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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.029
 wR factor = 0.073
Data-to-parameter ratio = 8.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(S)-Methyl 2-[(furan-2-carbonyl)amino]-
3-phenylpropanoate**

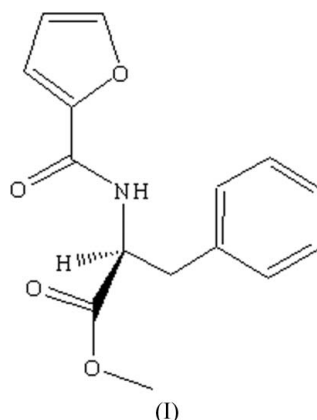
The title compound, $\text{C}_{15}\text{H}_{15}\text{NO}_4$, was synthesized by acylation of methyl L-2-amino-3-phenylpropanoate with furan-2-carbonyl chloride at room temperature. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into extended chains parallel to the b axis.

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Comment

Furan derivatives are well known in many marine organisms (Faulkner, 2001), and some have important bioactivities, such as antitumor activity (Phuwapraisiran *et al.*, 2004) and diabetes treatment activity (Hwang *et al.*, 2002). In our search for bio-active compounds, a series of furan-2-carboxamido acids and their esters, including the title compound, (I), have been synthesized by reaction of amino acid esters with furan-2-carbonyl chloride. We report here the crystal structure of (I).



Bond lengths and angles are unexceptional and are in good agreement with the corresponding values in methyl 2-(4,5-dibromo-1-methylpyrrole-2-carboxylamino)-3-phenylpropanoate (Zeng *et al.*, 2006) and 4-[(furan-2-ylmethylene)amino]-1,5-dimethyl-2-phenyl-1,2-dihydropyrazol-3-one (Li *et al.*, 2005).

In the crystal structure, molecules are connected by $\text{N}-\text{H}\cdots\text{O}$ hydrogen-bond interactions (Table 1), generating chains running parallel to the b axis (shown in Fig. 2).

Experimental

Methyl L-2-amino-3-phenylpropanoate hydrochloride (1.08 g, 5 mmol) was added to dichloromethane (6 ml), followed by the addition of triethylamine (1.5 ml); after stirring for 15 min, the precipitate was filtered off. Furan-2-carbonyl chloride (0.5 ml, 5 mmol) in dichloromethane (3 ml) was added to the filtrate dropwise at 288–293 K. The mixture reacted at room temperature for 2 h and was then filtered; the filtrate was collected and washed with water

(5 ml). The organic phase was dried with anhydrous sodium sulfate overnight and the solvent removed by distillation under reduced pressure. The pale brown solid residue was dissolved in 95% ethanol at room temperature. Colorless crystals suitable for X-ray analysis (m. p. 345 K, in 84.2% yield) grew over a period of 7 days when the solution was exposed to air.

Crystal data

$C_{15}H_{15}NO_4$	$Z = 4$
$M_r = 273.28$	$D_x = 1.286 \text{ Mg m}^{-3}$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 8.5817 (12) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$b = 8.9505 (14) \text{ \AA}$	$T = 173 (2) \text{ K}$
$c = 18.375 (3) \text{ \AA}$	Block, colorless
$V = 1411.4 (4) \text{ \AA}^3$	$0.48 \times 0.46 \times 0.32 \text{ mm}$

Data collection

Bruker SMART 1K CCD area-detector diffractometer	5884 measured reflections
φ and ω scans	1612 independent reflections
Absorption correction: multi-scan	1492 reflections with $I > 2\sigma(I)$
SADABS (Sheldrick, 1996)	$R_{\text{int}} = 0.019$
$T_{\text{min}} = 0.870$, $T_{\text{max}} = 0.971$	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.265P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.073$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
1612 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
184 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.042 (3)

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots O2^i$	0.88	2.12	2.930 (2)	154

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

H atoms were positioned geometrically [$C-H = 1.00 \text{ \AA}$ for CH, $C-H = 0.99 \text{ \AA}$ for CH_2 , 0.98 \AA for CH_3 , 0.95 \AA for CH(aromatic), and $N-H = 0.88 \text{ \AA}$] and refined using a riding model, with $U_{\text{iso}} = 1.2U_{\text{eq}}$ ($1.5U_{\text{eq}}$ for the methyl group) of the parent atom. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT-Plus* (Bruker, 1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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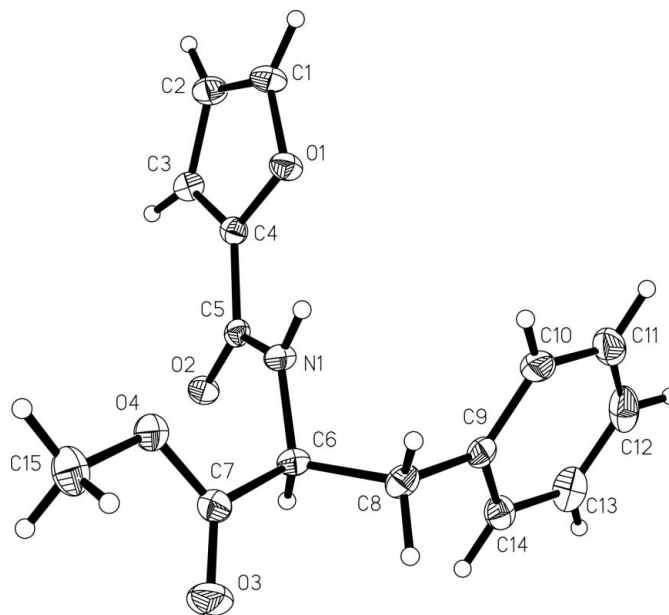


Figure 1

The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

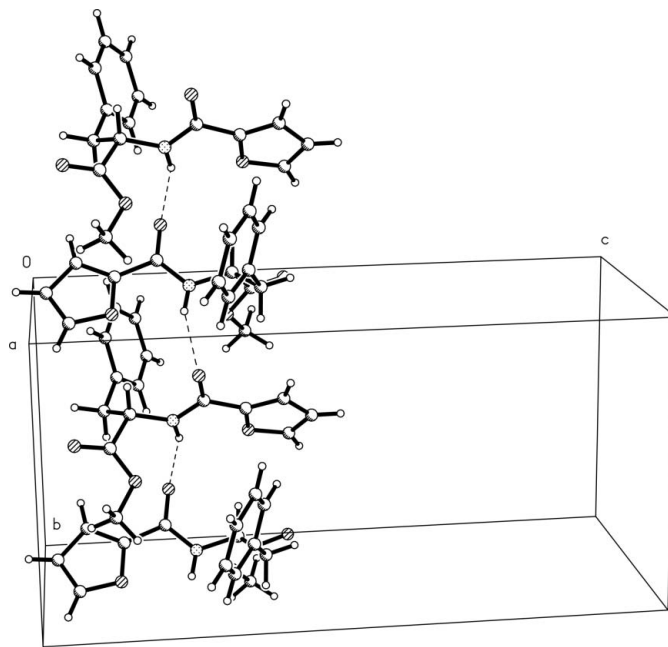


Figure 2

Part of the crystal structure of (I), showing the hydrogen-bonded dashed lines chains.

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