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N-Acetyl-L-valine

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The title compound, $C_7H_{13}NO_3$, was prepared by acetylation of L-valine. The C(carbonyl)—N bond length is 1.324 (2) Å, which corresponds to the C—N bond length of a typical acylamine group.

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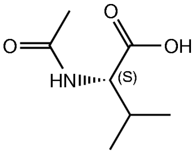
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.072
Data-to-parameter ratio = 10.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

N-Acetyl-L-valine, (I), is a versatile synthon in the synthesis of several pharmaceuticals and their key intermediates (Reddy *et al.*, 1999; Heavner, 1997). In a continuation of our work on the structure–activity relationship of the avermectin B1 derivatives, we have obtained a colourless crystalline compound that was the product of acetylation of L-valine. The structural identity of our product, (I), was resolved using single-crystal X-ray diffraction to determine the molecular structure.



(I)

The molecular structure of (I) is illustrated in Fig. 1. Selected bond lengths, angles and torsion angles are listed in Table 1. In (I), the C(carbonyl)—N bond length is 1.324 (2) Å, which corresponds to the C—N bond length of a typical acylamine group (Ganis *et al.*, 1971). Atoms C2, C3, N1 and C1 are coplanar [deviations within 0.0136 (9) Å], and atoms N1, C1, C4 and O3 are also coplanar [deviations within 0.0290 (8) Å]. The dihedral angle between the two planes is 49.75 (13)°.

Experimental

Compound (I) was obtained by acetylating L-valine with acetic anhydride and was recrystallized from ethanol to give colourless prisms (m.p. 437–438 K), $[\alpha]^{D}_{25}$ +4.1 (H_2O, 1%) (Cadogan *et al.*, 1996). L-Valine was purchased from the Shanghai Chemical Reagents Co.

Crystal data

$C_7H_{13}NO_3$
M_r = 159.18
Orthorhombic, $P2_12_12_1$
a = 6.654 (1) Å
b = 9.444 (2) Å
c = 13.182 (3) Å
V = 828.4 (3) $Å^3$
Z = 4
D_x = 1.276 Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 3.1–27.5°
μ = 0.10 mm^{-1}
T = 293 (2) K
Prism, colourless
0.20 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1841 measured reflections
1099 independent reflections
830 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\rm max} = 27.5°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 12$
$l = -16 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.072$
$S = 0.91$
1099 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0340P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.12$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.052 (4)

Table 1
Selected geometric parameters (Å, °).

O1—C3	1.245 (2)	O3—C4	1.326 (2)
N1—C3	1.324 (2)	O2—C4	1.191 (2)
N1—C1	1.452 (2)		
C3—N1—C1	124.54 (14)	N1—C3—C2	116.12 (16)
O1—C3—N1	122.83 (17)	N1—C1—C4	107.37 (15)
O1—C3—C2	121.05 (17)	N1—C1—C5	112.91 (15)
C1—N1—C3—C2	177.95 (17)	C3—N1—C1—C5	104.6 (2)
C3—N1—C1—C4	−129.47 (18)	O3—C4—C1—N1	−175.47 (15)

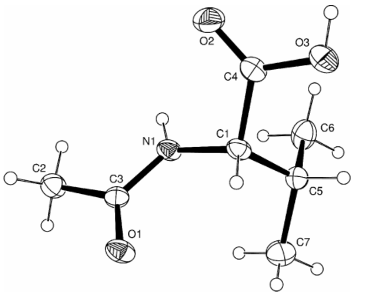


Figure 1
The structure of (I), drawn with 30% probability displacement ellipsoids.

H atoms were included at calculated positions and refined using a riding model, with $U_{\rm iso}$ = 1.2 (or 1.5 for methyl H atoms) times $U_{\rm eq}$(parent atom). C—H distances were constrained to 0.96 Å for methyl H atoms and 0.98 Å for the remainder. The O—H distance was constrained to 0.82 Å and the N—H distance to 0.86 Å. In the absence of significant anomalous scattering effects, the Friedel pairs were merged. The absolute configuration was assumed to be that of the starting material.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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