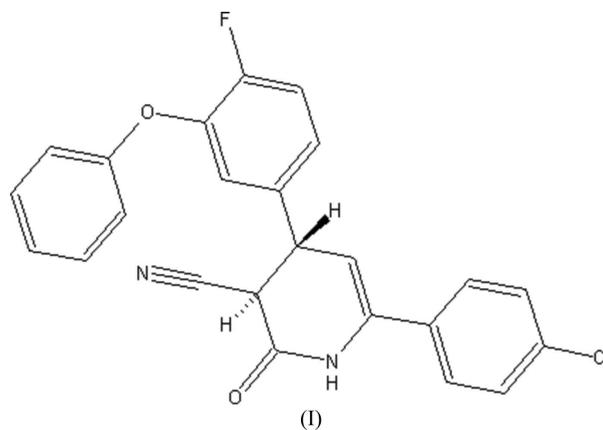


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## Key indicators

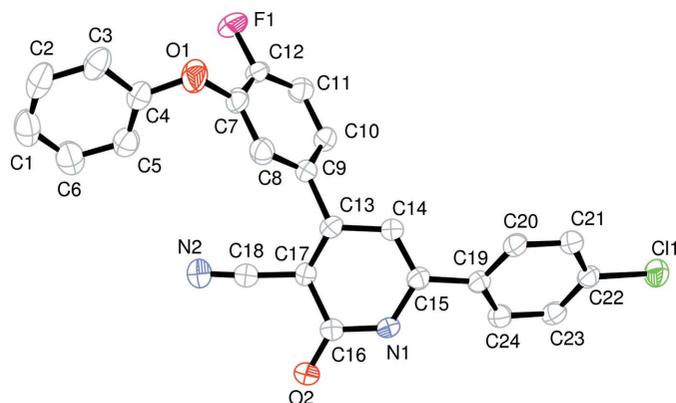
Single-crystal X-ray study  
*T* = 290 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$   
*R* factor = 0.053  
*wR* factor = 0.120  
Data-to-parameter ratio = 10.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.6-(4-Chlorophenyl)-4-(4-fluoro-3-phenoxy-  
phenyl)-2-oxo-1,2,3,4-tetrahydropyridine-  
3-carbonitrileThe crystal structure of the title compound,  $\text{C}_{24}\text{H}_{16}\text{ClFN}_2\text{O}_2$ , reveals a half-chair conformation of the central tetrahydropyridine (THP) ring. The supramolecular structure is stabilized by strong  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, weak intermolecular interactions involving the chloro and fluoro substituents and aromatic  $\pi-\pi$  interactions.Received 23 May 2006  
Accepted 25 May 2006

## Comment

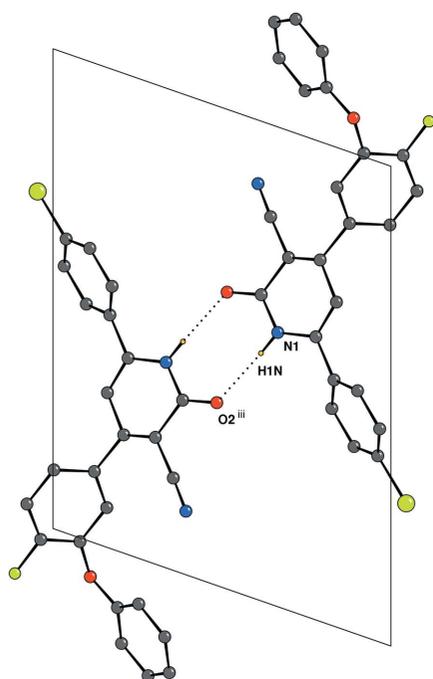
1,2,3,4-Tetrahydropyridine-3-carbonitrile derivatives with varying substituents on the THP ring have been synthesized (Wang, 2006; Patel *et al.*, 2002) and their agrochemical activity investigated (Mohan, 2006). The structure of the title THP derivative (I) is reported here (Fig. 1).The THP ring is almost planar, with atoms C17 and C13 deviating by only 0.193 (3) and  $-0.101$  (4)  $\text{\AA}$ , respectively, from the C14/C15/N1/C16 least-squares plane.A short  $\text{Cl}^{\text{iv}}\cdots\text{F}^{\text{iv}}$  intermolecular contact of 3.196 (2)  $\text{\AA}$  [symmetry code: (iv)  $x, y, z - 1$ ] is observed in the crystal structure and strong  $\text{N}^{\text{i}}-\text{H}^{\text{i}}\cdots\text{O}^{\text{iii}}$  hydrogen bonds form inversion-related dimers in the *ac* plane (Fig. 2 and Table 1). The structure is further stabilized by  $\text{C}-\text{H}\cdots\text{Cl}$  and  $\text{C}-\text{H}\cdots\text{F}$  interactions, forming molecular chains along the crystallographic *c* glide plane, and  $\pi-\pi$  interactions between the chlorophenyl rings [ $\text{Cg}^4\cdots\text{Cg}^{4^{\text{v}}}$  = 3.922 (3)  $\text{\AA}$ ;  $\text{Cg}^4$  is the centroid of the C19–C24 ring; symmetry code: (v)  $1 - x, -y, -z$ ] (Fig. 3).

## Experimental

Single crystals of (I) (Mohan, 2006) were grown by slow evaporation of an acetone solution at 275–277 K.



**Figure 1**  
A view of the title compound, shown with 50% probability displacement ellipsoids.



**Figure 2**  
The formation of a centrosymmetric dimer by N—H...O hydrogen bonds (dotted lines). Symmetry code as in Table 1.

#### Crystal data

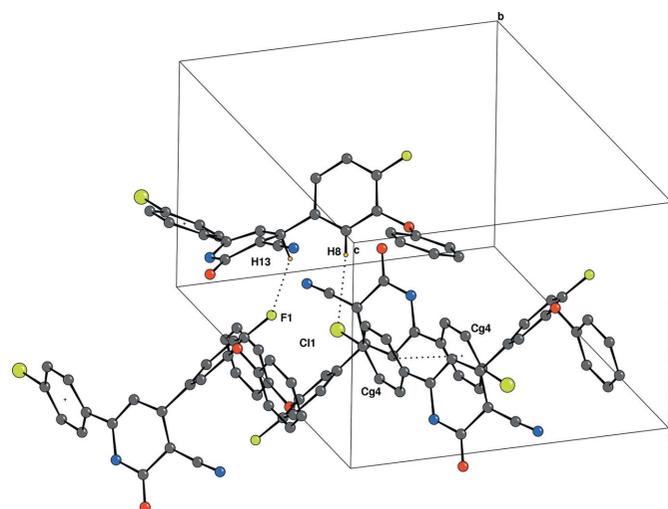
$C_{24}H_{16}ClFN_2O_2$   
 $M_r = 418.84$   
Monoclinic,  $P2_1/n$   
 $a = 11.316$  (6) Å  
 $b = 11.899$  (7) Å  
 $c = 15.109$  (8) Å  
 $\beta = 109.088$  (9)°  
 $V = 1922.6$  (18) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.447$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.23$  mm<sup>-1</sup>  
 $T = 290$  (2) K  
Block, colourless  
0.14 × 0.12 × 0.10 mm

#### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.928$ ,  $T_{\max} = 0.977$

14458 measured reflections  
3387 independent reflections  
3145 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.022$   
 $\theta_{\text{max}} = 26.4^\circ$



**Figure 3**  
The C—H...Cl, C—H...F and  $\pi$ — $\pi$  interactions in (I). Hydrogen bonds and the interactions between the C19—C24 ring centroids are shown as dotted lines.

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.053$   
 $wR(F^2) = 0.120$   
 $S = 1.22$   
3387 reflections  
335 parameters  
H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0267P)^2 + 1.6131P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\text{max}} = 0.001$$

$$\Delta\rho_{\text{max}} = 0.18 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\text{min}} = -0.20 \text{ e } \text{Å}^{-3}$$

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C8—H8...Cl1 <sup>i</sup>	0.93	2.80	3.701 (2)	163
C13—H13...F1 <sup>ii</sup>	0.98	2.48	3.274 (5)	138
N1—H1N...O2 <sup>iii</sup>	0.86 (3)	2.11 (3)	2.963 (4)	177

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

Amino atom H1N and H14 on the THP ring were located in a difference Fourier map and refined isotropically. All other H atoms were refined using a riding model, with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1999) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

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