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Crystal structure of 2-(5-chloro-quinolin-8-yloxy)-*N*-quinolin-8-yl-acetamide, C₂₀H₁₄N₃O₂Cl

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.25 × 0.18 × 0.15 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.25 mm ⁻¹
Diffractometer, scan mode:	SMART, φ and ω
$\theta_{\max}$, completeness:	25.0°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	7607, 2970, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2305
$N(\text{param})_{\text{refined}}$:	235
Programs:	Bruker [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	1.37482(3)	0.59180(7)	1.02415(5)	0.0847(2)
O1	0.99629(7)	0.35932(12)	0.91121(9)	0.0522(3)
O2	0.85161(8)	0.02429(14)	0.87801(11)	0.0758(4)
N1	1.01771(9)	0.64942(15)	0.85088(10)	0.0512(3)
N2	0.82200(8)	0.28954(15)	0.83867(10)	0.0471(3)
H2A	0.8493	0.3822	0.8485	0.057*
N3	0.74690(10)	0.56434(16)	0.74687(11)	0.0564(4)
C1	1.02877(13)	0.7962(2)	0.82335(13)	0.0583(4)
H1B	0.9753	0.8562	0.7842	0.070*
C2	1.11432(14)	0.8680(2)	0.84840(14)	0.0621(5)
H2B	1.1176	0.9734	0.8272	0.075*
C3	1.19299(13)	0.7832(2)	0.90388(14)	0.0588(5)
H3B	1.2512	0.8296	0.9215	0.071*
C4	1.18649(11)	0.62391(19)	0.93503(12)	0.0472(4)
C5	1.26297(11)	0.5229(2)	0.99161(13)	0.0550(4)
C6	1.25081(12)	0.3734(2)	1.02066(14)	0.0599(5)
H6A	1.3027	0.3088	1.0582	0.072*
C7	1.16193(12)	0.3135(2)	0.99557(13)	0.0559(4)
H7A	1.1548	0.2102	1.0170	0.067*
C8	1.08570(10)	0.40544(18)	0.93997(12)	0.0444(4)
C9	1.09599(10)	0.56358(18)	0.90752(11)	0.0434(4)
C10	0.98043(11)	0.19559(18)	0.92655(13)	0.0491(4)
H10A	1.0076	0.1722	1.0002	0.059*
H10B	1.0101	0.1260	0.8955	0.059*
C11	0.87781(11)	0.16225(18)	0.87853(12)	0.0486(4)
C12	0.72521(11)	0.29172(19)	0.78317(12)	0.0472(4)
C13	0.66768(12)	0.1642(2)	0.77282(14)	0.0606(5)
H13A	0.6925	0.0659	0.8049	0.073*
C14	0.57134(13)	0.1811(3)	0.71406(17)	0.0747(6)
H14A	0.5327	0.0930	0.7073	0.090*
C15	0.53291(13)	0.3210(3)	0.66713(17)	0.0778(6)
H15A	0.4684	0.3288	0.6286	0.093*
C16	0.58979(12)	0.4558(2)	0.67592(14)	0.0625(5)

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Abstract

C₂₀H₁₄N₃O₂Cl, monoclinic, *P*₂/c (no. 14), *a* = 15.954(8) Å, *b* = 8.246(4) Å, *c* = 14.383(7) Å, β = 116.313(8)°, *V* = 1696.1(15) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0331, *wR*_{ref}(*F*²) = 0.0909, *T* = 296 K.

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The molecular structure is shown in the figure (hydrogen atoms are omitted for clarity). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

5-Chloro-8-hydroxyquinoline (1.79 g, 10 mmol) and anhydrous potassium carbonate (1.60 g, 11.6 mmol) were added to DMF (30 mL), then 2-chloro-*N*-quinolin-8-yl-acetamide (2.20 g, 10.0 mmol) and a small quantity of KI were added. The reaction mixture was stirred for 5 h at 100–110 °C. After cooling, 150 mL water was added and stirred for 2 h. The precipitate was collected by filtration and washed with water. Recrystallization from CH₃CN gave colorless block crystals.

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C17	0.55674(15)	0.6065(3)	0.62992(18)	0.0836(6)
H17A	0.4929	0.6222	0.5899	0.100*
C18	0.61644(17)	0.7285(3)	0.64318(19)	0.0873(7)
H18A	0.5944	0.8292	0.6131	0.105*
C19	0.71158(14)	0.7029(2)	0.70247(16)	0.0717(5)
H19A	0.7523	0.7886	0.7110	0.086*
C20	0.68685(11)	0.4417(2)	0.73451(12)	0.0493(4)

Experimental details

The structure was solved by direct methods and refined with the SHELX crystallographic software package [3]. The hydrogen atoms were placed at calculated positions and refined as riding atoms with isotropic displacement parameters.

Comment

The quinoline-based amide compounds have attracted much attention mainly due to their excellent coordination ability [4–7] and high selectivity to metal ions [8].

There is one title molecule in the asymmetric unit (see the Figure). In the title compound, all bond lengths are comparable with those observed in a similar compound [7]. This is also true for the parent compound [9] as well as for a related salt [10]. The dihedral angle between two quinoline ring moieties (N1/C1–C9, r.m.s. deviation 0.0142 Å; N3/C12–C20, r.m.s. deviation 0.0020 Å) is 7.8°. In the crystal structure, intramolecular N–H···O hydrogen bonds between amide N and phenolic O atoms are present.

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