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Ethyl 6-chloro-2-methyl-4-phenylquinoline-3-carboxylate

R. Subashini,^a F. Nawaz Khan,^a Suganya Mittal,^a
Venkatesha R. Hathwar^b and Seik Weng Ng^{c*}

^aChemistry Division, School of Science and Humanities, VIT University, Vellore 632 014, Tamil Nadu, India, ^bSolid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and ^cDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

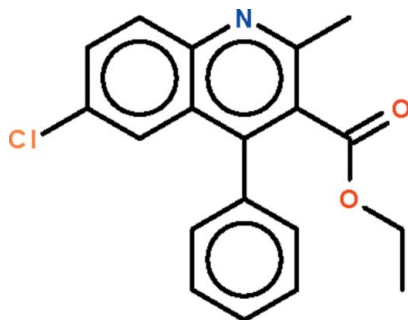
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Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.048; wR factor = 0.147; data-to-parameter ratio = 18.0.

In the title compound, $\text{C}_{19}\text{H}_{16}\text{ClNO}_2$, the quinoline ring system is planar (r.m.s. deviation = 0.008 Å). The phenyl group and the $-\text{CO}_2$ fragment of the ester unit form dihedral angles of 60.0 (1) and 60.5 (1)°, respectively, with the quinoline ring system.

Related literature

For related structures, see: Baumer *et al.* (2001); Subashini *et al.* (2009).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{16}\text{ClNO}_2$
 $M_r = 325.78$
 Triclinic, $P\bar{1}$
 $a = 8.3622$ (3) Å
 $b = 10.1971$ (3) Å
 $c = 10.7052$ (3) Å
 $\alpha = 110.440$ (2)°
 $\beta = 101.588$ (2)°
 $\gamma = 94.860$ (2)°
 $V = 825.91$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹
 $T = 290$ K
 $0.24 \times 0.18 \times 0.13$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.945$, $T_{\max} = 0.970$
 15008 measured reflections
 3775 independent reflections
 2854 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.147$
 $S = 1.04$
 3775 reflections
 210 parameters
 1 restraint
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.33$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2957).

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supporting information

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Ethyl 6-chloro-2-methyl-4-phenylquinoline-3-carboxylate

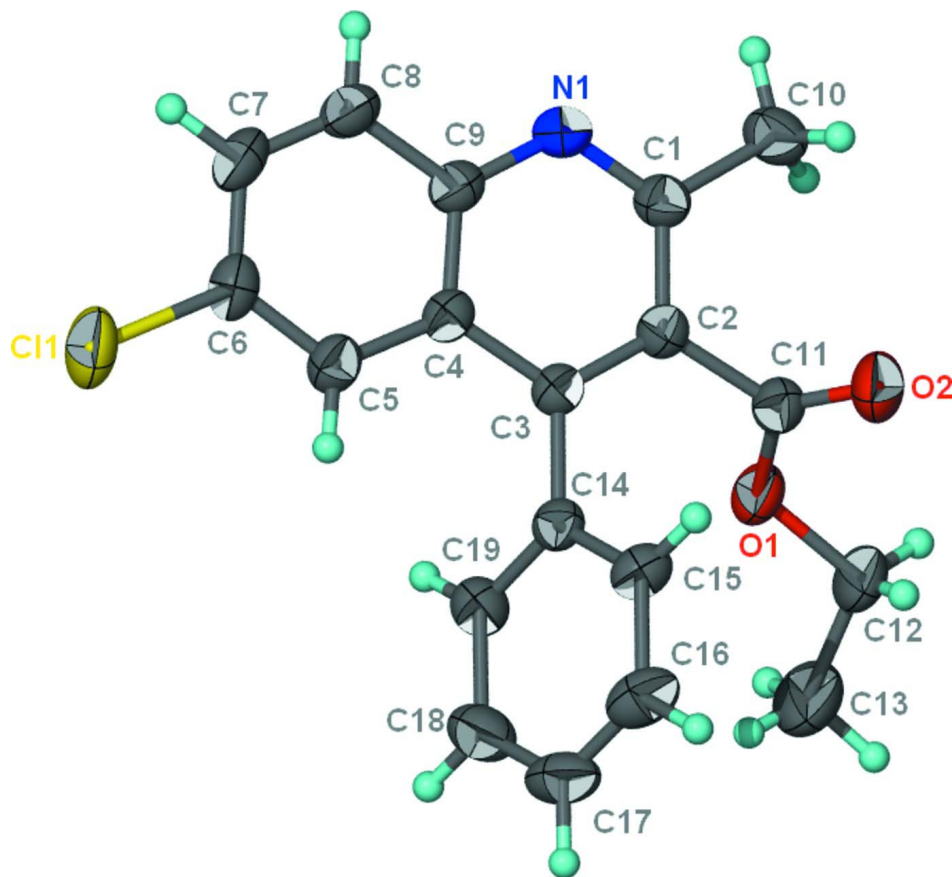
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S1. Experimental

2-Amino-5-chlorobenzophenone (0.5 mmol), ethyl acetoacete (0.6 mmol, 1.2 equiv.) and iodine (1 mol %) in ethanol (1 ml) were stirred until the reaction was completed, as indicated by TLC. The reaction was quenched with water (15 ml). The organic product was extracted with ethyl acetate. Evaporation of the solvent gave a solid that was recrystallized from DMSO.

S2. Refinement

C-bound H-atoms were placed in calculated positions (C-H = 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with $U_{iso}(\text{H})$ set to $1.2U_{eq}(\text{C})$. The C—C distance of the ethyl chain was tightly restrained to 1.500 (2) Å.

**Figure 1**

Displacement ellipsoid plot (Barbour, 2001) of $C_{19}H_{16}ClNO_2$ at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

Ethyl 6-chloro-2-methyl-4-phenylquinoline-3-carboxylate

Crystal data

$C_{19}H_{16}ClNO_2$

$M_r = 325.78$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.3622(3)\ \text{\AA}$

$b = 10.1971(3)\ \text{\AA}$

$c = 10.7052(3)\ \text{\AA}$

$\alpha = 110.440(2)^\circ$

$\beta = 101.588(2)^\circ$

$\gamma = 94.860(2)^\circ$

$V = 825.91(4)\ \text{\AA}^3$

$Z = 2$

$F(000) = 340$

$D_x = 1.310\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1153 reflections

$\theta = 1.7\text{--}24.3^\circ$

$\mu = 0.24\ \text{mm}^{-1}$

$T = 290\ \text{K}$

Block, colourless

$0.24 \times 0.18 \times 0.13\ \text{mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.945$, $T_{\max} = 0.970$

15008 measured reflections

3775 independent reflections

2854 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.025$
 $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.1^\circ$
 $h = -10 \rightarrow 10$

$k = -12 \rightarrow 13$
 $l = -13 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.048$
 $wR(F^2) = 0.147$
 $S = 1.04$
 3775 reflections
 210 parameters
 1 restraint
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.1903P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.33 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.38 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.59565 (8)	0.80991 (7)	0.87661 (5)	0.0711 (2)
N1	0.79494 (19)	0.38099 (15)	0.42954 (15)	0.0465 (4)
O1	0.93549 (17)	0.66715 (14)	0.21071 (12)	0.0523 (3)
O2	0.7449 (2)	0.48238 (16)	0.06011 (14)	0.0690 (4)
C1	0.8150 (2)	0.40465 (18)	0.31986 (18)	0.0433 (4)
C2	0.7883 (2)	0.53430 (18)	0.30236 (17)	0.0407 (4)
C3	0.7375 (2)	0.63972 (17)	0.40021 (16)	0.0387 (4)
C4	0.71546 (19)	0.61552 (17)	0.52007 (16)	0.0387 (4)
C5	0.6644 (2)	0.7151 (2)	0.62823 (17)	0.0451 (4)
H5	0.6412	0.8009	0.6230	0.054*
C6	0.6496 (2)	0.6845 (2)	0.74006 (17)	0.0481 (4)
C7	0.6778 (2)	0.5543 (2)	0.74986 (18)	0.0523 (5)
H7	0.6647	0.5352	0.8264	0.063*
C8	0.7245 (2)	0.4561 (2)	0.64596 (19)	0.0508 (4)
H8	0.7428	0.3696	0.6520	0.061*
C9	0.7459 (2)	0.48359 (18)	0.52871 (17)	0.0422 (4)
C10	0.8700 (3)	0.2882 (2)	0.2144 (2)	0.0569 (5)
H10A	0.8926	0.2145	0.2484	0.085*
H10B	0.9685	0.3259	0.1968	0.085*
H10C	0.7839	0.2500	0.1307	0.085*
C11	0.8176 (2)	0.55604 (19)	0.17664 (18)	0.0465 (4)
C12	0.9625 (4)	0.7067 (2)	0.0980 (2)	0.0733 (7)
H12A	0.8579	0.6918	0.0321	0.088*
H12B	1.0348	0.6487	0.0514	0.088*
C13	1.0409 (5)	0.8617 (3)	0.1562 (3)	0.1064 (11)
H13A	1.0569	0.8904	0.0826	0.160*
H13B	1.1459	0.8749	0.2191	0.160*
H13C	0.9696	0.9181	0.2038	0.160*
C14	0.7035 (2)	0.77328 (18)	0.38081 (17)	0.0408 (4)
C15	0.5843 (2)	0.7689 (2)	0.26713 (19)	0.0492 (4)
H15	0.5239	0.6823	0.2036	0.059*

C16	0.5557 (3)	0.8940 (2)	0.2488 (2)	0.0609 (5)
H16	0.4755	0.8908	0.1733	0.073*
C17	0.6458 (3)	1.0230 (2)	0.3421 (3)	0.0625 (6)
H17	0.6263	1.1064	0.3293	0.075*
C18	0.7641 (3)	1.0279 (2)	0.4538 (2)	0.0629 (5)
H18	0.8251	1.1147	0.5165	0.075*
C19	0.7927 (2)	0.9034 (2)	0.4729 (2)	0.0521 (4)
H19	0.8731	0.9075	0.5487	0.063*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0823 (4)	0.0947 (5)	0.0429 (3)	0.0315 (3)	0.0267 (2)	0.0238 (3)
N1	0.0520 (9)	0.0403 (8)	0.0503 (8)	0.0080 (6)	0.0129 (7)	0.0206 (7)
O1	0.0608 (8)	0.0592 (8)	0.0419 (6)	0.0060 (6)	0.0191 (6)	0.0223 (6)
O2	0.0949 (12)	0.0642 (9)	0.0385 (7)	0.0010 (8)	0.0144 (7)	0.0118 (6)
C1	0.0431 (9)	0.0404 (9)	0.0472 (9)	0.0068 (7)	0.0130 (7)	0.0163 (7)
C2	0.0416 (9)	0.0427 (9)	0.0395 (8)	0.0072 (7)	0.0117 (7)	0.0164 (7)
C3	0.0387 (8)	0.0410 (9)	0.0380 (8)	0.0071 (7)	0.0089 (6)	0.0170 (7)
C4	0.0372 (8)	0.0431 (9)	0.0374 (8)	0.0062 (7)	0.0080 (6)	0.0179 (7)
C5	0.0446 (9)	0.0547 (10)	0.0413 (8)	0.0146 (8)	0.0125 (7)	0.0221 (8)
C6	0.0439 (9)	0.0630 (11)	0.0366 (8)	0.0080 (8)	0.0109 (7)	0.0176 (8)
C7	0.0528 (10)	0.0662 (12)	0.0395 (9)	−0.0035 (9)	0.0069 (7)	0.0274 (9)
C8	0.0581 (11)	0.0494 (10)	0.0470 (9)	0.0005 (8)	0.0069 (8)	0.0260 (8)
C9	0.0418 (9)	0.0440 (9)	0.0422 (8)	0.0033 (7)	0.0077 (7)	0.0201 (7)
C10	0.0645 (12)	0.0455 (10)	0.0657 (12)	0.0169 (9)	0.0276 (10)	0.0186 (9)
C11	0.0557 (10)	0.0464 (10)	0.0422 (9)	0.0155 (8)	0.0176 (8)	0.0177 (8)
C12	0.113 (2)	0.0663 (14)	0.0491 (11)	0.0044 (13)	0.0366 (12)	0.0246 (10)
C13	0.165 (3)	0.086 (2)	0.0744 (17)	−0.011 (2)	0.0446 (19)	0.0358 (15)
C14	0.0453 (9)	0.0429 (9)	0.0410 (8)	0.0124 (7)	0.0171 (7)	0.0192 (7)
C15	0.0503 (10)	0.0527 (10)	0.0515 (10)	0.0093 (8)	0.0119 (8)	0.0280 (8)
C16	0.0559 (11)	0.0731 (14)	0.0729 (13)	0.0208 (10)	0.0185 (10)	0.0469 (12)
C17	0.0709 (13)	0.0522 (12)	0.0866 (15)	0.0251 (10)	0.0355 (12)	0.0407 (11)
C18	0.0757 (14)	0.0423 (10)	0.0725 (13)	0.0136 (10)	0.0271 (11)	0.0180 (10)
C19	0.0583 (11)	0.0474 (10)	0.0488 (10)	0.0107 (8)	0.0128 (8)	0.0158 (8)

Geometric parameters (Å, °)

C11—C6	1.7414 (19)	C10—H10A	0.96
N1—C1	1.317 (2)	C10—H10B	0.96
N1—C9	1.364 (2)	C10—H10C	0.96
O1—C11	1.329 (2)	C12—C13	1.513 (2)
O1—C12	1.450 (2)	C12—H12A	0.97
O2—C11	1.206 (2)	C12—H12B	0.97
C1—C2	1.428 (2)	C13—H13A	0.96
C1—C10	1.503 (3)	C13—H13B	0.96
C2—C3	1.380 (2)	C13—H13C	0.96
C2—C11	1.501 (2)	C14—C19	1.383 (3)

C3—C4	1.432 (2)	C14—C15	1.394 (2)
C3—C14	1.489 (2)	C15—C16	1.389 (3)
C4—C5	1.416 (2)	C15—H15	0.93
C4—C9	1.421 (2)	C16—C17	1.381 (3)
C5—C6	1.364 (2)	C16—H16	0.93
C5—H5	0.93	C17—C18	1.373 (3)
C6—C7	1.404 (3)	C17—H17	0.93
C7—C8	1.362 (3)	C18—C19	1.387 (3)
C7—H7	0.93	C18—H18	0.93
C8—C9	1.419 (2)	C19—H19	0.93
C8—H8	0.93		
C1—N1—C9	118.67 (14)	H10B—C10—H10C	109.5
C11—O1—C12	115.60 (15)	O2—C11—O1	124.32 (17)
N1—C1—C2	122.09 (16)	O2—C11—C2	124.75 (18)
N1—C1—C10	116.33 (15)	O1—C11—C2	110.93 (14)
C2—C1—C10	121.57 (15)	O1—C12—C13	108.36 (17)
C3—C2—C1	120.68 (15)	O1—C12—H12A	110.0
C3—C2—C11	119.90 (15)	C13—C12—H12A	110.0
C1—C2—C11	119.42 (15)	O1—C12—H12B	110.0
C2—C3—C4	117.83 (14)	C13—C12—H12B	110.0
C2—C3—C14	121.20 (14)	H12A—C12—H12B	108.4
C4—C3—C14	120.96 (14)	C12—C13—H13A	109.5
C5—C4—C9	119.10 (15)	C12—C13—H13B	109.5
C5—C4—C3	123.49 (15)	H13A—C13—H13B	109.5
C9—C4—C3	117.41 (15)	C12—C13—H13C	109.5
C6—C5—C4	119.64 (16)	H13A—C13—H13C	109.5
C6—C5—H5	120.2	H13B—C13—H13C	109.5
C4—C5—H5	120.2	C19—C14—C15	118.78 (16)
C5—C6—C7	122.02 (17)	C19—C14—C3	120.68 (15)
C5—C6—C11	119.74 (15)	C15—C14—C3	120.52 (16)
C7—C6—C11	118.23 (13)	C16—C15—C14	120.00 (18)
C8—C7—C6	119.22 (16)	C16—C15—H15	120.0
C8—C7—H7	120.4	C14—C15—H15	120.0
C6—C7—H7	120.4	C17—C16—C15	120.37 (19)
C7—C8—C9	121.19 (17)	C17—C16—H16	119.8
C7—C8—H8	119.4	C15—C16—H16	119.8
C9—C8—H8	119.4	C18—C17—C16	119.94 (18)
N1—C9—C8	117.90 (15)	C18—C17—H17	120.0
N1—C9—C4	123.31 (15)	C16—C17—H17	120.0
C8—C9—C4	118.79 (16)	C17—C18—C19	119.9 (2)
C1—C10—H10A	109.5	C17—C18—H18	120.0
C1—C10—H10B	109.5	C19—C18—H18	120.0
H10A—C10—H10B	109.5	C14—C19—C18	120.97 (19)
C1—C10—H10C	109.5	C14—C19—H19	119.5
H10A—C10—H10C	109.5	C18—C19—H19	119.5
C9—N1—C1—C2	0.5 (3)	C7—C8—C9—C4	-0.8 (3)

C9—N1—C1—C10	179.69 (16)	C5—C4—C9—N1	179.81 (15)
N1—C1—C2—C3	-1.0 (3)	C3—C4—C9—N1	0.2 (2)
C10—C1—C2—C3	179.86 (16)	C5—C4—C9—C8	-0.2 (2)
N1—C1—C2—C11	178.43 (16)	C3—C4—C9—C8	-179.76 (15)
C10—C1—C2—C11	-0.7 (3)	C12—O1—C11—O2	6.4 (3)
C1—C2—C3—C4	1.1 (2)	C12—O1—C11—C2	-174.03 (17)
C11—C2—C3—C4	-178.39 (15)	C3—C2—C11—O2	-119.9 (2)
C1—C2—C3—C14	-177.78 (15)	C1—C2—C11—O2	60.7 (3)
C11—C2—C3—C14	2.8 (2)	C3—C2—C11—O1	60.5 (2)
C2—C3—C4—C5	179.76 (15)	C1—C2—C11—O1	-118.93 (17)
C14—C3—C4—C5	-1.4 (2)	C11—O1—C12—C13	156.4 (2)
C2—C3—C4—C9	-0.7 (2)	C2—C3—C14—C19	-119.39 (19)
C14—C3—C4—C9	178.17 (15)	C4—C3—C14—C19	61.8 (2)
C9—C4—C5—C6	1.7 (3)	C2—C3—C14—C15	58.7 (2)
C3—C4—C5—C6	-178.74 (16)	C4—C3—C14—C15	-120.12 (18)
C4—C5—C6—C7	-2.3 (3)	C19—C14—C15—C16	-0.7 (3)
C4—C5—C6—C11	177.19 (13)	C3—C14—C15—C16	-178.83 (17)
C5—C6—C7—C8	1.3 (3)	C14—C15—C16—C17	0.5 (3)
C11—C6—C7—C8	-178.20 (14)	C15—C16—C17—C18	-0.1 (3)
C6—C7—C8—C9	0.3 (3)	C16—C17—C18—C19	-0.2 (3)
C1—N1—C9—C8	179.84 (16)	C15—C14—C19—C18	0.5 (3)
C1—N1—C9—C4	-0.1 (3)	C3—C14—C19—C18	178.57 (18)
C7—C8—C9—N1	179.20 (17)	C17—C18—C19—C14	0.0 (3)
