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N-(4-Ethoxyphenyl)-2-(quinolin-8-yloxy)-acetamide monohydrate

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Molecules of the title compound, $C_{19}H_{18}N_2O_3\cdot H_2O$, form inversion-related dimers through C—H···O hydrogen bonds. The crystal packing is further stabilized by intermolecular N—H···O and C—H···O hydrogen bonds involving the solvent water molecule, and by C—H···π interactions.

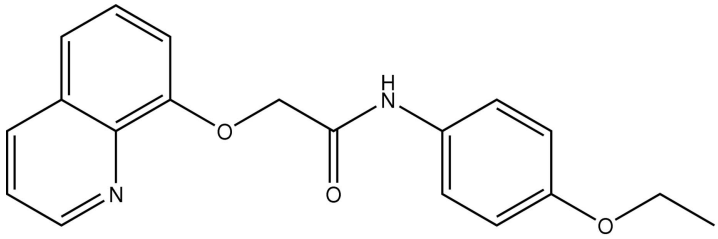
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.135
Data-to-parameter ratio = 14.5

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

Comment

We report here the synthesis and structure of the title compound, (I) (Fig. 1), as part of our studies on amide compounds.



$\cdot H_2O$

(I)

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those in the related compound, *N*-(4-methoxyphenyl)-2-(quinolin-8-yloxy)-acetamide monohydrate, (II) (Wen *et al.*, 2005). The non-H atoms in (I) show a nearly planar conformation, with a dihedral angle of 4.03 (1)° between the benzene ring and the quinoline moiety, while the corresponding value in (II) is 67.06 (7)°. There are two intramolecular hydrogen bonds, *viz*. N2—H26···O1 and C17—H17*A*···O2, forming five- and six-membered rings, respectively (Fig. 1), which contribute to the overall planarity of the molecule.

In the crystal structure, molecules are linked into inversion-related dimers by C7—H7*A*···O2 intermolecular hydrogen

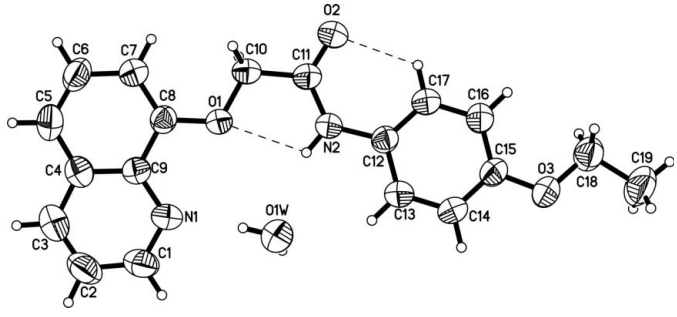


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Dashed lines indicate hydrogen bonds.

bonds (Table 1 and Fig. 2). The crystal packing is also stabilized by intermolecular N2—H2*A*···O1*W*, O1*W*—H2*W*1···N1 and C13—H13*A*···O1*W* hydrogen bonds, involving the solvent water molecule, and C—H···π interactions.

Experimental

The title compound was prepared according to the literature method of Wen *et al.* (2005). Colourless single crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether–ethyl acetate (1:3 *v*/*v*) solution over 5 d.

Crystal data

$C_{19}H_{18}N_2O_3\cdot H_2O$
M_r = 340.37
Monoclinic, $P2_1/c$
a = 14.603 (2) Å
b = 5.0837 (7) Å
c = 24.349 (3) Å
β = 107.143 (3)°
V = 1727.3 (4) Å^3
Z = 4
D_x = 1.309 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.37 × 0.12 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.993
9166 measured reflections
3396 independent reflections
1758 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.135
S = 0.99
3396 reflections
234 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···*Cg*2^{i}	0.97	2.82	3.524	130
O1*W*—H1*W*1···*Cg*3^{ii}	0.85 (3)	2.81	3.452	133
C18—H18*A*···*Cg*3^{i}	0.97	2.94	3.851	158
N2—H2*A*···O1	0.86	2.28	2.707 (3)	111
N2—H2*A*···O1*W*	0.86	2.18	2.997 (3)	159
O1*W*—H2*W*1···N1	0.86 (3)	1.90 (3)	2.752 (3)	172 (3)
C7—H7*A*···O2^{iii}	0.93	2.43	3.235 (3)	146
C13—H13*A*···O1*W*	0.93	2.37	3.177 (4)	145
C17—H17*A*···O2	0.93	2.23	2.842 (3)	122

Symmetry codes: (i) $x, y+1, z$; (ii) $x, y-1, z$; (iii) $-x, -y, -z$. *Cg*2 and *Cg*3 denote the centroids of the C4–C9 and C12–C17 rings, respectively.

All H atoms were located in difference Fourier maps. The water H atoms were refined isotropically with the O1*W*—H1*W*1 and O1*W*—H2*W*1 distances restrained to 0.85 (1) Å. The remaining H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 times U_{eq}(methyl C).

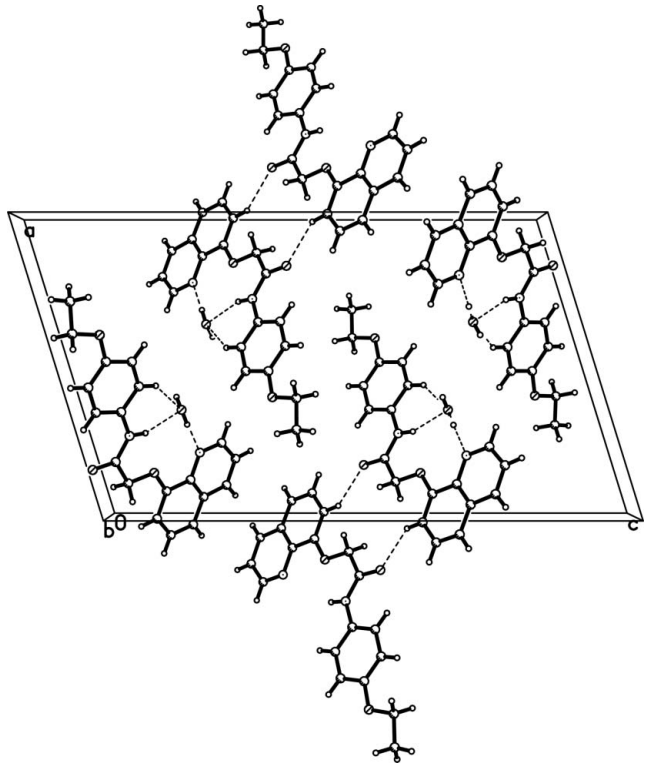


Figure 2
Packing diagram of (I), showing the intermolecular hydrogen bonds (dashed lines), viewed down the *b* axis,

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*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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