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Ethyl N-(2-pyridyl)carbamate

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.109
Data-to-parameter ratio = 15.1

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

The title compound, $C_8H_{10}N_2O_2$, is nearly planar. The crystal packing is stabilized by N—H···N hydrogen bonds.

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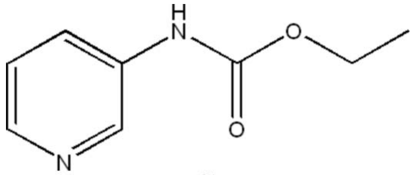
Comment

Pyridine-containing compounds are used extensively as bridging ligands in coordination and metallosupramolecular chemistry (Steel, 1990, 2005). Moreover, pyridine derivatives are often used as intermediates in synthetic chemistry. The title compound, (I), is a precursor used in the preparation of tricyclic amide and urea compounds for the inhibition of G-protein function and the treatment of proliferative diseases (Bishop *et al.*, 1995). We report here the crystal structure of (I).


(I)

All the bond distances and angles are normal (Kennedy *et al.*, 2004). The overall molecule is extended and nearly planar, with an r.m.s. derivation of 0.0383 Å. The terminal ethoxycarbonyl group is slightly twisted, by 5.1 (5)°, away from the pyridine ring. Hydrogen-bond interactions between the amino H and pyridyl N atoms link the molecules into an infinite chain along the *c* axis.

Experimental

The title compound was synthesized according to the modified method of Katritzky (1956). Ethyl chloroformate (10.85 g, 0.10 mol) was added dropwise to a solution of 3-aminopyridine (9.42 g,

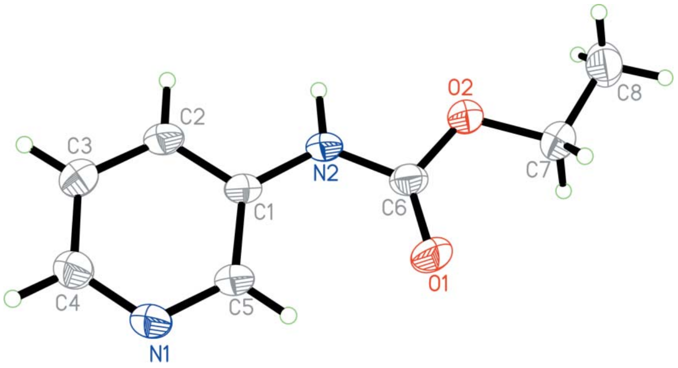


Figure 1
A view of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

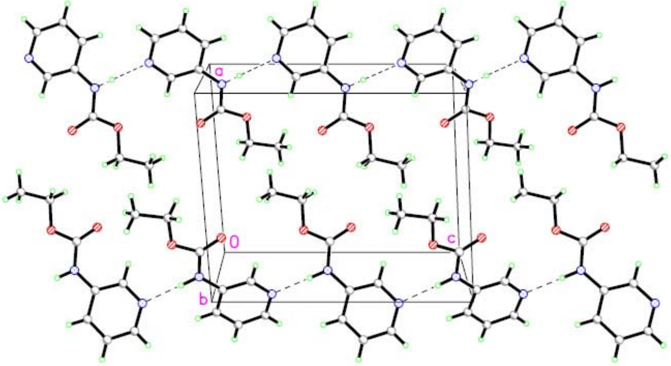


Figure 2
The unit-cell packing, viewed down the *c* axis, with hydrogen bonds shown as dashed lines.

0.10 mol) in dry pyridine (30 ml) and stirred at 273–278 K for 6 h. After another 8 h at room temperature, the reaction mixture was hydrolysed with ice water (60 ml). The solid was filtered off and recrystallized from ethanol/water, giving 9.96 g (60%) of colourless solid (m.p. 363–364 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of the mother liquor.

Crystal data

$C_8H_{10}N_2O_2$
$M_r = 166.18$
Monoclinic, $P2_1/c$
$a = 9.621$ (4) Å
$b = 7.497$ (3) Å
$c = 11.839$ (5) Å
$\beta = 93.211$ (6)°
$V = 852.6$ (6) Å^3
$Z = 4$

$D_x = 1.295$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1352 reflections
$\theta = 3.2$–$24.8°$
$\mu = 0.10$ mm^{-1}
$T = 294$ (2) K
Block, colourless
$0.30 \times 0.26 \times 0.20$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.972$, $T_{max} = 0.981$
4629 measured reflections

1741 independent reflections
1090 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 26.4°$
$h = -11 \rightarrow 12$
$k = -9 \rightarrow 7$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.109$
$S = 1.01$
1741 reflections
115 parameters
H atoms treated by a mixture of independen and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.0996P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.027 (4)

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.2042 (19)	N2—C6	1.351 (2)
O2—C6	1.342 (2)	N2—C1	1.394 (2)
O2—C7	1.442 (2)		
O1—C6—N2	127.08 (16)	O2—C6—N2	108.87 (13)
N2—C1—C5—N1	179.69 (16)	C1—N2—C6—O2	−174.15 (15)
C7—O2—C6—N2	−178.59 (15)	C6—O2—C7—C8	179.11 (17)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···N1^{i}	0.94 (1)	1.98 (1)	2.914 (4)	178 (1)

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

All H atoms were positioned geometrically and refined as riding, with C—H distances of 0.93 (pyridyl H), 0.96 (CH_2) and 0.97 Å (CH_3), and with $U_{iso}(H) = 1.2U_{eq}(C)$. The amino H atom was refined freely [N—H = 0.936 (9)].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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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