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N-Benzoylalanine

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.144
Data-to-parameter ratio = 9.7

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

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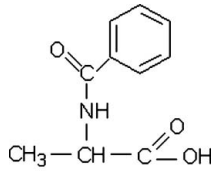
In the crystal structure of the title compound, $C_{10}H_{11}NO_3$, there are O—H···O and N—H···O hydrogen bonds, connecting the molecules into planes parallel to the *bc* plane.

Comment

As a result of systematic studies on new complexes of metallic ions with amino-acid derivatives (Fu *et al.*, 2004), we have focused our attention on amino-acid derivatives. In this paper, we present an X-ray crystallographic analysis of the title compound, (I) (Fig. 1).



(I)

The title compound, (I), is an amino-acid derivative with a free carboxylic acid group. The torsion angles for O1—C1—C2—N1, C1—C2—N1—C4, C2—N1—C4—C5 and N1—C4—C5—C6 are 165.54 (15), −150.82 (18), 174.47 (14) and −32.4 (2)°, respectively. The hydrogen bond between the carboxylic acid group and the O atom of the acetyl group (Table 1) connects the molecules into an infinite chain along the *b* axis. The hydrogen bond between the amido N atom and the carboxylic C=O connects the chains into a plane parallel to the *bc* plane (Table 1 and Fig. 2). There are unequal distances for the C1—O1 [1.314 (4) Å] and C1=O2 [1.204 (3) Å] bonds, with unequal O1—C1—C2 [124.4 (2)°] and O2—C1—C2 [111.33 (17)°] angles. We could not detect

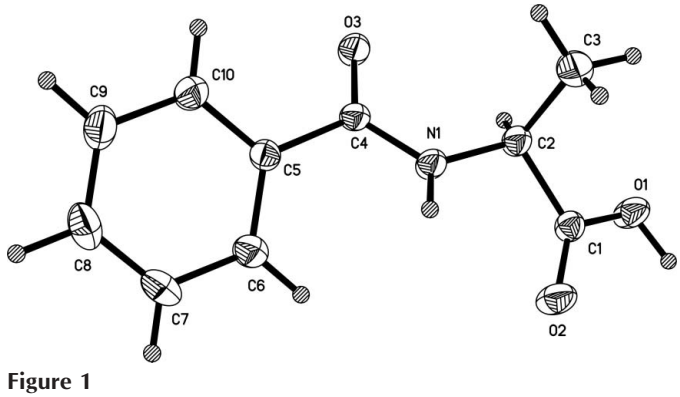


Figure 1
An *ORTEPIII* (Burnett & Johnson, 1996) view of the molecular structure of (I), showing the labelling of all non-H atoms. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as circles of arbitrary radius.

any significant stacking interactions, the distances between planes being close to the sums of van der Waals radii.

Experimental

Compound (I) was synthesized according to the literature (Steiger, 1944). Crystals appropriate for data collection were obtained by slow evaporation of an ethanol solution at 293 K.

Crystal data

$C_{10}H_{11}NO_3$
M_r = 193.20
Monoclinic, $P2_1/c$
a = 9.263 (2) Å
b = 10.308 (3) Å
c = 10.974 (3) Å
β = 112.872 (3)°
V = 965.5 (4) Å^3
Z = 4
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2314 reflections
θ = 2.4–28.3°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, yellow
0.39 × 0.31 × 0.27 mm

Data collection

Bruker SMART CCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.962, T_{max} = 0.974
4307 measured reflections
1659 independent reflections
1352 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 25.1°
$h = -10 \rightarrow 11$
$k = -12 \rightarrow 11$
$l = -13 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.144
S = 1.08
1659 reflections
171 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0948P)^2 + 0.0352P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{i}	0.93 (3)	1.74 (3)	2.604 (5)	154 (3)
N1—H2···O2^{ii}	0.86 (2)	2.29 (2)	3.076 (5)	153 (2)

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

All H atoms were located in a difference map and refined freely; C—H distances are in the range 0.92 (2)–1.04 (3) Å.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

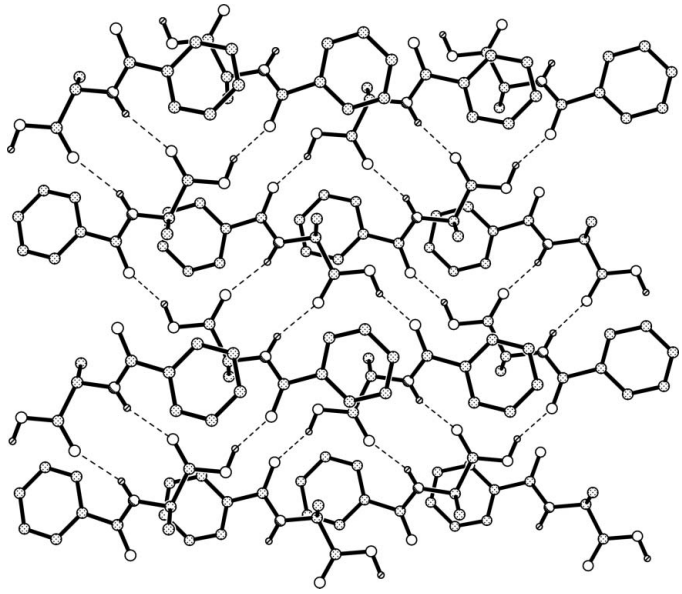


Figure 2
A *PLATON* (Spek, 2003) view of the hydrogen bonding (dashed lines) in (I). H atoms not involved in hydrogen bonding have been omitted.

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