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N-(4-Iodophenyl)quinoline-2-carboxamide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.031
wR factor = 0.072
Data-to-parameter ratio = 17.5

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

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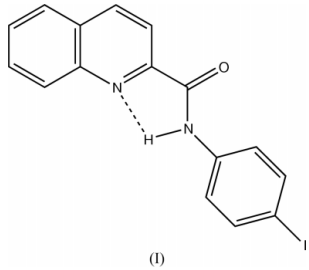
The quinolyl and phenyl rings in the title compound, $C_{16}H_{11}IN_2O$, are almost coplanar. There is an intramolecular hydrogen bond between the quinoline N atom and amide N atom [N···N = 2.659 (3) Å and N—H···N = 112°].

Comment

We have previously reported the structure of the bidentate ligand (*R*)-*N*-(1-phenylethyl)quinoline-2-carboxamide (Yang *et al.*, 2001). The quinolyl and phenyl rings in that compound form a dihedral angle of 89.07 (5)°, while the two rings in the title compound, (I), are coplanar. It is predicted that the N atom of the quinoline ring and the amide N atom or carbonyl O atom will coordinate to a metal ion and form a complex with a five-membered ring structure. There is an intramolecular hydrogen bond involving the quinoline and amide N atoms [N2···N1 = 2.659 (3) Å and N2—H2*A*···N1 = 112°]. The structure of *N*-(4-methoxyphenyl)quinoline-2-carboxamide is reported in the preceding paper (Qi *et al.*, 2003).



(I)

Experimental

The title compound was synthesized from 2-quinolinecarboxylic acid and 4-iodoaniline according to the general procedure of Johnson *et al.* (1960). The crystal used for the data collection was obtained by slow evaporation of a saturated DMF–H_2O solution of (I) at room temperature.

Crystal data

$C_{16}H_{11}IN_2O$
M_r = 374.17
Monoclinic, $P2_1/n$
a = 6.5389 (10) Å
b = 17.036 (3) Å
c = 12.702 (2) Å
β = 102.377 (3)°
V = 1382.1 (4) Å^3
Z = 4
D_x = 1.798 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 4725 reflections
θ = 1–27.5°
μ = 2.31 mm^{-1}
T = 294 (2) K
Prism, yellow
0.20 × 0.18 × 0.14 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.655, T_{max} = 0.738
9337 measured reflections
3169 independent reflections
2153 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 27.6°
h = −8 → 6
k = −22 → 20
l = −16 → 16

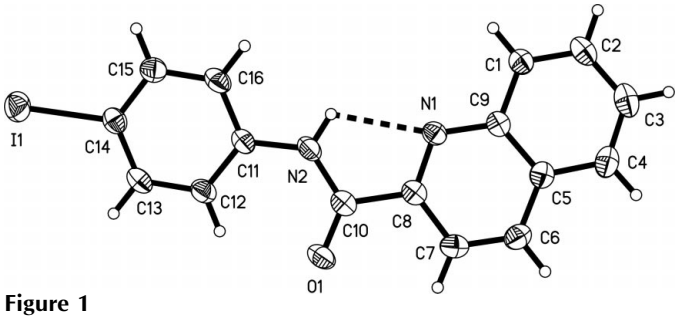


Figure 1
The molecular structure of (I), showing ellipsoids at the 30% probability level (Siemens, 1995).

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.031$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.61$ e Å^{-3}
3169 reflections	$\Delta\rho_{min} = -0.33$ e Å^{-3}
181 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.86	2.22	2.659 (3)	112

The C-bound H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation. The H atom on N2 was initially refined but was constrained in the final refinement.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SHELXTL-NT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL-NT*; software used to prepare material for publication: *SHELXTL-NT*.

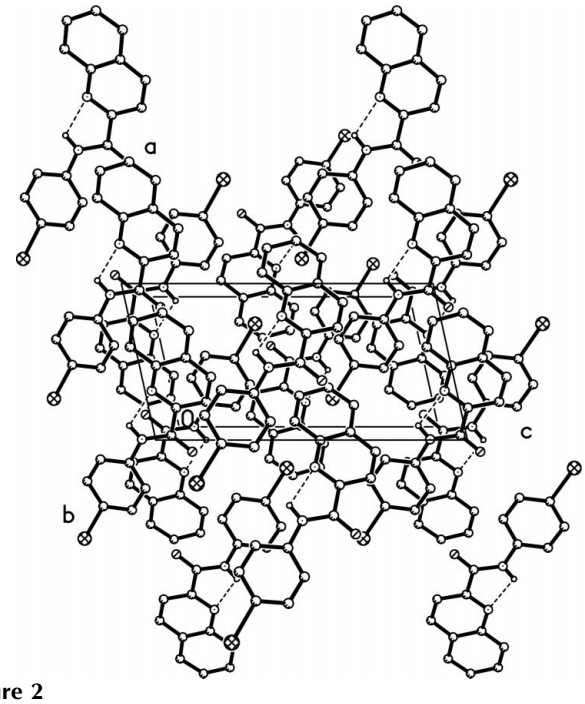


Figure 2
The molecular packing along the *b* axis.

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