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N-(Quinolin-8-yl)-2-(quinolin-8-yloxy)acetamide

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Key indicators

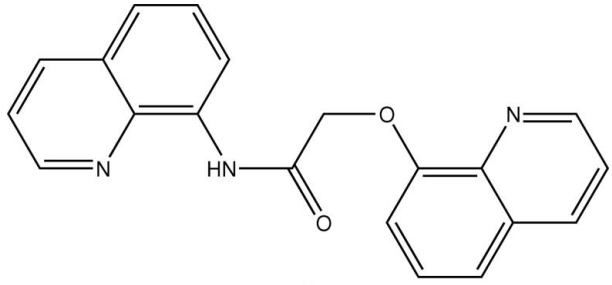
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.129
Data-to-parameter ratio = 13.5

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

In the crystal structure of the title compound, $C_{20}H_{15}N_3O_2$, molecules are linked into dimers by C—H···O intermolecular hydrogen bonds. The crystal packing is also stabilized by C—H···π and π–π interactions involving the quinoline units.

Comment

We have reported the structure of *N*-(4-methoxyphenyl)-2-(quinolin-8-yloxy)acetamide monohydrate, (II), (Wen *et al.*, 2005). As part of our studies on amide compounds, the title compound, (I), has been synthesized and the structure is reported here.



(I)

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and comparable with those in the related compound, (II). The two quinoline units are essentially planar, the dihedral angle between them being 83.07 (1)°. There are three intramolecular hydrogen bonds, *viz*. N2—H2*A*···O1 and N2—H2*A*···N3 and C20—H20*A*···O2 (Table 1), forming three five-membered rings. In the crystal structure, molecules are linked into dimers by a C10—H10*A*···O2^{i} intermolecular hydrogen bond (Table 1 and Fig. 2). The crystal packing is also stabilized by C—H···π (Table 1) and π–π interactions involving the quinoline units, with *Cg*2···*Cg*2^{iii}, *Cg*2···*Cg*4^{iii} and *Cg*1···*Cg*3^{iv} distances of 3.642 (2), 3.849 (2) and 3.694 (2) Å, respectively [*Cg*1, *Cg*2, *Cg*3 and *Cg*4 denote the centroids of the N1/C1–C5, N3/C13–C17, C1/C5–C9 and C12/C13/C17–C20 rings, respectively; symmetry codes: (iii) $1-x, 2-y, 2-z$; (iv) $1-x, 1-y, 1-z$].

Experimental

To a solution of 8-hydroxyquinoline (2.9 g, 20 mmol) in acetone (40 ml) were added 2-chloro-*N*-(quinolin-8-yl)acetamide (4.42 g, 20 mmol), K_2CO_3 (3.04 g, 22 mmol) and KI (0.5 g), and the resulting mixture was stirred at 333 K for 5 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 colourless powder at room temperature for 48 h. Colourlesss single crystals

suitable for X-ray diffraction study were obtained by slow evaporation of an ethyl acetate solution over a period of one week.

Crystal data

$C_{20}H_{15}N_3O_2$
M_r = 329.35
Triclinic, $P\overline{1}$
a = 8.256 (3) Å
b = 10.017 (4) Å
c = 10.181 (4) Å
α = 85.629 (7)°
β = 85.187 (7)°
γ = 77.572 (8)°
V = 817.8 (5) Å^3
Z = 2
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Column, colourless
0.36 × 0.12 × 0.11 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.969, T_{max} = 0.990
4030 measured reflections
3047 independent reflections
1876 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.129
S = 0.98
3047 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0597P)^2 + 0.0383P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	2.27	2.711 (2)	111
N2—H2A···N3	0.86	2.24	2.654 (3)	110
C10—H10A···O2^{i}	0.97	2.50	3.466 (3)	173
C20—H20A···O2	0.93	2.32	2.903 (3)	121
C4—H4A···$Cg2^{ii}$	0.93	2.89	3.780 (2)	160
C6—H6A···$Cg4^{ii}$	0.93	2.70	3.611 (1)	169
C16—H16A···$Cg3^{iii}$	0.93	2.63	3.549 (2)	169

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x, y-1, z$; (iii) $-x+1, -y+2, -z+2$. $Cg1$, $Cg2$, $Cg3$ and $Cg4$ denote the centroids of the N1/C1–C5, N3/C13–C17, C1/C5–C9 and C12/C13/C17–C20 rings, respectively

All H atoms were located in difference Fourier maps and constrained to ride on their parent atoms, with C—H = 0.93–0.97 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: *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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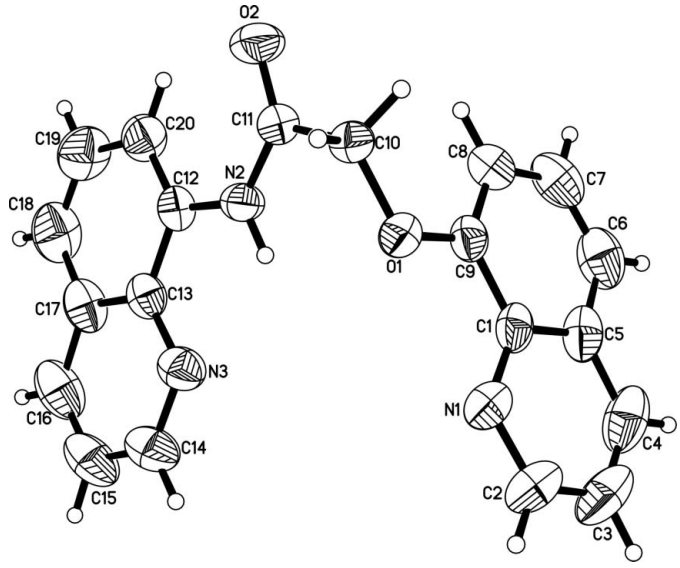

Figure 1
The molecular structure of the compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

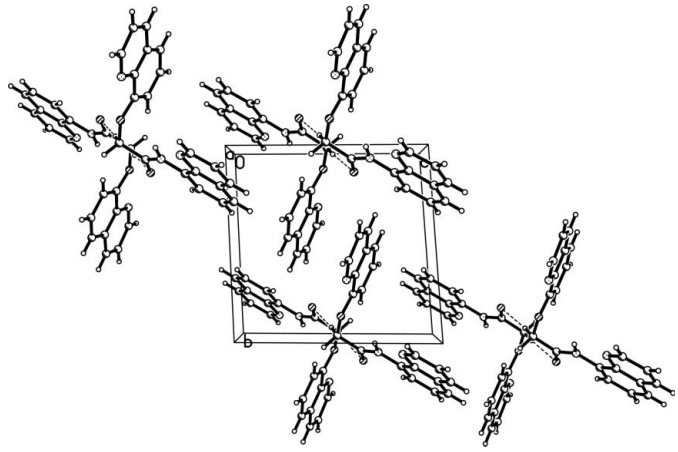

Figure 2
Packing diagram of (I), viewed down the *a* axis, showing the intermolecular hydrogen bonds (dashed lines).

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