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

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.111
Data-to-parameter ratio = 16.5

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

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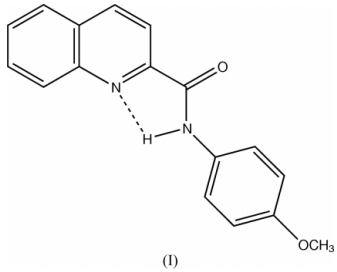
The quinolyl and phenyl rings in the title compound, $C_{17}H_{14}N_2O_2$, are almost coplanar. There is an intramolecular hydrogen bond between the quinoline N atom and the amide N atom [N···N = 2.6602 (17) Å and N—H···N = 112°].

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 corresponding 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 between the quinoline N atom and the amide N atom [N2···N1 = 2.6602 (17) Å and N2—H2*A*···N1 = 112°]. The structure of *N*-(4-iodophenyl)-quinoline-2-carboxamide is reported in the following paper (Qi *et al.*, 2003).



(I)

Experimental

The title compound was synthesized from 2-quinolinecarboxylic acid and 4-methoxyaniline 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

$C_{17}H_{14}N_2O_2$
M_r = 278.30
Monoclinic, $P2_1/n$
a = 6.6372 (11) Å
b = 18.109 (3) Å
c = 11.4921 (19) Å
β = 92.867 (3)°
V = 1379.6 (4) Å^3
Z = 4
D_x = 1.340 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3598 reflections
θ = 1–27.5°
μ = 0.09 mm^{-1}
T = 294 (2) K
Prism, colorless
0.38 × 0.28 × 0.26 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.977
9204 measured reflections
3167 independent reflections
1829 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 27.5°
$h = -8 \rightarrow 8$
$k = -13 \rightarrow 23$
$l = -14 \rightarrow 14$

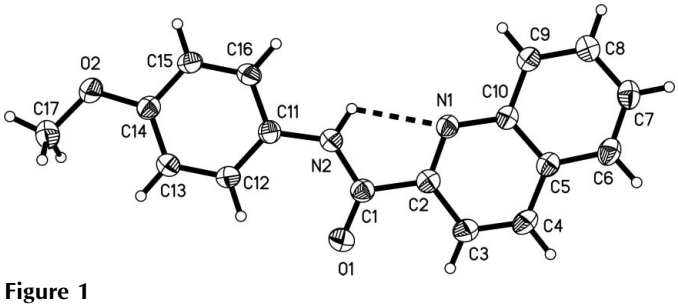


Figure 1
The molecular structure of (I), showing ellipsoids at the 30% probability level (Siemens, 1995).

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
3167 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
192 parameters	Extinction correction: *SHELXL*97
H-atom parameters constrained	Extinction coefficient: 0.020 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N1	0.86	2.21	2.6602 (17)	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*.

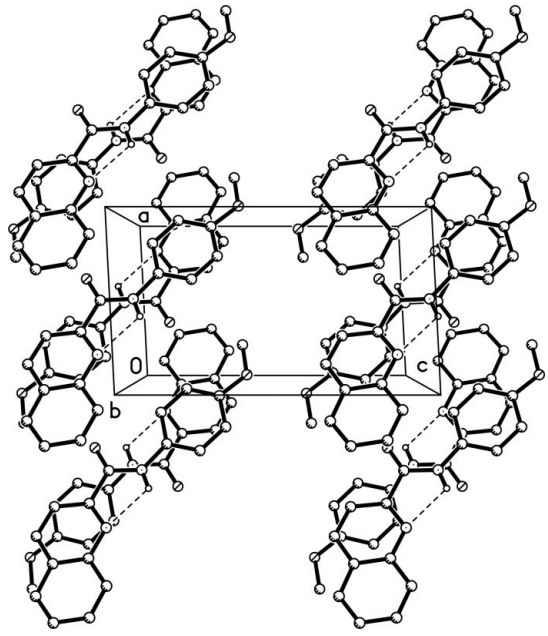


Figure 2
The molecular packing along the *b* axis.

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