Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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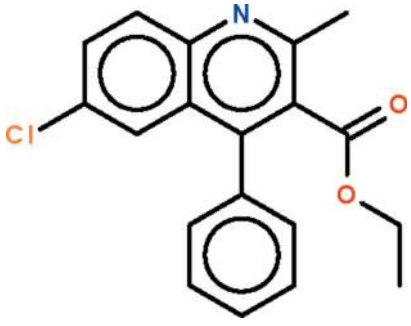
Received 27 October 2009; accepted 29 October 2009

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).

The authors thank the Department of Science and Technology, India, for use of the diffraction facility set up under the IRHPA–DST programme at IISc. FNK thanks the DST for Fast Track Proposal funding. The authors also thank VIT University and the University of Malaya for supporting this study.

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

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Baumer, V. N., Shishkin, O. V., Ukrainets, I. V., Taran, S. G. & Amin, J. N. (2001). *Acta Cryst.* E**57**, o254–o255.
Bruker (2004). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Subashini, R., Hathwar, V. R., Manivel, P., Prabakaran, K. & Khan, F. N. (2009). *Acta Cryst.* E**65**, o370.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

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

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

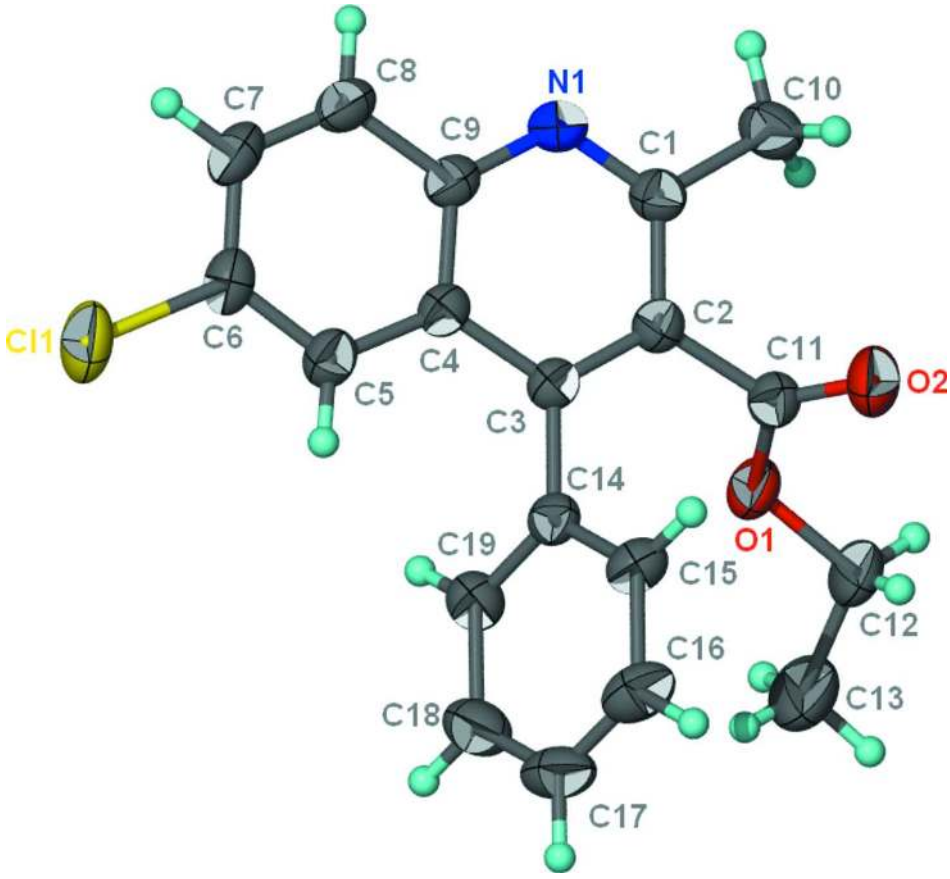

Figure 1

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.

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Crystal data

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$M_r = 325.78$
Triclinic, $P\overline{1}$
Hall symbol: -P 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) Å^3
$Z = 2$
$F(000) = 340$
$D_x = 1.310$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1153 reflections
$\theta = 1.7$–24.3°
$\mu = 0.24$ mm^{-1}
$T = 290$ K
Block, colourless
0.24 × 0.18 × 0.13 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_{int} = 0.025
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −10→10
k = −12→13
l = −13→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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	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 (Å²)

	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, º)

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)