

## 4-Chloro-8-(trifluoromethyl)quinoline

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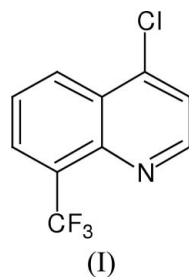
## Key indicators

Single-crystal X-ray study  
 $T = 173$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.037  
 $wR$  factor = 0.105  
Data-to-parameter ratio = 12.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound,  $\text{C}_{10}\text{H}_5\text{ClF}_3\text{N}$ , crystallizes with two almost identical molecules in the asymmetric unit. Geometric parameters are in the usual ranges. The crystal packing is characterized by  $\text{C}-\text{H}\cdots\text{N}$  weak hydrogen bonds and  $\pi-\pi$  stacking interactions.

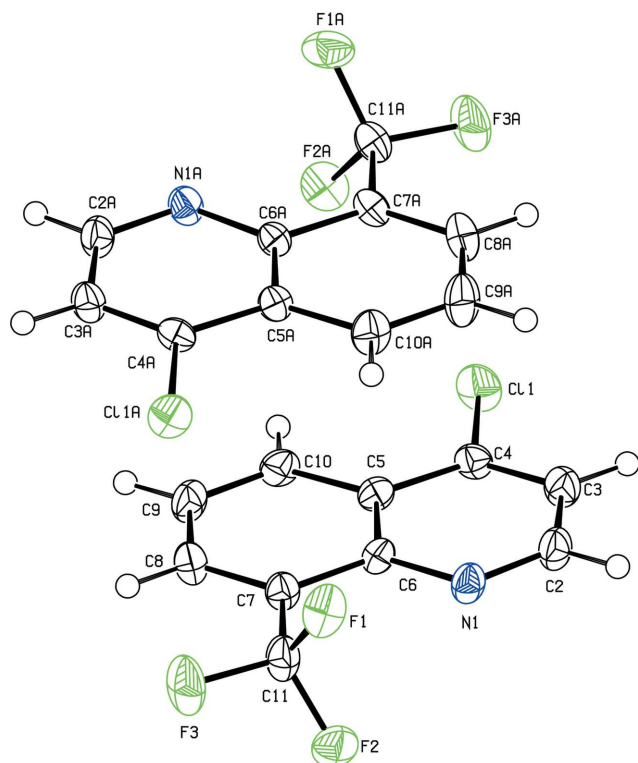
## Comment

Quinolines have been interesting to researchers for many years because a large number of natural products contain these heterocycles. They are found in numerous commercial 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  $\text{CF}_3$  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 (Küçüküzgel *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.

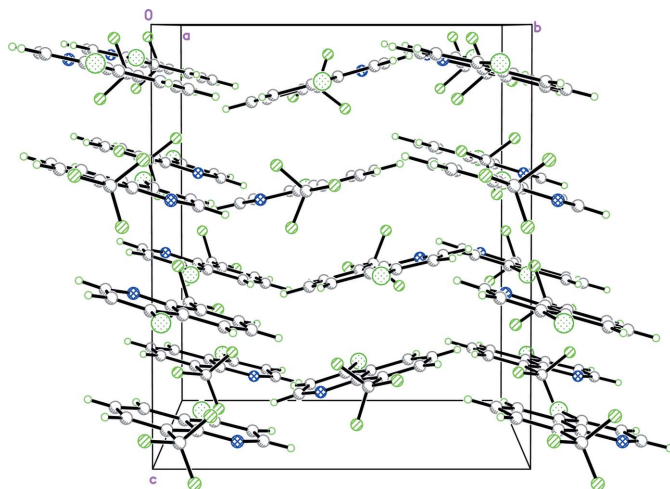


A perspective view of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November

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**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 (*C<sub>g</sub>* = centre of gravity): *C<sub>g</sub>*(C5–10)···*C<sub>g</sub>*(N1A, C2A–C6A) 3.825 Å, *C<sub>g</sub>*(N1A, C2A–C6A)···*C<sub>g</sub>*<sup>i</sup>(N1A, C2A–C6A) 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  
 $\beta = 95.023$  (9)°  
 $V = 1861.4$  (3) Å<sup>3</sup>

$Z = 8$   
 $D_x = 1.653$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.42$  mm<sup>-1</sup>  
 $T = 173$  (2) K  
 Block, colourless  
 0.49 × 0.49 × 0.48 mm

### Data collection

Stoe IPDS-II two-circle diffractometer  
 $\omega$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$   
 $\theta_{\max} = 25.6^\circ$

### 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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.0089 (11)

**Table 1**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C3A–H3A···N1 <sup>i</sup>	0.95	2.61	3.546 (3)	168
C3–H3···N1A <sup>ii</sup>	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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

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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