goodman, Marsh, Rapoport & Musich, 1975); *cyclo*(-L-prolyl-D-*tert*-leucyl-) (Sklenář & Ječný, 1979). Azetidine ($n = 2$) and pipecoline ($n = 4$) analogues were not found. The *cyclo*(-L-prolyl-D-neopentyl-) was determined earlier (Symerský, Bláha & Langer, 1987). A paper on the interpretation of the CD spectra of 2,5-piperazinediones is being prepared and will be published elsewhere (Fričˇ & Bláha, 1987). The title compounds are commonly designated as *cyclo*(-D-Aze-D-Leu-) and *cyclo*(-D-Pip-L-Leu-).



(I) n=2, R_1=H, R_2=$CH_2CH(CH_3)_2$

(II) n=4, R_1=$CH_2CH(CH_3)_2$, R_2=H

Experimental. Title compounds synthetized at the Institute of Organic Chemistry and Biochemistry, Praha. Colorless thick tabular crystal of (I) grown from a methanol–butanol mixture, thin tabular crystals of (II) from a solution in chloroform by slow evaporation. Density measurement could not be performed owing to the insufficient amount of the crystals. In both cases Weissenberg and oscillation photographs were taken with Cu $K\alpha$ radiation and preliminary cell dimensions and space groups were determined. Intensity measurement on Syntex $P2_1$ diffractometer with graphite monochromator, Mo $K\alpha$ radiation, $[(\sin\theta)/\lambda]_{max} = 0{\cdot}7042$ and $0{\cdot}6497$ Å^{-1}. Crystal (I) $0{\cdot}25 \times 0{\cdot}45 \times 0{\cdot}60$ (cut from monocrystal block), crystal (II) $0{\cdot}15 \times 0{\cdot}45 \times 0{\cdot}80$ mm (without treatment). Final cell dimensions refined on 25 diffractometer reflections with $4{\cdot}0 < 2\theta < 23{\cdot}0°$ for (I) and on 15 reflections with $4{\cdot}0 < 2\theta < 25°$ for (II). θ–2θ scan technique, $0 \le h \le 12$, $0 \le k \le 24$, $0 \le l \le 9$, in a range up to $2\theta = 60°$ for (I) and $0 \le h \le 13$, $0 \le k \le 26$, $0 \le l \le 8$, up to $2\theta = 55°$ for (II). For (I) 1796 unique reflections measured, 221 unobserved with $I < 1{\cdot}96\sigma_I$, standard reflections 002, 040, 400 monitored after every 47 reflections did not show a significant decrease of intensity or sharp deviations throughout data collection. For (II) 1742 unique reflections measured, 425 unobserved with $I < 1{\cdot}96\sigma_I$, standard reflections 002, 040, 200 monitored in the same way also did not show any decrease or instability. The measurements were reduced to the same scale with the program *INTER* (Langer, 1973). Corrections for Lorentz and polarization factors were made, not for absorption. The measurement of (I) evaluated with the classic BPB method, of (II) with a combined method of profile analysis (Lehmann & Larsen, 1974) and mask procedure (Sjölin & Wlodawer, 1981) without background measurement. The phase problem was solved by direct methods (*MULTAN*80; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). All non-H atoms of both structures were revealed on E maps. The enantiomorphs used here agreed with the declared stereochemistry known from chemical syntheses. Refinement on $|F|$ by the full-matrix LS method with the program *SHELX*76 (Sheldrick, 1976). H atoms bonded to nitrogens located from $\Delta\rho$ maps and refined without constraints, the others calculated in theoretical positions and for (I) refined without constraints. For (II) a riding model for methyl H atoms was used. For both structures an empirical correction for secondary extinction was included as $F_c^{corr} = F_c(1 - gF_c^2/\sin\theta)$, where $g = 0{\cdot}0\ (2) \times 10^{-6}$ and $g = 0{\cdot}3\ (1) \times 10^{-6}$ for (I) and (II) respectively. 192 parameters refined for (I), $(\Delta/\sigma)_{max} = 0{\cdot}151$, final $R = 0{\cdot}0459$, $wR = 0{\cdot}0489$, $w = 8{\cdot}159/[\sigma_F^2 + (0{\cdot}03F)^2]$ for observed reflections; $R = 0{\cdot}0535$, $wR = 0{\cdot}052$, $w = 1/[\sigma_F^2 + (0{\cdot}03F)^2]$ for all reflections. $w = k/[\sigma_F^2 + (gF)^2]$, k is a factor redetermined after each structure-factor calculation, g is an

ignorance factor with fixed value derived experimentally from analysis of variance. This weighting scheme is included in the program system *SHELX*76 (Sheldrick, 1976). σ_F is taken from counting statistics. $\sigma_F^2 = \sigma_I^2/[4(\mathrm{Lp})^2F_o^2]$, Lp being the Lorentz–polarization factor. 214 parameters refined for (II), $(\Delta/\sigma)_{max} = 0.009$, final $R = 0.0543$, $wR = 0.0568$, $w = 1.706/[\sigma_F^2 + (0.03F)^2]$ for observed reflections; $R = 0.0724$, $wR = 0.072$, $w = 1/[\sigma_F^2 + (0.03F)^2]$ for all reflections, σ_F taken from counting statistics. The residuals on final $\Delta\rho$ maps were 0.27, −0.29 and 0.24, −0.24 e Å^{-3} for (I) and (II) respectively. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Geometrical interpretations of the structures calculated with program *PARST*83 (Nardelli, 1983).

Discussion. The minimum-overlap views of the molecules investigated are shown in Figs. 1(*a*) and 1(*b*). The fractional atomic coordinates and B_{eq} values are listed in Table 1, selected bond lengths and angles in Table 2.* The crystal packing and hydrogen bonds are shown in Figs. 2(*a*) and 2(*b*). The molecules are connected by hydrogen bonds in two antiparallel helices along **a**. This screw type of hydrogen bonding seems to be common for 2,5-piperazinediones in the crystalline state which have one H-donating nitrogen atom, *e.g.* Sklenář & Ječný (1979), Mazza *et al.* (1984). The six-membered 2,5-piperazinedione ring always keeps a twist-boat conformation in cyclodipeptides (I) and (II). The search of proline-analogues in the Cambridge Structural Database also showed the boat conformation with more or less twisting. The sense of the boat is consistent with the bridge-carbon-atom chirality. Only the structure of *cyclo*(-L-prolyl-α-aminoisobutyryl-) (Gdaniec, 1981) with two symmetrically independent molecules shows one molecule with a 2,5-piperazinedione ring in a sofa conformation.

The value $\chi^2 = \sum_1^6(w\Delta)^2$ indicating an overall degree of non-planarity of the 2,5-piperazinedione ring decreases in the series: (I); *cyclo*(-L-Pro-D-Neo-) (Symerský *et al.*, 1987); (II): 63 278, 6360, 2308. Δ is the distance of an atom from the least-squares weighted plane, w is the reciprocal value of the e.s.d of Δ. The oriented interplanar angle (Karle, 1981) between the planes $C_\alpha^1C'N'C_\alpha^2$ and $C_\alpha^2C''N''C_\alpha^1$ also decreases in its absolute value: −38·1 (1), 26·9 (2), −21·5 (3)°. The overall non-planarity and fold of the ring along a line joining the two C_α atoms increase with decreasing side-ring size. The description of the peptide-group geometry of (I) and (II) following Winkler & Dunitz (1971) and Warshel, Levitt & Lifson (1970) is summarized in Table 3. All peptide groups are pronouncedly non-planar. The highly pyramidal bond

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and thermal parameters and hydrogen-bond parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43931 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

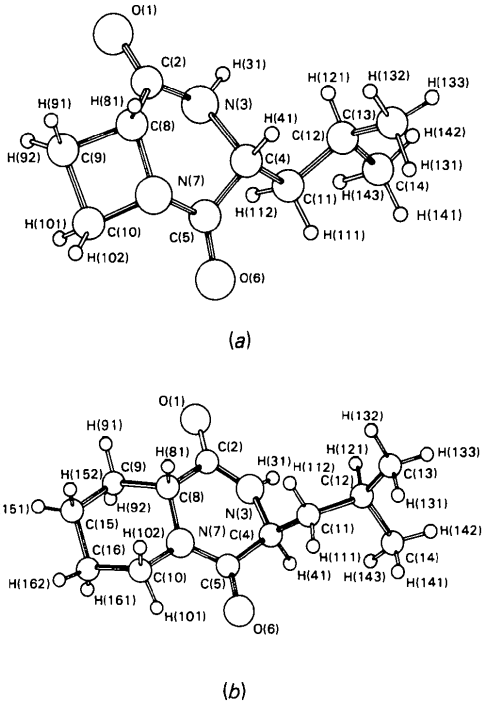


Fig. 1. View of (*a*) structure (I) and (*b*) structure (II) with the numbering scheme.

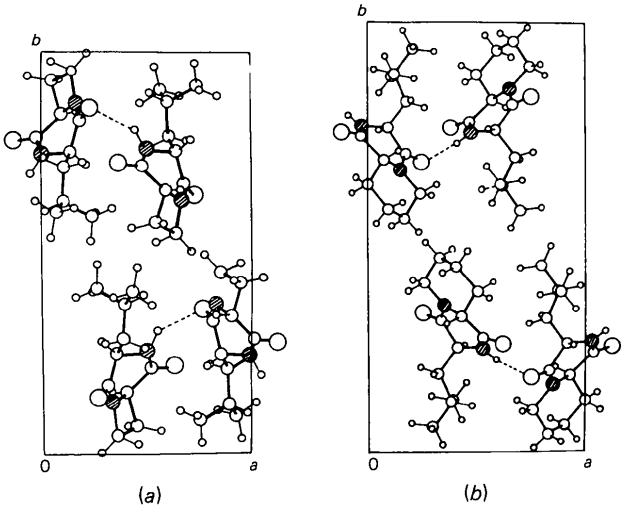


Fig. 2. (*a*) The crystal packing of (I) and H bonds in projection along the *c* axis. N atoms shaded. Symmetry relation for connected molecules: $x+\frac{1}{2}$, $-y+\frac{1}{2}$, $-z+1$. (*b*) The crystal packing of (II) and H bonds in projection along the *c* axis. N atoms shaded. Symmetry relation for connected molecules: $x+\frac{1}{2}$, $-y+\frac{1}{2}$, $-z+1$.

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and* B_{eq} ($Å^2$) *values with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{8}{3}\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
(I) *cyclo*(-D-Aze-D-Leu-)				
C(13)	7575 (4)	886 (2)	4785 (7)	5·24 (8)
C(11)	8875 (2)	2111 (1)	4000 (3)	2·65 (4)
C(5)	8163 (2)	3317 (1)	5819 (3)	2·74 (4)
C(4)	8610 (2)	2479 (1)	6065 (3)	2·46 (3)
O(1)	11311 (2)	2787 (1)	10083 (2)	3·80 (4)
C(2)	10216 (2)	2854 (1)	9003 (3)	2·73 (4)
N(7)	8317 (2)	3702 (1)	7548 (3)	3·05 (4)
C(12)	8982 (2)	1244 (1)	4002 (4)	3·32 (5)
C(8)	9042 (2)	3438 (1)	9417 (3)	2·94 (4)
O(6)	7687 (2)	3586 (1)	4211 (3)	3·89 (4)
N(3)	9954 (2)	2433 (1)	7328 (3)	2·82 (3)
C(9)	9511 (3)	4261 (2)	9844 (5)	4·37 (7)
C(10)	8586 (4)	4507 (1)	7991 (5)	4·36 (7)
C(14)	9317 (3)	980 (1)	1834 (5)	4·41 (6)
(II) *cyclo*(-D-Pip-L-Leu-)				
C(5)	8336 (3)	1916 (2)	3905 (5)	3·07 (7)
N(3)	10289 (3)	2578 (1)	2856 (5)	3·59 (7)
C(2)	10345 (3)	2321 (2)	910 (6)	3·21 (7)
C(11)	8239 (3)	3145 (2)	4088 (6)	3·68 (9)
O(1)	11222 (3)	2464 (1)	−372 (5)	5·12 (7)
C(8)	9302 (3)	1807 (2)	299 (5)	3·02 (7)
N(7)	8507 (2)	1570 (1)	2112 (4)	3·08 (6)
C(4)	9142 (3)	2529 (2)	4265 (5)	3·22 (7)
C(10)	7585 (4)	1027 (2)	1602 (7)	4·1 (1)
O(6)	7521 (2)	1742 (1)	5281 (4)	4·44 (7)
C(12)	8824 (4)	3784 (2)	5008 (7)	4·2 (1)
C(15)	9065 (4)	666 (2)	−1317 (7)	4·6 (1)
C(16)	8308 (5)	449 (2)	631 (8)	4·9 (1)
C(9)	10011 (4)	1228 (2)	−771 (7)	4·07 (9)
C(13)	7984 (6)	4370 (2)	4263 (13)	7·7 (2)
C(14)	8892 (5)	3766 (3)	7407 (7)	6·1 (1)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

(I) *cyclo*(-D-Aze-D-Leu-)

C(13)–C(12)	1·518 (4)	C(2)–C(8)	1·510 (3)
C(11)–C(4)	1·522 (3)	C(2)–N(3)	1·348 (3)
C(11)–C(12)	1·536 (3)	N(7)–C(8)	1·468 (3)
C(5)–C(4)	1·545 (3)	N(7)–C(10)	1·473 (3)
C(5)–N(7)	1·330 (3)	C(12)–C(14)	1·527 (4)
C(5)–O(6)	1·235 (3)	C(8)–C(9)	1·542 (4)
C(4)–N(3)	1·479 (3)	C(9)–C(10)	1·541 (5)
O(1)–C(2)	1·228 (2)		

C(4)–C(11)–C(12)	115·8 (2)	C(5)–N(7)–C(8)	126·6 (2)
N(7)–C(5)–O(6)	124·6 (2)	C(8)–N(7)–C(10)	93·9 (2)
C(4)–C(5)–O(6)	123·4 (2)	C(13)–C(12)–C(11)	111·3 (2)
C(4)–C(5)–N(7)	112·0 (2)	C(11)–C(12)–C(14)	108·5 (2)
C(11)–C(4)–C(5)	111·0 (2)	C(13)–C(12)–C(14)	110·8 (2)
C(5)–C(4)–N(3)	109·2 (2)	C(2)–C(8)–N(7)	112·6 (2)
C(11)–C(4)–N(3)	110·1 (2)	N(7)–C(8)–C(9)	88·6 (2)
O(1)–C(2)–N(3)	124·1 (2)	C(2)–C(8)–C(9)	118·8 (2)
O(1)–C(2)–C(8)	122·4 (2)	C(4)–N(3)–C(2)	124·9 (2)
C(8)–C(1)–N(3)	113·5 (2)	C(8)–C(9)–C(10)	88·4 (2)
C(5)–N(7)–C(10)	132·9 (2)	N(7)–C(10)–C(9)	88·5 (2)

(II) *cyclo*(-D-Pip-L-Leu-)

C(5)–N(7)	1·348 (5)	C(8)–N(7)	1·481 (5)
C(5)–C(4)	1·498 (6)	C(8)–C(9)	1·530 (6)
C(5)–O(6)	1·248 (4)	N(7)–C(10)	1·472 (5)
N(3)–C(2)	1·342 (6)	C(10)–C(16)	1·508 (7)
N(3)–C(4)	1·462 (5)	C(12)–C(13)	1·530 (7)
C(2)–O(1)	1·234 (5)	C(12)–C(14)	1·526 (7)
C(2)–C(8)	1·526 (6)	C(15)–C(16)	1·517 (7)
C(11)–C(4)	1·545 (6)	C(15)–C(9)	1·521 (6)
C(11)–C(12)	1·535 (7)		

C(4)–C(5)–O(6)	118·7 (5)	C(8)–N(7)–C(10)	114·2 (4)
N(7)–C(5)–O(6)	122·0 (5)	C(5)–N(7)–C(10)	119·5 (4)
N(7)–C(5)–C(4)	119·3 (4)	N(3)–C(4)–C(11)	111·3 (4)
C(2)–N(3)–C(4)	124·8 (4)	C(5)–C(4)–C(11)	109·8 (4)
N(3)–C(2)–C(8)	118·0 (4)	C(5)–C(4)–N(3)	112·9 (5)
N(3)–C(2)–O(1)	123·2 (5)	N(7)–C(10)–C(16)	111·4 (4)
O(1)–C(2)–C(8)	118·8 (4)	C(11)–C(12)–C(14)	112·2 (6)
C(4)–C(11)–C(12)	115·2 (4)	C(11)–C(12)–C(13)	108·8 (5)
C(2)–C(8)–C(9)	108·3 (4)	C(13)–C(12)–C(14)	110·6 (6)
C(2)–C(8)–N(7)	113·1 (4)	C(16)–C(15)–C(9)	110·1 (5)
N(7)–C(8)–C(9)	110·4 (5)	C(10)–C(16)–C(15)	110·6 (6)
C(5)–N(7)–C(8)	123·9 (5)	C(8)–C(9)–C(15)	112·5 (4)

arrangement at N(7) of (I) [$\chi_N = -36·4$ (4) °] as a consequence of the four-membered-ring constraints is the main contribution to the puckering of the 2,5-piperazinedione ring. A similar but smaller non-planarity at N(7) of (II) is due to the chair conformation of the side ring [$\chi_N = 18·6$ (9)°]. But the analogous N atom of *cyclo*(-L-Pro-D-Neo-) (Symerský *et al.*, 1987) has the smallest non-planarity [$\chi_N = -5·2$ (8)°] because the near C_2 symmetry of the five-membered side ring does not require pronounced pyramidicity at the N atom. The C—N (peptide) and C—O (carbonyl) bond lengths of the three compounds are given in Table 4. *cyclo*(-D-Pip-L-Leu-) has the closest lengths of both peptide groups. The difference between these homoconjugated bonds increases with decreasing side-ring size. The carbonyl bond lengths which participate in hydrogen bonding (C′—O) are pronouncedly longer. But there is one length here, C(5)—O(6) of *cyclo*(-D-Aze-D-Leu-), which is relatively shorter in this series of bond lengths, and it can be correlated with the highly non-planar bond arrangement at the N(7) atom.

The influences of the intramolecular environment on the peptide group demonstrated here by the side-ring size and by the side-ring conformation evidently determine the geometry of the peptide group.

The authors thank Dr K. Bláha for his stimulating suggestions.

Table 3. *Parameters and angles* (°) *describing the geometry of the peptide groups with e.s.d.'s in parentheses*

Parameter definition
$\omega_1(C_\alpha^1–C–N–C_\alpha^2)$, $\omega_2(O–C–N–X)$
$\omega_3(O–C–N–C_\alpha)$, $\omega_4(C_\alpha–C–N–X)$
X = C or H
$\tau' = \omega_1 + \omega_2$
$\chi_C = \omega_1 - \omega_3 + 180$ mod 360°
$\chi_N = \omega_2 - \omega_3 + 180$

Upper values are related to the peptide group with N bridge atom, lower values to the second one

	cyclo(-D-Aze-D-Leu-)	*cyclo*(D-Pip-L-Leu)
τ'	−18·4 (4)	−0·6 (6)
	2 (2)	−17 (3)
χ_C	1·6 (3)	0·2 (9)
	−1·4 (3)	−2·5 (9)
χ_N	−36·4 (4)	18·6 (9)
	10 (2)	11 (3)

Table 4. *Comparison of peptide and carbonyl bond lengths* (Å) *with e.s.d.'s in parentheses*

	cyclo(-D-Aze-D-Leu-)	*cyclo*(-L-Pro-D-Neo-)	*cyclo*(-D-Pip-L-Leu-)
N–C′	1·330 (3)	1·321 (6)	1·348 (5)
HN–C″	1·348 (5)	1·334 (7)	1·342 (6)
C′–O	1·235 (3)	1·250 (6)	1·248 (4)
C″–O	1·228 (2)	1·227 (6)	1·234 (5)

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tert-Butyloxycarbonyl-L-aminosuccinyl-glycyl-L-alanine Methyl Ester (Boc-L-Asu-Gly-L-Ala-OMe)

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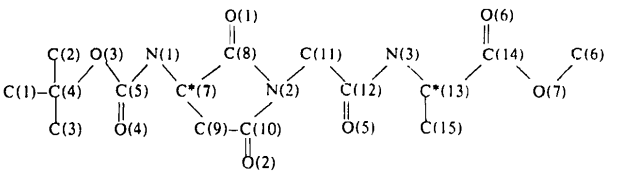
Abstract. $C_{15}H_{23}N_3O_7$, $M_r = 357{\cdot}36$, orthorhombic, $P2_12_12_1$, $a = 9{\cdot}251\ (5)$, $b = 11{\cdot}179\ (1)$, $c = 35{\cdot}113\ (4)$ Å, $V = 3631\ (3)$ Å^3, $Z = 8$, $D_x = 1{\cdot}307$ Mg m^{-3}, λ(Cu $K\alpha$) $= 1{\cdot}5418$ Å, $\mu = 0{\cdot}84$ mm^{-1}, $F(000) = 1520$, room temperature, $R = 0{\cdot}045$ for 3330 observed reflections. In agreement with our previous potential-energy calculations [Capasso, Mattia, Mazzarella & Zagari (1984) *Int. J. Pept. Protein Res.* **24**, 85–95], both molecules in the asymmetric unit adopt a type II′ β-turn conformation, with an intramolecular 4→1 hydrogen bond. In the crystal, chains of hydrogen-bonded molecules wind up around the screw axes parallel to **a**.

Introduction. In protein chemistry, the role played by the succinimide ring in the non-enzymatic deamidation of the asparaginyl side chain has been examined by an increasing number of studies (Graf, Bajusz, Patthy, Barat & Cseh, 1971; Aswad, 1984). Moreover, recent studies (Clarke, 1984) have indicated that the succinimide ring is an intermediate in the repair or selective degradation of deamidated proteins. The biological relevance of the succinimide ring has prompted us to study systematically the conformational parameters of model peptides containing the cyclic imide structure, in solution and the solid state (Capasso, Mattia, Mazzarella & Zagari, 1984*a*,*b*; Capasso, Mazzarella, Sica & Zagari, 1984). In this paper we describe the crystal and molecular structure of the fully blocked tripeptide Boc-L-Asu-Gly-L-Ala-OMe.



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