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

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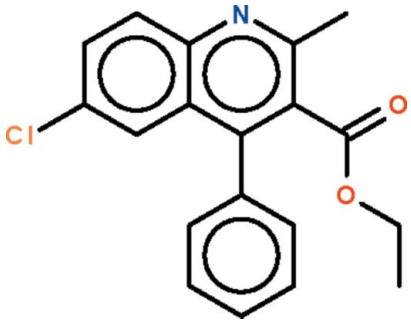
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.147; data-to-parameter ratio = 18.0.

In the title compound, $C_{19}H_{16}ClNO_2$, the quinoline ring system is planar (r.m.s. deviation = 0.008 Å). The phenyl group and the $-CO_2$ 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

$C_{19}H_{16}ClNO_2$
M_r = 325.78
Triclinic, $P\overline{1}$
a = 8.3622 (3) Å
b = 10.1971 (3) Å
c = 10.7052 (3) Å
α = 110.440 (2)°
β = 101.588 (2)°
γ = 94.860 (2)°
V = 825.91 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 290 K
0.24 × 0.18 × 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_{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
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −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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supplementary materials

Acta Cryst. (2009). E**65**, o2986 [**doi:10.1107/S160053680904536X**]

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

R. Subashini, F. N. Khan, S. Mittal, V. R. Hathwar and S. W. Ng

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.

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}(H) set to 1.2U_{eq}(C). The C—C distance of the ethyl chain was tightly restrained to 1.500 (2) Å.

Figures

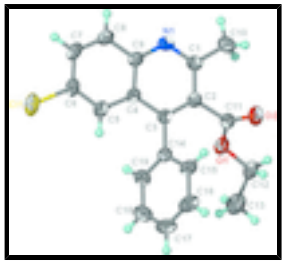


Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $C_{19}H_{16}ClNO_2$ at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

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

Crystal data

$C_{19}H_{16}ClNO_2$	$Z = 2$
$M_r = 325.78$	$F_{000} = 340$
Triclinic, $P\overline{1}$	$D_x = 1.310$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 8.3622$ (3) Å	Cell parameters from 1153 reflections
$b = 10.1971$ (3) Å	$\theta = 1.7$–24.3°
$c = 10.7052$ (3) Å	$\mu = 0.24$ mm^{-1}
$\alpha = 110.440$ (2)°	$T = 290$ K
$\beta = 101.588$ (2)°	Block, colourless
$\gamma = 94.860$ (2)°	0.24 × 0.18 × 0.13 mm
$V = 825.91$ (4) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3775 independent reflections
Radiation source: fine-focus sealed tube	2854 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 290$ K	$\theta_{max} = 27.5^o$
φ and ω scans	$\theta_{min} = 2.1^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.945$, $T_{max} = 0.970$	$k = -12 \rightarrow 13$
15008 measured reflections	$l = -13 \rightarrow 10$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.147$	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2 + 0.1903P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} = 0.001$
3775 reflections	$\Delta\rho_{max} = 0.33$ e Å^{-3}
210 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	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 (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	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)

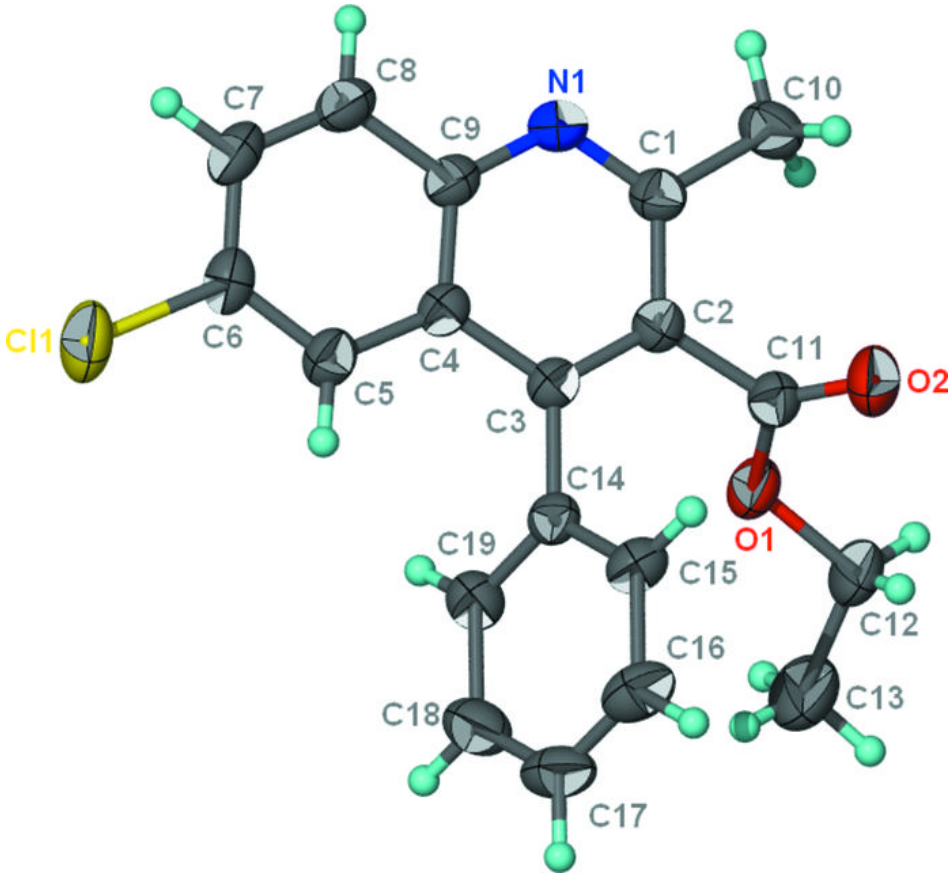
C18	0.0757 (14)	0.0423 (10)	0.0725 (13)	0.0136 (10)	0.0271 (11)	0.0180 (10)
C19	0.0583 (11)	0.0474 (10)	0.0488 (10)	0.0107 (8)	0.0128 (8)	0.0158 (8)

Geometric parameters (Å, °)

Cl1—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—Cl1	119.74 (15)	C15—C14—C3	120.52 (16)
C7—C6—Cl1	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—Cl1	177.19 (13)	C3—C14—C15—C16	−178.83 (17)
C5—C6—C7—C8	1.3 (3)	C14—C15—C16—C17	0.5 (3)
Cl1—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)

Fig. 1


C8
N1
C10
C7
C9
C1
C2
Cl1
C6
C4
C11
O2
C5
C3
C14
O1
C19
C15
C12
C16
C13
C18
C17