Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Acetyl-*N*-phenylglycine

Ai-Yun Fu[a,b]* and Da-Qi Wang[b]

[a]Department of Chemistry, Dezhou University, Shandong Dezhou 253023, People's Republic of China, and [b]Department of Chemistry, Liaocheng University, Shandong Liaocheng 252059, People's Republic of China

Correspondence e-mail: aiyunfu@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.006 Å
R factor = 0.049
wR factor = 0.143
Data-to-parameter ratio = 10.9

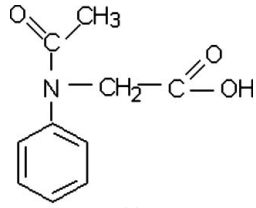
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 June 2005
Accepted 7 July 2005
Online 13 July 2005

The structure of the title amino acid, $C_{10}H_{11}NO_3$, is stabilized by O—H···O hydrogen bonds, connecting the molecules into infinite chains along the *b* axis.

Comment

As a result of systematic studies on new complexes of metal ions with amino acid derivatives (Fu, Wang & Shen, 2004; Fu, Wang, Shen & Zhang, 2004; Fu, Fu & Yu, 2005), we have focused our attention on amino-acid structures. In this paper, we present the structure of the title compound, (I) (Fig. 1), an amino acid derivative with a free carboxylic acid group.



(I)

Atom O1 of the carboxylic acid group acts as a hydrogen-bond donor, forming an O1—H2···O3 hydrogen bond and connecting the molecules into infinite chains along the *b* axis. Atom O2 of the carboxylic acid group acts as an acceptor, forming a non-classical C2—H2···O2 hydrogen bond which links the chains parallel to the *bc* plane (Table 1 and Fig. 2). There are unequal distances and angles within the carboxylic acid unit [C1═O1 = 1.183 (4), C1—O2 = 1.315 (4) Å; O1—

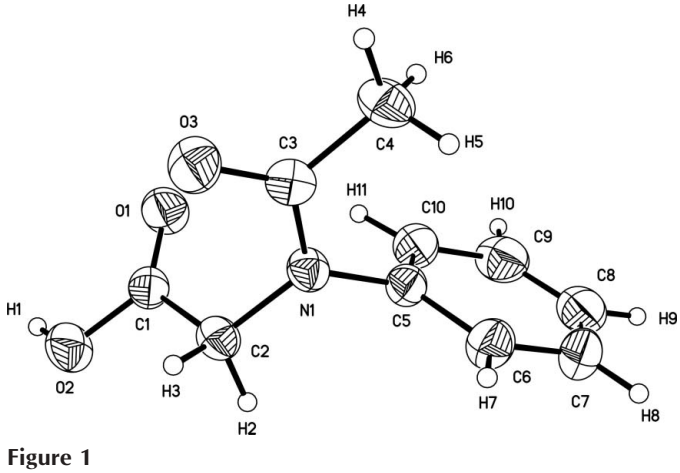


Figure 1
An *ORTEPIII* (Burnett & Johnson, 1996) view of the molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as circles of arbitrary radius.

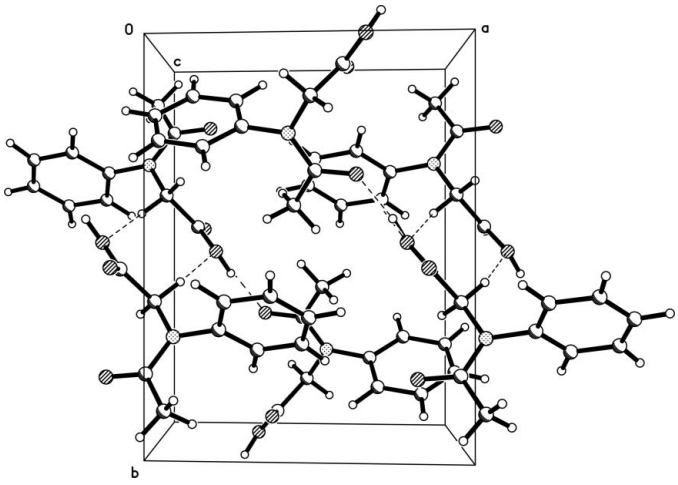


Figure 2
A *PLATON* (Spek, 2003) view of the hydrogen-bonding motif for (I). Hydrogen bonds are drawn as dashed lines.

C1—C2 = 125.3 (3) and O2—C1—C2 = 109.1 (3)°]. The C1═O1 distance here is shorter than the distance of 1.204 (3) Å found for *N*-benzoylalanine (Fu & Wang, 2005). The bond lengths and angles for (I) are comparable to and consistent with the corresponding values found in complexes containing the *N*-acetyl-*N*-phenylglycinate ligand (Fu, Wang & Shen, 2004; Fu, Wang, Shen & Zhang, 2004; Fu, Fu & Yu, 2005). The sum of angles C3—N1—C5 [122.2 (3)°], C3—N1—C2 [118.0 (3)°] and C5—N1—C2 [119.5 (3)°] is close to 360°, indicating a planar conformation at atom N1. We could not detect any significant stacking interactions, the distances between the aromatic ring planes being close to the sum of the van der Waals radii.

Experimental

An analytically pure commercially available sample of *N*-acetyl-*N*-phenylglycine (POCH, Poland) was used. Single crystals were grown by slow evaporation of a methanol–chloroform (1:1) solution.

Crystal data

$C_{10}H_{11}NO_3$
M_r = 193.20
Monoclinic, $P2_1/n$
a = 8.889 (14) Å
b = 11.523 (18) Å
c = 9.677 (15) Å
β = 95.58 (3)°
V = 987 (3) Å^3
Z = 4
D_x = 1.301 Mg m^{-3}
Mo- $K\alpha$ radiation
Cell parameters from 863 reflections
θ = 2.9–21.8°
μ = 0.10 mm^{-1}
T = 273 (2) K
Block, yellow
0.35 × 0.31 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.967, T_{max} = 0.984
5022 measured reflections
1749 independent reflections
802 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 25.0°
$h = -7 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.143
S = 0.97
1749 reflections
160 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O3^{i}	0.90 (1)	1.71 (1)	2.592 (4)	169 (3)
C2—H2···O2^{ii}	1.01 (3)	2.53 (3)	3.388 (6)	143 (2)

Symmetry codes: (i) $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (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 0.96 (1)–1.01 (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*).

The authors thank the Science and Technology Office of Dezhou City, Shandong Province, People's Republic of China, for research grant No. 030701.

References

Fu, A.-Y., Fu, S.-Z. & Yu, T. (2005). *Acta Cryst.* E**61**, m223–m225.
Fu, A.-Y. & Wang, D.-Q. (2005). *Acta Cryst.* E**61**, o2336–o2337.
Fu, A.-Y., Wang, D.-Q. & Shen, Q.-J. (2004). *Acta Cryst.* E**60**, m1346–m1348.
Fu, A.-Y., Wang, D.-Q., Shen, Q.-J. & Zhang, C.-L. (2004). *Acta Cryst.* E**60**, m1337–m1339.
Bruker (1997). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997*a*). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.