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1-Phenyl-2-trifluoromethyl-4-quinolone

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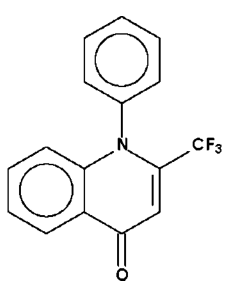
Key indicators: single-crystal X-ray study; *T* = 295 K; mean σ(C–C) = 0.003 Å; *R* factor = 0.041; *wR* factor = 0.147; data-to-parameter ratio = 15.5.

In the title molecule, $C_{16}H_{10}F_3NO$, the N-bound phenyl ring is oriented nearly orthogonal to the quinolinyl ring in order to avoid steric clashes with the trifluoromethyl substituent [dihedral angle 89.7 (1)°].

Related literature

For synthesis, see: Sosnovskikh *et al.* (2005); Usachev & Sosnovskikh (2004).



Experimental

Crystal data

$C_{16}H_{10}F_3NO$
M_r = 289.25
Monoclinic, $P2_1/c$
a = 8.7403 (5) Å
b = 17.574 (1) Å
c = 8.7559 (6) Å
β = 103.931 (2)°
V = 1305.4 (1) Å^3
Z = 4
Mo *K*α radiation
μ = 0.12 mm^{-1}
T = 295 (2) K
0.35 × 0.25 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.843, T_{max} = 0.982
20310 measured reflections
2970 independent reflections
1882 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.147
S = 1.14
2970 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2227).

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S1. Comment

Compound (I) was isolated during an attempted reaction of the corresponding thione with $CuCl_2$ in THF solution, see Experimental. The N-bound aromatic ring in (I) occupies a position orthogonal to the quinolinyl ring so as to avoid steric clashes with the adjacent CF_3 group, Fig. 1.

S2. Experimental

The synthesis of (I) has been described by Usachev & Sosnovskikh (2004); also see Sosnovskikh *et al.* (2005). In the present study, (I) was obtained as a side-product when the thione was recrystallized from THF in the presence of copper(II) chloride.

S3. Refinement

Carbon-bound H atoms were included in the refinement in the riding-model approximation with C—H = 0.93 Å, and with U_{iso}(H) 1.2U_{eq}(C).

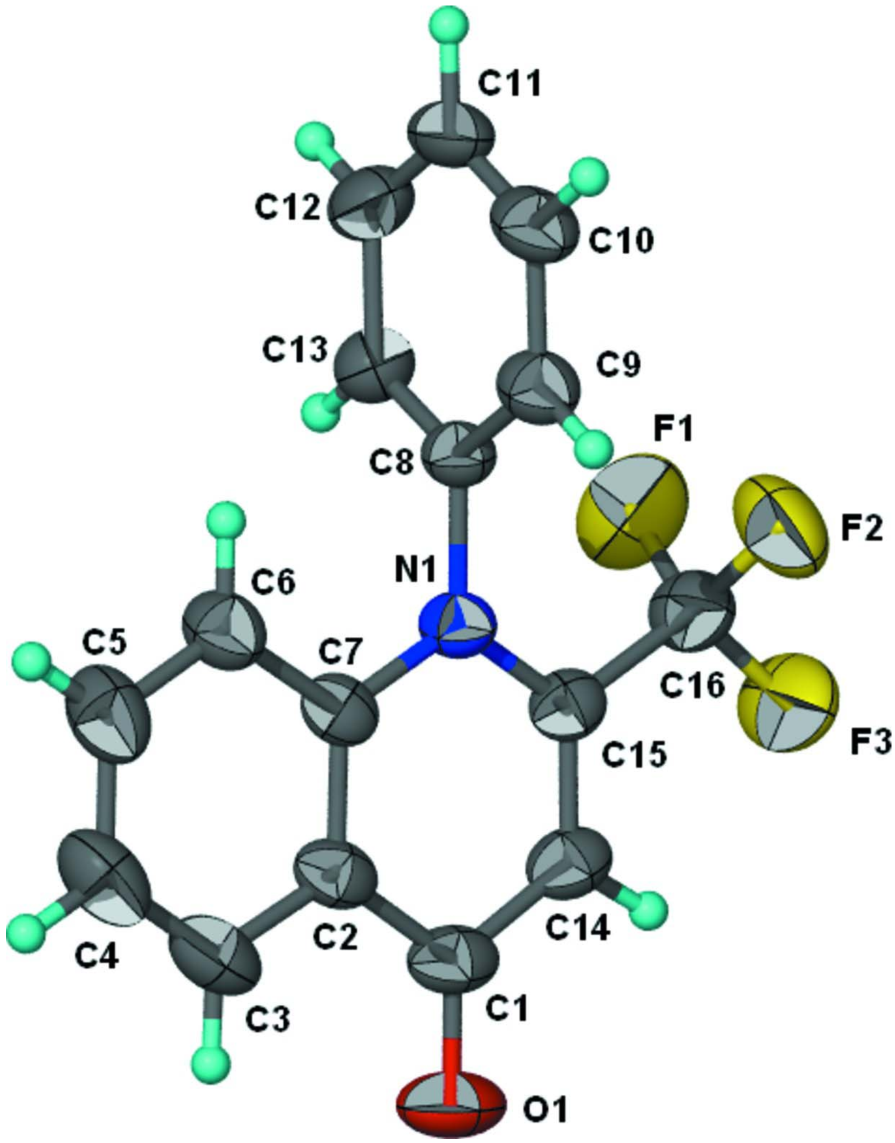

Figure 1

Molecular structure of (I) showing displacement ellipsoids at the 50% probability level and H atoms as spheres of arbitrary radius.

1-Phenyl-2-trifluoromethyl-4-quinolone

Crystal data

$C_{16}H_{10}F_3NO$
$M_r = 289.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.7403$ (5) Å
$b = 17.574$ (1) Å
$c = 8.7559$ (6) Å
$\beta = 103.931$ (2)°
$V = 1305.4$ (1) Å^3
$Z = 4$
$F(000) = 592$
$D_x = 1.472$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 12413 reflections
$\theta = 3.2$–27.5°
$\mu = 0.12$ mm^{-1}
$T = 295$ K
Prism, yellow
0.35 × 0.25 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.843, T_{max} = 0.982
20310 measured reflections
2970 independent reflections
1882 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 27.4°, θ_{min} = 3.2°
$h = -11 \rightarrow 10$
$k = -22 \rightarrow 22$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.147$
$S = 1.14$
2970 reflections
191 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0722P)^2 + 0.1288P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.005 (3)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.43638 (17)	0.24350 (8)	0.2257 (2)	0.1064 (6)
F2	0.43881 (16)	0.34786 (9)	0.10584 (14)	0.0941 (5)
F3	0.65236 (14)	0.30060 (9)	0.23970 (17)	0.0969 (5)
O1	0.72788 (16)	0.43177 (9)	0.73522 (17)	0.0794 (5)
N1	0.33546 (14)	0.36764 (7)	0.39971 (15)	0.0456 (3)
C1	0.6081 (2)	0.41335 (10)	0.6337 (2)	0.0560 (5)
C2	0.4482 (2)	0.42888 (9)	0.65010 (19)	0.0496 (4)
C3	0.4245 (2)	0.46671 (12)	0.7840 (2)	0.0660 (5)
H3	0.5114	0.4821	0.8618	0.079*
C4	0.2772 (3)	0.48118 (13)	0.8018 (2)	0.0768 (6)
H4	0.2639	0.5067	0.8907	0.092*
C5	0.1465 (3)	0.45791 (13)	0.6873 (2)	0.0721 (6)
H5	0.0458	0.4676	0.7004	0.086*
C6	0.1646 (2)	0.42053 (11)	0.5544 (2)	0.0590 (5)
H6	0.0764	0.4051	0.4781	0.071*
C7	0.31618 (19)	0.40578 (9)	0.53450 (18)	0.0461 (4)
C8	0.19504 (17)	0.34533 (9)	0.28127 (19)	0.0460 (4)
C9	0.1299 (2)	0.39618 (11)	0.1639 (2)	0.0557 (4)
H9	0.1768	0.4433	0.1582	0.067*
C10	−0.0070 (2)	0.37585 (13)	0.0544 (2)	0.0655 (5)
H10	−0.0520	0.4092	−0.0264	0.079*
C11	−0.0764 (2)	0.30637 (14)	0.0650 (2)	0.0701 (6)
H11	−0.1682	0.2931	−0.0086	0.084*

C12	−0.0110 (2)	0.25642 (13)	0.1837 (3)	0.0691 (6)
H12	−0.0589	0.2097	0.1904	0.083*
C13	0.1267 (2)	0.27569 (11)	0.2936 (2)	0.0575 (5)
H13	0.1719	0.2422	0.3741	0.069*
C14	0.61571 (19)	0.37504 (10)	0.4918 (2)	0.0547 (4)
H14	0.7140	0.3646	0.4733	0.066*
C15	0.48470 (18)	0.35353 (9)	0.3836 (2)	0.0472 (4)
C16	0.5026 (2)	0.31135 (12)	0.2388 (2)	0.0626 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1113 (11)	0.0740 (9)	0.1504 (14)	−0.0158 (7)	0.0641 (10)	−0.0509 (9)
F2	0.0938 (10)	0.1323 (13)	0.0570 (8)	0.0227 (8)	0.0197 (7)	−0.0097 (7)
F3	0.0547 (7)	0.1408 (13)	0.1002 (10)	0.0159 (7)	0.0283 (6)	−0.0278 (9)
O1	0.0612 (8)	0.0894 (10)	0.0712 (10)	−0.0143 (7)	−0.0163 (7)	−0.0032 (8)
N1	0.0397 (7)	0.0496 (7)	0.0446 (8)	0.0023 (5)	0.0043 (5)	−0.0038 (6)
C1	0.0524 (10)	0.0504 (9)	0.0553 (10)	−0.0051 (7)	−0.0062 (8)	0.0093 (8)
C2	0.0587 (10)	0.0425 (8)	0.0412 (8)	−0.0009 (7)	−0.0004 (7)	0.0039 (7)
C3	0.0828 (14)	0.0647 (12)	0.0432 (10)	−0.0016 (9)	0.0010 (9)	−0.0027 (9)
C4	0.1019 (16)	0.0793 (14)	0.0482 (11)	0.0114 (12)	0.0165 (11)	−0.0099 (10)
C5	0.0777 (13)	0.0850 (14)	0.0563 (12)	0.0204 (11)	0.0217 (10)	−0.0009 (10)
C6	0.0551 (10)	0.0703 (12)	0.0495 (10)	0.0102 (8)	0.0088 (8)	−0.0035 (9)
C7	0.0514 (9)	0.0436 (8)	0.0405 (8)	0.0058 (6)	0.0054 (7)	0.0028 (7)
C8	0.0382 (8)	0.0549 (9)	0.0427 (9)	0.0013 (6)	0.0056 (6)	−0.0053 (7)
C9	0.0509 (9)	0.0630 (11)	0.0500 (10)	0.0054 (7)	0.0057 (7)	−0.0019 (8)
C10	0.0516 (10)	0.0912 (15)	0.0481 (10)	0.0131 (10)	0.0013 (8)	−0.0037 (10)
C11	0.0439 (9)	0.1105 (18)	0.0526 (11)	−0.0076 (10)	0.0052 (8)	−0.0243 (11)
C12	0.0532 (10)	0.0841 (14)	0.0708 (13)	−0.0185 (9)	0.0163 (9)	−0.0180 (11)
C13	0.0509 (9)	0.0637 (11)	0.0569 (10)	−0.0061 (8)	0.0111 (8)	−0.0016 (8)
C14	0.0406 (9)	0.0570 (10)	0.0621 (11)	0.0011 (7)	0.0039 (7)	0.0049 (8)
C15	0.0428 (8)	0.0460 (9)	0.0510 (10)	0.0028 (6)	0.0081 (7)	0.0027 (7)
C16	0.0502 (10)	0.0700 (12)	0.0682 (12)	0.0045 (9)	0.0157 (8)	−0.0098 (10)

Geometric parameters (Å, º)

F1—C16	1.318 (2)	C6—C7	1.402 (2)
F2—C16	1.328 (2)	C6—H6	0.9300
F3—C16	1.321 (2)	C8—C9	1.377 (2)
O1—C1	1.2421 (19)	C8—C13	1.377 (2)
N1—C15	1.368 (2)	C9—C10	1.389 (2)
N1—C7	1.402 (2)	C9—H9	0.9300
N1—C8	1.4569 (19)	C10—C11	1.376 (3)
C1—C14	1.429 (3)	C10—H10	0.9300
C1—C2	1.464 (3)	C11—C12	1.375 (3)
C2—C7	1.400 (2)	C11—H11	0.9300
C2—C3	1.405 (3)	C12—C13	1.390 (3)
C3—C4	1.358 (3)	C12—H12	0.9300

C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.388 (3)	C14—C15	1.353 (2)
C4—H4	0.9300	C14—H14	0.9300
C5—C6	1.378 (3)	C15—C16	1.509 (3)
C5—H5	0.9300		

C15—N1—C7	118.97 (13)	C8—C9—C10	118.76 (19)
C15—N1—C8	122.58 (13)	C8—C9—H9	120.6
C7—N1—C8	118.45 (12)	C10—C9—H9	120.6
O1—C1—C14	122.49 (18)	C11—C10—C9	120.14 (19)
O1—C1—C2	122.78 (18)	C11—C10—H10	119.9
C14—C1—C2	114.73 (14)	C9—C10—H10	119.9
C7—C2—C3	118.62 (17)	C10—C11—C12	120.51 (17)
C7—C2—C1	121.02 (16)	C10—C11—H11	119.7
C3—C2—C1	120.36 (16)	C12—C11—H11	119.7
C4—C3—C2	121.24 (18)	C11—C12—C13	120.06 (19)
C4—C3—H3	119.4	C11—C12—H12	120.0
C2—C3—H3	119.4	C13—C12—H12	120.0
C3—C4—C5	120.03 (19)	C8—C13—C12	118.78 (18)
C3—C4—H4	120.0	C8—C13—H13	120.6
C5—C4—H4	120.0	C12—C13—H13	120.6
C6—C5—C4	120.56 (19)	C15—C14—C1	122.15 (16)
C6—C5—H5	119.7	C15—C14—H14	118.9
C4—C5—H5	119.7	C1—C14—H14	118.9
C5—C6—C7	119.82 (18)	C14—C15—N1	122.97 (16)
C5—C6—H6	120.1	C14—C15—C16	118.99 (15)
C7—C6—H6	120.1	N1—C15—C16	118.04 (14)
C2—C7—N1	120.14 (15)	F1—C16—F3	106.56 (16)
C2—C7—C6	119.74 (15)	F1—C16—F2	106.15 (17)
N1—C7—C6	120.13 (14)	F3—C16—F2	106.31 (17)
C9—C8—C13	121.74 (16)	F1—C16—C15	112.65 (16)
C9—C8—N1	118.85 (15)	F3—C16—C15	111.59 (15)
C13—C8—N1	119.34 (15)	F2—C16—C15	113.10 (16)

O1—C1—C2—C7	−178.65 (16)	C13—C8—C9—C10	−0.9 (3)
C14—C1—C2—C7	1.2 (2)	N1—C8—C9—C10	−177.78 (15)
O1—C1—C2—C3	0.6 (3)	C8—C9—C10—C11	0.7 (3)
C14—C1—C2—C3	−179.60 (16)	C9—C10—C11—C12	−0.1 (3)
C7—C2—C3—C4	−0.3 (3)	C10—C11—C12—C13	−0.4 (3)
C1—C2—C3—C4	−179.56 (19)	C9—C8—C13—C12	0.5 (3)
C2—C3—C4—C5	0.6 (3)	N1—C8—C13—C12	177.32 (16)
C3—C4—C5—C6	−0.5 (3)	C11—C12—C13—C8	0.2 (3)
C4—C5—C6—C7	0.1 (3)	O1—C1—C14—C15	178.37 (17)
C3—C2—C7—N1	−179.75 (15)	C2—C1—C14—C15	−1.4 (2)
C1—C2—C7—N1	−0.5 (2)	C1—C14—C15—N1	1.1 (3)
C3—C2—C7—C6	−0.1 (3)	C1—C14—C15—C16	−178.30 (16)
C1—C2—C7—C6	179.14 (15)	C7—N1—C15—C14	−0.3 (2)
C15—N1—C7—C2	0.0 (2)	C8—N1—C15—C14	178.98 (15)

C8—N1—C7—C2	−179.28 (14)	C7—N1—C15—C16	179.08 (15)
C15—N1—C7—C6	−179.62 (15)	C8—N1—C15—C16	−1.6 (2)
C8—N1—C7—C6	1.1 (2)	C14—C15—C16—F1	120.25 (19)
C5—C6—C7—C2	0.2 (3)	N1—C15—C16—F1	−59.1 (2)
C5—C6—C7—N1	179.87 (17)	C14—C15—C16—F3	0.4 (3)
C15—N1—C8—C9	−91.06 (19)	N1—C15—C16—F3	−178.97 (16)
C7—N1—C8—C9	88.22 (19)	C14—C15—C16—F2	−119.37 (18)
C15—N1—C8—C13	92.0 (2)	N1—C15—C16—F2	61.2 (2)
C7—N1—C8—C13	−88.73 (19)		