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Phenyl 2-picolinamidobenzoate

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In the title compound, $C_{19}H_{14}N_2O_3$, all bond lengths and angles show normal values. The molecules are linked by C—H···O hydrogen bonds, forming dimers which are arranged parallel to the *a* axis.

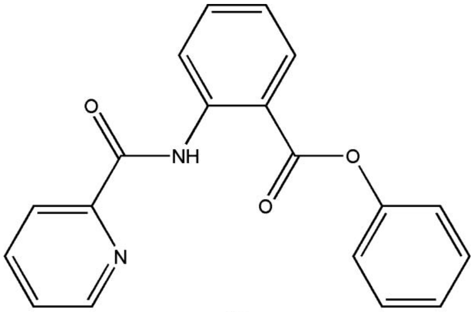
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.100
Data-to-parameter ratio = 13.7

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

Comment

Pyridine-containing amide compounds have been intensively studied due to their potential biological activities (Belokon *et al.*, 2003). The title compound, (I), is a pyridine-amide compound containing a phenoxycarbonylphenyl ester group attached to the amide N atom (Fig. 1). The bond lengths and angles are in normal ranges (Allen *et al.*, 1987).



(I)

Both the 2-picolinamidobenzoyl (C7–C19/O2/O3/N1/N2) and phenoxy (O1/C1–C6) fragments are essentially planar, with maximum deviations of 0.072 (3) Å for atom C7 and 0.027 (1) Å for O1 from their respective least-squares planes. The O1/C1–C6 fragment makes a dihedral angle of 71.49 (6)° with the C7–C19/O2/O3/N1/N2 fragment.

There are two intramolecular hydrogen bonds (N1—H1···O2 and N1—H1···N2) (Table 1). In the crystal structure, the molecules are linked by C—H···O hydrogen bonds (Table 1), forming dimers that are are arranged parallel to the *a* axis (Fig. 2).

Experimental

Pyridine (15 ml, 185.8 mmol) was added to a mixture of picolinic acid (3 g, 24.4 mmol) and *o*-aminobenzoic acid (3 g, 21.9 mmol). The solution was stirred for 30 min at room temperature, and then the temperature was gradually increased to about 373 K. To the solution, triphenyl phosphite (6.6 ml, 25.2 mmol) was slowly added dropwise under reflux with continuous stirring. After 10 h, the reaction mixture was cooled to room temperature and some yellow lumps formed. After filtration, the solid was washed with cold diethyl ether, water and methanol. Crystals suitable for X-ray diffraction were obtained from water–methanol (1:1) over a period of about two weeks.

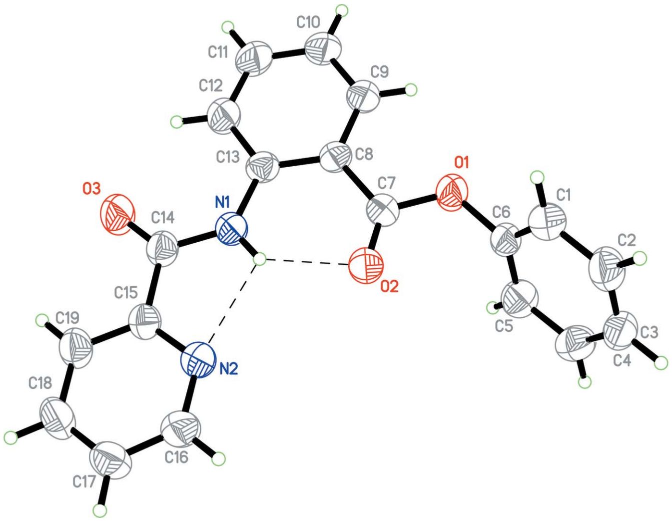


Figure 1
The molecular structure of the title compound, (I), shown with 50% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

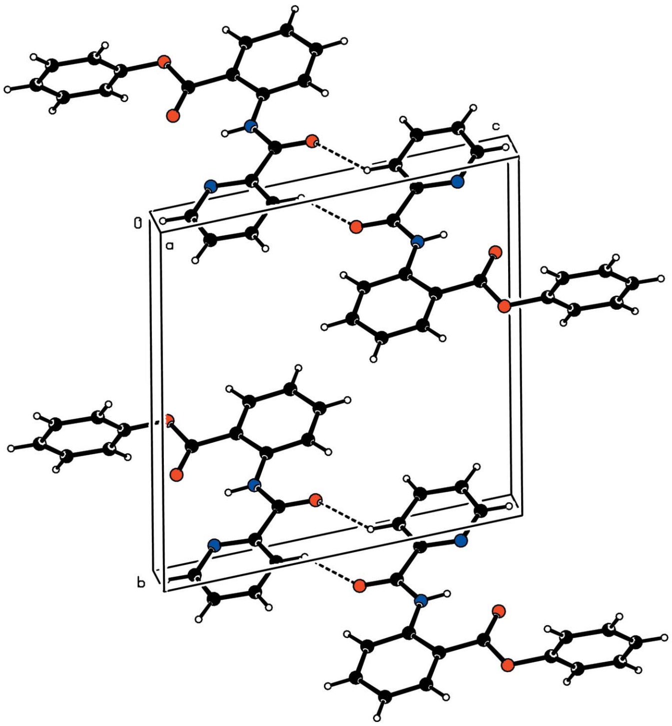


Figure 2
Packing diagram of compound (I), viewed approximately down the *a* axis. Dashed lines denote C—H···O hydrogen bonds.

Crystal data

$C_{19}H_{14}N_2O_3$
$M_r = 318.32$
Triclinic, $P\overline{1}$
$a = 5.657$ (2) Å
$b = 11.700$ (4) Å
$c = 11.793$ (4) Å
$\alpha = 98.910$ (8)°
$\beta = 97.291$ (9)°
$\gamma = 96.008$ (7)°

$V = 758.7$ (5) Å^3
$Z = 2$
$D_x = 1.393$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 292$ (2) K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.971$, $T_{\max} = 0.990$

8013 measured reflections
2965 independent reflections
1895 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.059$
$\theta_{\max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.100$
$S = 0.91$
2965 reflections
217 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C6	1.412 (2)	N1—C14	1.363 (2)
C7—O1—C6	117.79 (13)	C14—N1—C13	128.46 (14)
C7—O1—C6—C1	−103.79 (19)	C13—N1—C14—O3	1.3 (3)
C6—O1—C7—C8	179.06 (14)	C13—N1—C14—C15	−179.28 (14)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O2	0.86	2.02	2.708 (2)	137
N1—H1*B*···N2	0.86	2.26	2.693 (2)	111
C19—H19*A*···O3$^{\rm i}$	0.93	2.54	3.269 (2)	133

Symmetry code: (i) $-x + 3, -y + 2, -z + 1$.

After their location in a difference map, all H atoms were positioned geometrically at ideal positions and allowed to ride on their parent C or N atoms, with C—H = 0.93 Å, N—H = 0.86 Å and $U_{\rm iso}$(H)= 1.2$U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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