The crystal structure of ethyl 3-(1-methyl-1H-indole-2-carbonyl)-2-phenylquinoline-4-carboxylate, C28H22N2O3

Abstract

C28H22N2O3, triclinic, P1 (no. 2), a = 9.7431(6) Å, b = 12.2795(6) Å, c = 12.6009(6) Å, α = 71.454(2)°, β = 68.694(2)°, γ = 72.563(2)°, V = 1,302.36(12) Å3, Z = 2, Rgt(F) = 0.0655, wRref(F2) = 0.1988, T = 293(2) K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

In a Schlenk tube ethyl-1H-indole-2-carboxylate (0.20 mmol, 37.8 mg), 2,2,6,6-tetramethylpiperidine-1-oxotetrafluoroborate (0.4 mmol, 49.0 mg), copper(II) chloride (0.2 mmol, 26.9 mg) and DMAc (2.0 mL) were stirred at room temperature in air. After 15 h, Cs2CO3 (0.2 mmol, 65.2 mg) and 1-(1-methyl-1H-indol-2-yl)-3-phenylprop-2-yn-1-one (0.2 mmol, 51.9 mg) were added. After the completion of the addition, the reaction mixture was allowed to react at 60 °C for 2 h in air. The residue was purified by chromatography on silica gel (PE:EA = 5:1) to afford the desired compound (yellow solid, 50.3 mg, 58 %). Single crystals were obtained by crystallization from a mixture of dichloromethane (10 mL) and petroleum ether (2 mL).

2 Experimental details

Using Olex2, the structure was solved with the SHELXT structure solution program and refined with the SHELXL refinement package.
3 Comment

Quinolines are an important class of heterocycles occurring in many natural products, biologically active compounds and functionalized materials.4–6 Therefore, the synthesis of various quinoline derivatives is an important synthetic target which has received extensive attention. This structure consists of a quinoline ring, an indole ring and a benzene ring. There is one ketone carbonyl and one ester carbonyl in this structure. The bond lengths of the two carbonyl groups are almost the same (1.223 Å and 1.198 Å). These values agree with literature values.7–9

The complete set of X-ray diffraction data for the title compound was deposited to the Cambridge Crystallographic Data Centre (CCDC entry no. 2351774).

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

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References


