

Gao-Ning Li,^a Jian Li^b and Zu-Pei Liang^{b*}

^aCollege of Chemical Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China, and

^bDepartment of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China

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

Key indicators

Single-crystal X-ray study
 T = 294 K
 Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
 R factor = 0.035
 wR factor = 0.088
 Data-to-parameter ratio = 8.3

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

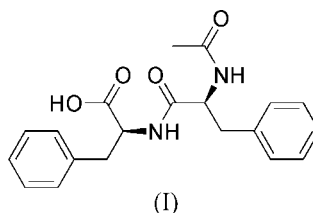
(S)-2-[(S)-2-Acetamido-3-phenylpropanamido]-3-phenylpropanoic acid

In the title compound, $\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_4$, the two phenyl rings form a dihedral angle of $89.2(2)^\circ$. The crystal structure is stabilized by weak $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Received 26 November 2006
 Accepted 12 December 2006

Comment

N-Acetyl amino acids play an important role in methylation, sulfuration, detoxication and antioxidation. They are very useful in the pharmaceutical and food industries.



The molecular structure of the title compound, (I), is illustrated in Fig. 1. The geometry of the *N*-acetyl-*L*-phenylalanine system is comparable to that reported for *N*-acetyl-*L*-phenylalanine (Stout *et al.*, 2000). The dihedral angle between the two phenyl rings is $89.2(2)^\circ$. The crystal structure is stabilized by weak $\text{N}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds (Fig. 2 and Table 1).

Experimental

A mixture of (*S*)-2-amino-3-phenylpropanoic acid (0.1 mol), acetic anhydride (0.2 mol) in water (30 ml) was stirred for 20 min at 298 K. After cooling, filtration and drying, the title compound was obtained. 10 mg of (I) was dissolved in 10 ml ethanol-*N,N*-dimethylacetamide (1:1 *v/v*) and the solution was allowed to evaporate at room temperature. Colourless single crystals of the title compound were formed after 35 d.

Crystal data

$\text{C}_{20}\text{H}_{22}\text{N}_2\text{O}_4$	$Z = 2$
$M_r = 354.40$	$D_x = 1.292 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 10.185(3) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 8.633(2) \text{ \AA}$	$T = 294(2) \text{ K}$
$c = 10.427(3) \text{ \AA}$	Block, colourless
$\beta = 96.364(5)^\circ$	$0.34 \times 0.30 \times 0.24 \text{ mm}$
$V = 911.1(4) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	5164 measured reflections
φ and ω scans	1978 independent reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Bruker, 1997)	1573 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.970$, $T_{\max} = 0.979$	$R_{\text{int}} = 0.028$
	$\theta_{\text{max}} = 26.4^\circ$

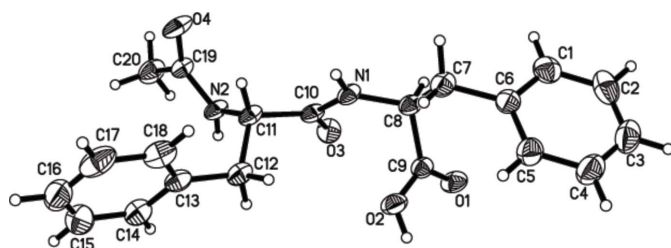


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.035$
 $wR(F^2) = 0.088$
 $S = 1.06$
 1978 reflections
 237 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.0961P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.12 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.14 \text{ e } \text{\AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O2-H2A\cdots O3^i$	0.82	1.79	2.598 (2)	169
$N1-H1\cdots O4^{ii}$	0.86	1.98	2.819 (3)	166
$N2-H2\cdots O1^{iii}$	0.86	2.02	2.872 (3)	168

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

The absolute configuration was known from the synthesis and assumed for the structure. H atoms were initially located in difference maps and then refined in a riding model, with $C-H = 0.93-0.98 \text{ \AA}$ and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ or $1.5 U_{\text{eq}}(\text{methyl } C)$. In the absence of significant anomalous dispersion effects, Friedel pairs were merged prior to refinement.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine

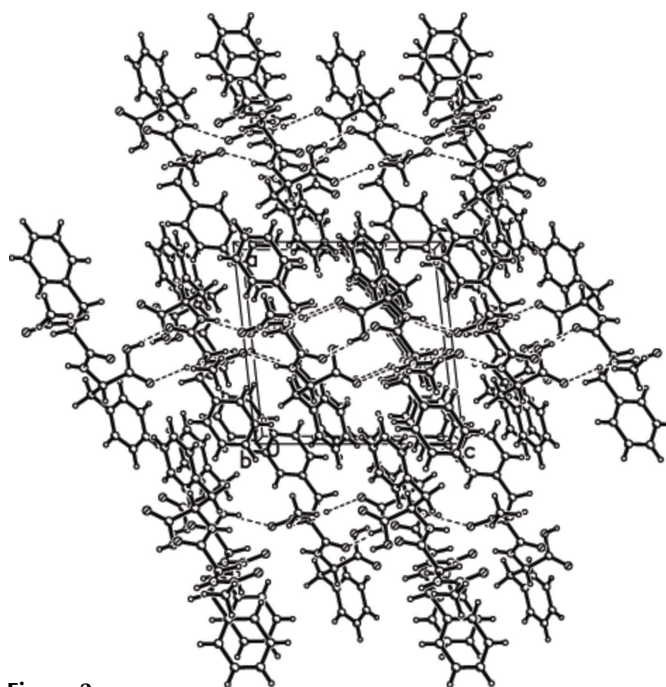


Figure 2
The crystal packing of (I), viewed along the b axis. Dashed lines indicate hydrogen bonds.

structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Doctoral Fund of Weifang University.

References

- Bruker (1997). *SADABS*, *SMART*, *SAINTE* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
 Stout, K. L., Hallock, K. J., Kampf, J. W. & Ramamoorthy, A. (2000). *Acta Cryst.* **C56**, e100.