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4-Chloro-8-(trifluoromethyl)quinoline

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.105
Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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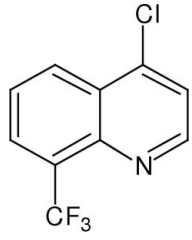
The title compound, $C_{10}H_5ClF_3N$, crystallizes with two almost identical molecules in the asymmetric unit. Geometric parameters are in the usual ranges. The crystal packing is characterized by C—H···N weak hydrogen bonds and π–π stacking interactions.

Comment

Quinolines have been interesting to researchers for many years because a large number of natural products contain these heterocycles. They are found in numerous commericial products, including pharmaceuticals, fragrances and dyes (Padwa *et al.*, 1999). Quinoline alkaloids such as quinine, chloroquin, mefloquine and amodiaquine are used as efficient drugs for the treatment of malaria (Robert & Meunier, 1998). Quinoline has been reported to have excellent antibiotic properties. Papaverine is an opium alkaloid, which is a non-specific smooth muscle relaxant and vasodilator (Gilchrist, 1997). In recent years, fluorinated compounds have been very important in the pharmaceutical field. Incorporation of an F atom instead of an H atom can alter the course of the reaction as well as biological activities. Introduction of further F atoms in a CF_3 group provides better lipophilicity and the compounds might be pharmacologically more interesting compared to their non-fluorinated analogues. Trifluoromethyl-substituted compounds have been reported to possess biological activities as herbicides (Bravo *et al.*, 1994), fungicides (Jung *et al.*, 2002) and inhibitors for platelet aggregation (Küçükgüzel *et al.*, 2000). Several quinoline derivatives have been evaluated *in vitro* against several parasites and HTLV-1 transformed cells (Franck *et al.*, 2004). 7-(Trifluoromethyl)-quinoline derivatives have been evaluated for *in vitro* activity against some parasites in blood (Abadi & Brun, 2003). Prompted by the varied biological activities, the crystal structure of the title compound, (I), is reported.



(I)

A perspective view of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November

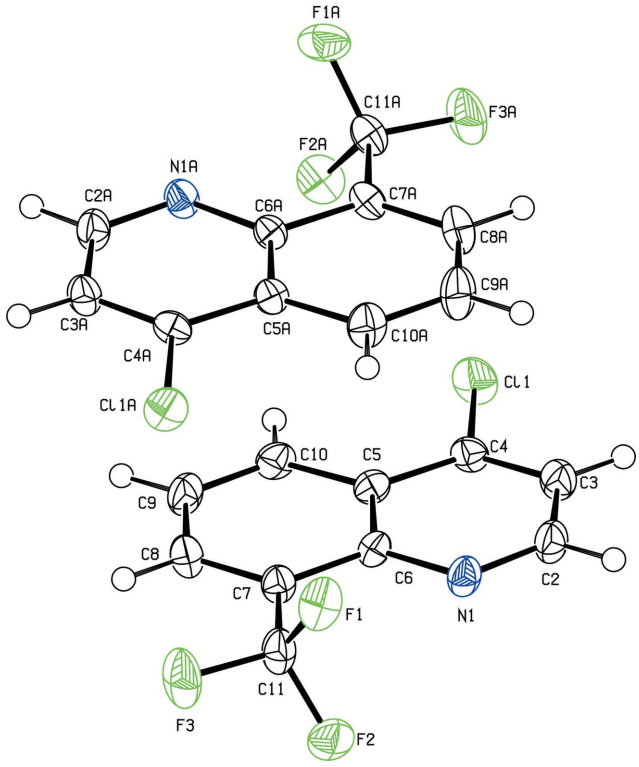


Figure 1
The asymmetric unit of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

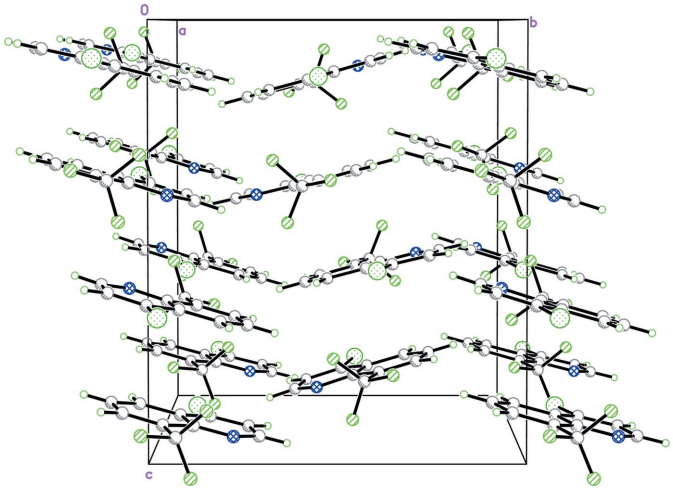


Figure 2
Packing diagram of the title compound, viewed perpendicular to the *bc* plane. H atoms have been omitted for clarity.

2005 update, August 2006; *MOGUL*, Version 1.1; Allen, 2002). The two molecules in the asymmetric unit are almost identical (r.m.s. deviation for all non-H atoms 0.022 Å). The crystal packing shows stacks of molecules (Fig. 2). The two symmetry-independent molecules are almost parallel [angle between the planes of the aromatic atoms = 2.33 (4)°]. The distances in a stack are (*Cg* = centre of gravity): *Cg*(C5–10)···*Cg*(N1*A*,C2*A*–C6*A*) 3.825 Å, *Cg*(N1*A*, C2*A*–C6*A*)···*Cg*^{i}(N1*A*, C2*A*–C6*A*) 3.610 Å [symmetry code: (i) $1-x, 1-y, 2-z$]. In addition to these π–π interactions, the molecules are linked by weak C—H···N hydrogen bonds (Table 1).

Experimental

The title compound was obtained as a gift sample from Strides Arco Laboratories, Mangalore, India. The sample was crystallized from a toluene–acetone (1:1) mixture by slow evaporation (m.p. 354–355 K).

Crystal data

$C_{10}H_5ClF_3N$
M_r = 231.60
Monoclinic, $P2_1/n$
a = 10.3179 (11) Å
b = 12.4319 (10) Å
c = 14.5673 (17) Å
β = 95.023 (9)°
V = 1861.4 (3) Å^3
Z = 8
D_x = 1.653 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 173 (2) K
Block, colourless
0.49 × 0.49 × 0.48 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.822, T_{max} = 0.825
11382 measured reflections
3486 independent reflections
2655 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.105
S = 1.06
3486 reflections
272 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.4196P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0089 (11)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3*A*—H3*A*···N1^{i}	0.95	2.61	3.546 (3)	168
C3—H3···N1*A*^{ii}	0.95	2.81	3.669 (3)	151

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

H atoms were found in a difference map, but they were repositioned geometrically and refined using a riding model, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 199); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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