

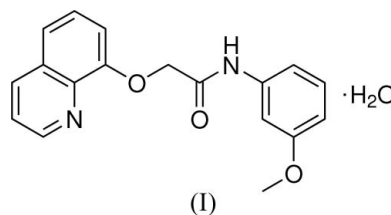
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.047
 wR factor = 0.097
Data-to-parameter ratio = 7.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*N*-(3-Methoxyphenyl)-2-(quinolin-8-yloxy)-
acetamide monohydrateIn the title compound, $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_3 \cdot \text{H}_2\text{O}$, the organic molecules and water molecules are linked by intermolecular $\text{N}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds. The structure is also stabilized by $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds.Received 8 June 2006
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Comment

In our ongoing studies of amide-type acyclic compounds with 8-hydroxyquinolate as the skeleton (Wen *et al.*, 2005), the title compound has been synthesized and its structure is reported here.All bond lengths and angles in (I) are normal (Allen *et al.*, 1987) and comparable with those in a related compound (Wen *et al.*, 2005). The molecules are linked by intermolecular hydrogen bonds, with N and O atoms acting as donors and acceptors (Table 1, Fig. 2). There are also three weak $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonds, one of them being intramolecular (Table 1). The angle between the mean planes of the benzene and quinoline rings is $56.2(1)^\circ$ (Nardelli, 1995).

Experimental

2-Chloro-*N*-(3-methoxyphenyl)acetamide (4.0 g, 20 mmol), K_2CO_3 (3.04 g, 22 mmol) and KI (0.5 g, 3 mmol) were added to a solution of 8-hydroxyquinoline (2.9 g, 20 mmol) in acetone (40 ml). The mixture was stirred at 333 K for 6 h. After cooling to room temperature, the mixture was washed three times with water and then filtered. The title compound was obtained after drying the resulting white powder at room temperature for 48 h (elemental analysis found: C 66.20, H 5.62, N 8.55, O 19.66; calculated: C 66.25, H 5.56, N 8.58, O 19.61 wt. %). Colourless single crystals suitable for X-ray diffraction studies were obtained by slow evaporation of an ethyl acetate solution over a period of 5 d.

Crystal data

 $\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_3 \cdot \text{H}_2\text{O}$
 $M_r = 326.34$
Monoclinic, $P2_1$
 $a = 8.1881(11)$ Å
 $b = 7.0491(10)$ Å
 $c = 14.094(2)$ Å
 $\beta = 100.553(2)^\circ$
 $V = 799.75(19)$ Å³ $Z = 2$
 $D_x = 1.355$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293(2)$ K
Block, colourless
 $0.26 \times 0.16 \times 0.12$ mm

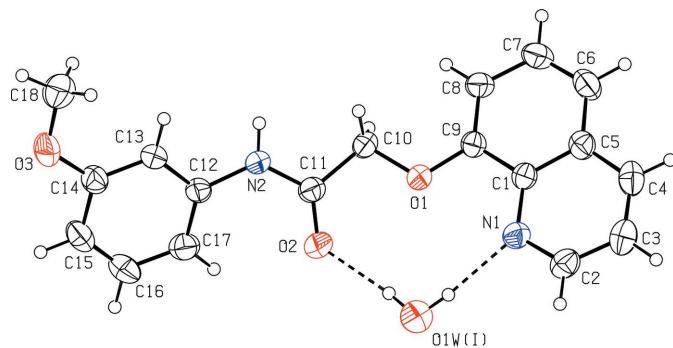


Figure 1
The structure of compound (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are shown as dashed lines. [Symmetry code: (I) $x, -1 + y, 1 + z$.]

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	4571 measured reflections
ω scans	1706 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1288 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.975, T_{\max} = 0.989$	$R_{\text{int}} = 0.026$
	$\theta_{\text{max}} = 26.1^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.0065P]$
$R[F^2 > 2\sigma(F^2)] = 0.047$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.098$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.14 \text{ e } \text{\AA}^{-3}$
1706 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e } \text{\AA}^{-3}$
224 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1W-H1W\cdots O2^i$	0.85 (3)	1.99 (3)	2.838 (4)	174 (4)
$N2-H2B\cdots O1W^{ii}$	0.86	2.00	2.844 (4)	167
$O1W-H2W\cdots N1^i$	0.86 (3)	1.98 (3)	2.830 (4)	173 (4)
$C8-H8A\cdots O2^{iii}$	0.93	2.50	3.365 (4)	154
$C13-H13A\cdots O1W^{ii}$	0.93	2.59	3.329 (4)	136
$C17-H17A\cdots O2$	0.93	2.37	2.906 (5)	116

Symmetry codes: (i) $x, y + 1, z - 1$; (ii) $x, y, z + 1$; (iii) $-x + 1, y + \frac{1}{2}, -z + 2$.

All H atoms were located in a difference Fourier map. Water H atoms were refined with $O1W-H1W$ and $O1W-H2W$ distance restraints of 0.85 \AA and with a common U_{iso} value. The remaining H atoms were placed in idealized positions and constrained to ride on their parent atoms, with $C_{\text{aryl}}-H = 0.93 \text{ \AA}$, $C_{\text{methyl}}-H = 0.96 \text{ \AA}$, $C_{\text{methylene}}-H = 0.97 \text{ \AA}$, and $N-H = 0.86 \text{ \AA}$, and with $U_{\text{iso}}(H) = 1.2 U_{\text{eq}}(C, N)$ or $1.5 U_{\text{iso}}(\text{methyl } C)$. 1307 Friedel pairs were merged

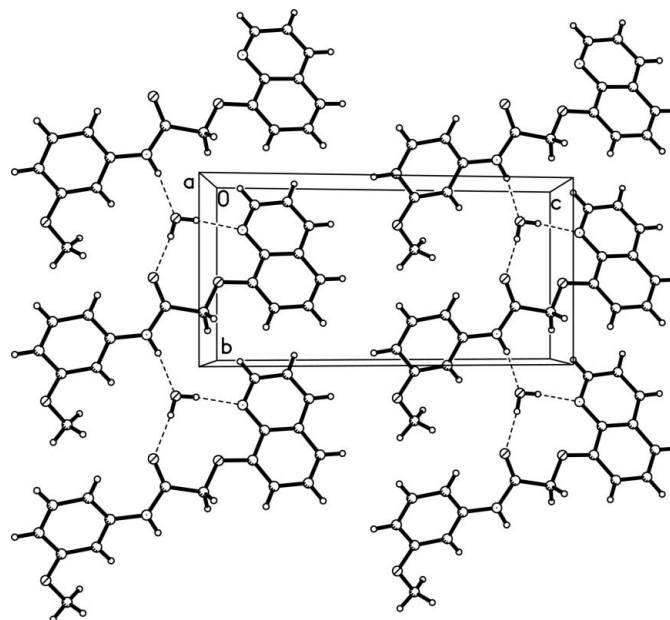


Figure 2
A packing diagram for (I), viewed down the a axis. Only the intermolecular hydrogen bonds with O or N donor atoms are shown, as dashed lines.

before the final refinement because of the absence of any significant anomalous scattering effects.

Data collection: *SMART* (Siemens, 1996); cell refinement: *S SAINT* (Siemens, 1996); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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