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N-(2-Chlorophenyl)-2-(quinolin-8-yloxy)acetamide

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Key indicators

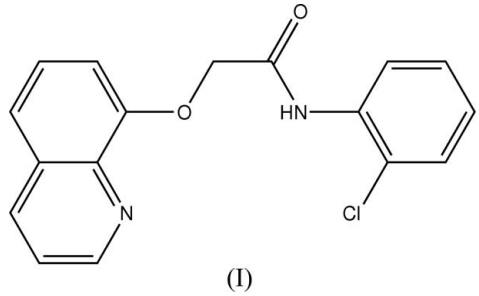
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.144
Data-to-parameter ratio = 14.3

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

In the title compound, $C_{17}H_{14}ClN_2O_3$, there are intramolecular hydrogen bonds of types N—H···O (2.634 and 2.570 Å), N—H···Cl (2.925 Å) and C—H···O (2.894 Å). The dihedral angle between the planes of the quinoline system and the benzene ring is 20.3 (1)°. The crystal packing is stabilized by π–π interactions.

Comment

In our ongoing studies of amide-type acyclic compounds with 8-hydroxyquinolinate as the skeleton (Li *et al.*, 2005), the title compound, (I), was synthesized and the structure is reported here.



(I)

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and comparable to those in a related compound (Li *et al.*, 2005). There are four intramolecular hydrogen bonds, forming three five-membered and one six-membered rings (Fig. 1 and Table 1). The packing is stabilized by π–π interactions between the aromatic rings [$Cg1\cdots Cg2(x, 1+y, z)$ = 3.706 Å; $Cg1$ and $Cg2$ are the centroids of the N1/C1–C5 and C1/C5–C9 rings, respectively].

Experimental

To a solution of 8-hydroxyquinoline (2.9 g, 20 mmol) in acetone (40 ml) were added 2-chloro-*N*-(2-chlorophenyl)acetamide (3.4 g, 20 mmol), K_2CO_3 (3.04 g, 22 mmol) and KI (0.5 g); the resulting mixture was stirred at 333 K for 6 h. After cooling to room temperature, the mixture was washed three times with water and filtered. The title compound was obtained after drying of the resulting white powder at room temperature for 48 h. Colourless single crystals suitable for X-ray structure analysis were obtained by slow evaporation of an ethyl acetate solution over a period of 5 d.

Crystal data

$C_{17}H_{14}ClN_2O_2$
M_r = 313.75
Monoclinic, $P2_1/c$
a = 20.245 (4) Å
b = 4.0211 (7) Å
c = 20.245 (4) Å
β = 117.38°
V = 1463.5 (5) Å^3
Z = 4
D_x = 1.424 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 293 (2) K
Plate, colourless
0.41 × 0.12 × 0.05 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.898, T_{max} = 0.987
7574 measured reflections
2853 independent reflections
1826 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.144
S = 1.01
2853 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 0.0875P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1	0.86	2.30	2.634 (3)	103
N2—H2A···Cl1	0.86	2.44	2.925 (2)	116
N2—H2A···O1	0.86	2.10	2.570 (3)	114
C17—H17A···O2	0.93	2.29	2.894 (4)	122

All H atoms were located in a difference Fourier map and then constrained to ride on their parent atoms, with C—H = 0.93 and 0.97 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *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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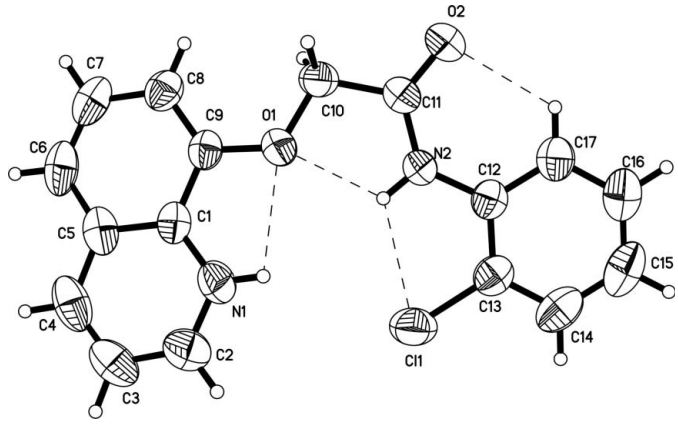

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom numbering scheme. Intramolecular hydrogen bonds are shown as dashed lines.

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