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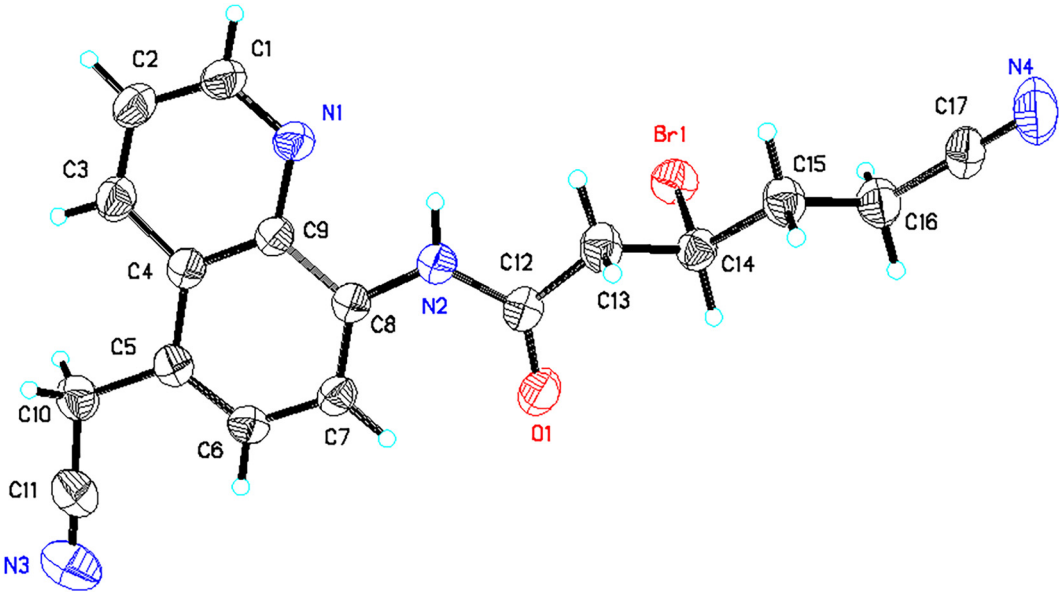
The crystal structure of 3-bromo-5-cyano–N-(5-(cyanomethyl)quinolin-8-yl)pentanamide, $C_{19}H_{15}BrN_4O$



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Abstract

$C_{18}H_{15}BrN_4O$, monoclinic, $C2/c$ (no. 15), a = 29.1892(14) Å, b = 5.3374(2) Å, c = 23.7466(10) Å, β = 116.732(1)°, V = 3304.2(2) Å^3, Z = 8, $R_{gt}(F)$ = 0.0355, $wR_{ref}(F^2)$ = 0.0954, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains the crystallographic data and the list of the atoms including atomic coordinates and displacement parameters can be found in the cif-file attached to this article.

Table 1: Data collection and handling.

Crystal:	Yellow prismatic
Size:	0.15 × 0.12 × 0.08 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.50 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω scans
θ_{max}, completeness:	26.0°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	15,706, 3,240, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,480
$N(param)_{refined}$:	208
Programs:	Bruker,[1] Olex2,[2] SHELX.[3]

1 Source of materials

In a Schlenk tube N-(quinolin-8-yl)but-3-enamide (42.5 mg, 0.20 mmol), 2-bromoacetonitrile (72.0 mg, 0.60 mmol), Na_2CO_3 (21.2 mg, 0.20 mmol), fac–Ir(ppy)3 (6.5 mg, 0.01 mmol) and

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CH_3CN (3.0 mL) were stirred at 40 W blue LED under N_2 for 24 h. Purification by chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) afforded desired compound. Single crystals suitable for X-ray diffraction were obtained by crystallization of the title compound from a mixture of dichloromethane (10 mL) and petroleum ether (2 mL).

2 Experimental details

Using Olex2,[2] the structure was solved with the Shelxt[3] structure solution program using Intrinsic Phasing and refined with the Olex2. refine[4] refinement package using Gauss–Newton minimisation.

3 Comment

Quinoline is considered one of the most privileged scaffolds due to its presence in many natural products, drugs, pesticides and dyes.[5–8] In the crystal structure, there are two cyano groups with almost identical bond lengths. Specifically, the bond length of C(11)–N(3) is 1.136(5) Å, and the bond length of C(17)–N(4) is 1.128(4) Å. This is consistent with the values reported in the literature.[8,9] There is a carbonyl group with a bond length of 1.216(3) Å, which is similar to that reported.[10,11] There are intramolecular hydrogen bonds present in the structure. N(2)–H(2)···N(1) and C(7)–(7)···O(1). The length of H(2)–N(1) bond is 2.20 Å. The bond length of H(7)–O(1) is 2.33 Å. The bond angle of N(2)–(2)···N(1) is 110.6 Å, while the bond angle of C(7)–(7)···O(1) is 120.3 Å. The bond lengths and bond angles of these two hydrogen bonds are also quite similar.

The complete set of X-ray diffraction data for the title compound was deposited to the Cambridge Crystallographic Data Centre (CCDC entry no. 2432057).

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