Final atomic parameters are given in Table 1.* Bond distances, bond angles and torsional angles are given in Table 2 (IUPAC–IUB Commission on Biochemical Nomenclature, 1970; IUPAC–IUB Joint Commission on Biochemical Nomenclature, 1974). Fig. 1 shows a thermal ellipsoid plot with the atomic numbering scheme. The two pseudo-centrosymmetrical molecules *A* and *B* form cyclic dimers by means of two hydrogen bonds [N(1)···O(4) and N(3)···O(2)]. The dimers are also connected in such a way that each *A* (or *B*) molecule is hydrogen bonded to two other *B* (or *A*) molecules [N(2)···O(3) and N(4)···O(1)].

* 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 54436 (10 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of MeCO-ψ[NH-CO]Val-NHMe

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(*Received* 6 *June* 1991; *accepted* 3 *July* 1991)

Abstract. *N,N'*-Dimethylisopropylmalonamide, $C_8H_{16}N_2O_2$, $M_r = 172.23$, orthorhombic, *Pbcm*, $a = 4.859$ (1), $b = 13.523$ (2), $c = 15.469$ (2) Å, $V = 1016.4$ Å^3, $Z = 4$, $D_x = 1.12$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu R_{max} \ll 1$, $\mu = 5.88$ cm^{-1}, $F(000) = 376$, $T = 293$ K, $R = 0.060$ for 665 observed reflections. Dimensions of this retropeptide molecule are quite similar to the standard values for peptides. The C^α and C^β atoms are in a mirror ($z = \frac{1}{4}$), so conformational angles are $\psi' = -\psi = -110.4°$ (2).

Experimental. Crystal size $0.24 \times 0.8 \times 0.04$ mm, X-ray data were collected at room temperature on an Enraf–Nonius CAD-4 automatic diffractometer, with Cu $K\alpha$ radiation up to a θ value of 70° ($\theta/2\theta$-scanning mode). Cell parameters refined by least squares on the basis of 25 independent θ values in the range 20–30°. 864 reflections measured ($h = 0$ to 4, $k = 0$ to 16, $l = 0$ to 18), 665 with $F_o > 3\sigma(F_o)$ were used for all calculations. Three standards (400, 2$\bar{1}$0, 200) measured every 2 h showed no deviations greater than 2% in intensity. Intensity data were corrected for Lorentz and polarization effects but not for absorption.

Structure solved by direct methods, using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined by full-matrix least-squares procedure on *F* (*SHELX*; Sheldrick, 1976). *E* maps revealed all non-H atoms, and H atoms appeared in difference maps. Refined parameters were calculated by using anisotropic temperature factors for non-H atoms and fixed isotropic temperature factors for H atoms. Final agreement factors were $R = 0.060$ and $wR = 0.070$ $\{w = 4.450/[\sigma^2(F_o) + 0.0009F_o^2]\}$. Goodness of fit = 2.25, $-0.31 < \Delta\rho < 0.19$ e Å^{-3}, shift/e.s.d.'s < 0.09. Following recommendations by Taylor & Kennard (1983), the NH H atoms were placed at 1.03 Å from N in the direction obtained by refinement. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV).

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Table 1. *Fractional coordinates with standard deviations and equivalent isotropic thermal parameters for* MeCO-ψ[NH-CO]Val-NHMe

	x	y	z	B_{eq} (Å^2)
O(1)	0.5808 (4)	0.0228 (2)	0.1500 (2)	5.98 (6)
N(1)	0.1422 (5)	0.0595 (2)	0.1237 (1)	3.85 (5)
C(1)	0.1990 (8)	0.1134 (3)	0.0451 (2)	5.32 (7)
C(2)	0.3370 (5)	0.0170 (2)	0.1704 (2)	3.39 (5)
C(3)	0.2447 (7)	−0.0390 (2)	0.250	3.12 (7)
C(6)	0.3499 (8)	−0.1456 (2)	0.250	4.33 (8)
C(7)	0.264 (1)	−0.1993 (3)	0.1687 (3)	6.68 (9)
H(N1)	−0.0595	0.0488	0.1418	

Table 2. *Bond lengths* (Å), *bond angles* (°) *and torsional angles* (°) *for* MeCO-ψ[NH-CO]Val-NHMe

N(1)—C(1)	1.445 (4)	C(2)—C(3)	1.514 (3)
N(1)—C(2)	1.322 (3)	C(3)—C(6)	1.530 (4)
O(1)—C(2)	1.230 (3)	C(6)—C(7)	1.511 (5)
C(1)—N(1)—C(2)	122.9 (2)	C(2)—C(3)—C(6)	111.9 (1)
O(1)—C(2)—N(1)	121.4 (3)	C(3)—C(6)—C(7)	111.1 (2)
O(1)—C(2)—C(3)	121.8 (2)	C(2)—C(3)—C(2^i)	108.9 (2)
N(1)—C(2)—C(3)	116.7 (3)	C(7)—C(6)—C(7^i)	112.7 (3)
	ψ	−110.4 (2)	
C(2)—C(3)—C(6)—C(7)	χ^1/C(7)	−55.6 (4)	
C(2)—C(3)—C(6)—C(7^i)	χ^1/C(7)′	178·1 (2)	
C(1)—N(1)—C(2)—O(1)	ω	3 (4)	

Final atomic parameters are given in Table 1.* Bond distances, bond angles and torsional angles are given in Table 2 (IUPAC–IUB Commission on Biochemical Nomeclature, 1970; IUPAC–IUB Joint Commission on Biochemical Nomenclature, 1984). Fig. 1 shows a thermal ellipsoid plot with the atomic numbering scheme. The conformation corresponds to a saddle point on the energy map (Stern, Chorev, Goodman & Hagler, 1983). Molecules are hydrogen bonded in such a way as to form a parallel β-sheet structure.

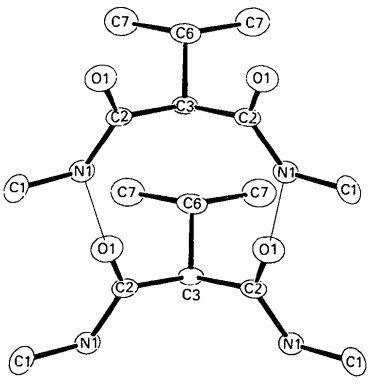

Fig. 1. *ORTEP* (Johnson, 1965) drawing of two associated MeCO-ψ[NH-CO]Val-NHMe molecules and interatomic distance (Å) associated with intermolecular hydrogen bond N—H···O [N(1)···O(1^i) = 2.803 (3); symmetry code: (i) $x-1, y, z$].

* 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 54437 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of the Guaianolide Derivative 9α-Thiophenoxy-11βH,13-dihydromicheliolide

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(*Received* 25 *June* 1991; *accepted* 9 *July* 1991)

Abstract. $C_{21}H_{26}O_3S$, $M_r = 358.5$, monoclinic, $P2_1$, $a = 10.4847$ (10), $b = 5.4915$ (6), $c = 17.145$ (2) Å, $\beta = 96.366$ (10)°, $V = 981.0$ (3) Å^3, $Z = 2$, $D_x = 1.214$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54184 Å, $\mu = 15.5$ cm^{-1}, $F(000) = 384$, $T = 297$ K, $R = 0.039$ for 1363 observations with $I > 1\sigma(I)$ (of 1590 unique data). The seven-membered ring is *trans* fused to the lactone ring and has a slightly distorted chair confor-

0108-2701/92/010179-03$03.00