

## 5-Benzyl-1-(4-fluorophenyl)-2-phenyl-4,5,6,7-tetrahydro-1H-pyrrolo[3,2-c]pyridine

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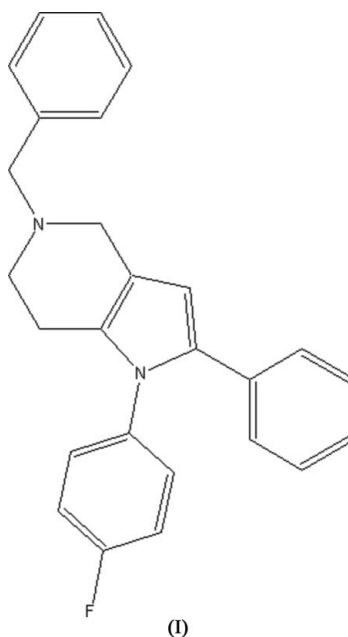
## Key indicators

Single-crystal X-ray study  
*T* = 290 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
*R* factor = 0.082  
*wR* factor = 0.137  
Data-to-parameter ratio = 11.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{26}\text{H}_{23}\text{FN}_2$ , the dihedral angle between the 4-fluorophenyl ring and the adjacent phenyl ring is  $62.3 (1)^\circ$ . The crystal structure is stabilized by  $\text{C}-\text{H}\cdots\pi$  interactions.

## Comment

Molecular organization and molecular interactions are the features that are responsible for molecules exhibiting different functional properties. An understanding of non-covalent interactions becomes essential for interpreting and predicting relationships between chemical structure and function (Hunter *et al.*, 2001). Crystal engineering *via* the manipulation of hydrogen bonding has attracted much attention in the recent literature (Aakeröy, 1997; Desiraju, 2000). Weak intermolecular forces of the type  $\text{C}-\text{H}\cdots\pi$  play an important role in various systems of biological and chemical interest (Nishio *et al.*, 2004). Intramolecular  $\text{C}-\text{H}\cdots\pi$  interactions are responsible for a molecule adopting a particular conformation in the solid state (Jennings *et al.*, 2001). 4-Keto-4,5,6,7-tetrahydroindoles have been tested for anti-implantation agents in rats and have been found to exhibit potent biological activity. Against this background, we have studied the crystal structure of the title compound (I).



A molecular view of (I), with the atom-labelling scheme, is shown in Fig. 1. Relevant bond distances and torsion angles are given in Table 1. Atom N1 deviates by  $0.604 (2) \text{ \AA}$  from

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the least-squares plane passing through atoms C5/C3/C4/C7/C6. The crystal structure is stabilized by C—H $\cdots\pi$  intermolecular interactions (Table 2), forming molecular dimers (Fig. 2).

## Experimental

The compound (I) was synthesized according to the procedure reported in the literature (Nagarajan *et al.*, 1985), and crystallized by slow evaporation of a chloroform/hexane (2:1 *v/v*) solution at 278 K.

### Crystal data

$C_{26}H_{23}FN_2$	$D_x = 1.264 \text{ Mg m}^{-3}$
$M_r = 382.46$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 650 reflections
$a = 13.220 (8) \text{ \AA}$	$\theta = 1.4\text{--}25.8^\circ$
$b = 18.431 (11) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 8.475 (5) \text{ \AA}$	$T = 290 (2) \text{ K}$
$\beta = 103.223 (11)^\circ$	Block, colourless
$V = 2010 (2) \text{ \AA}^3$	$0.25 \times 0.20 \times 0.15 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART APEX CCD area detector diffractometer	3975 independent reflections
$\varphi$ and $\omega$ scans	2935 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.043$
$T_{\text{min}} = 0.939$ , $T_{\text{max}} = 0.988$	$\theta_{\text{max}} = 26.4^\circ$
15238 measured reflections	$h = -16 \rightarrow 16$
	$k = -22 \rightarrow 22$
	$l = -10 \rightarrow 10$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0366P)^2 + 0.563P]$
$R[F^2 > 2\sigma(F^2)] = 0.082$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.137$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.23$	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
3975 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
354 parameters	
All H-atom parameters refined	

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

N2—C4	1.392 (3)	N1—C20	1.461 (3)
N2—C1	1.393 (3)	N1—C5	1.467 (3)
N2—C8	1.431 (3)	N1—C6	1.473 (3)
F1—C11	1.356 (3)		
C5—N1—C20—C26	60.4 (3)	C20—N1—C6—C7	169.2 (2)
C6—N1—C20—C26	−176.4 (3)	C5—N1—C6—C7	−67.5 (3)
C19—C14—C1—C2	−144.7 (3)		

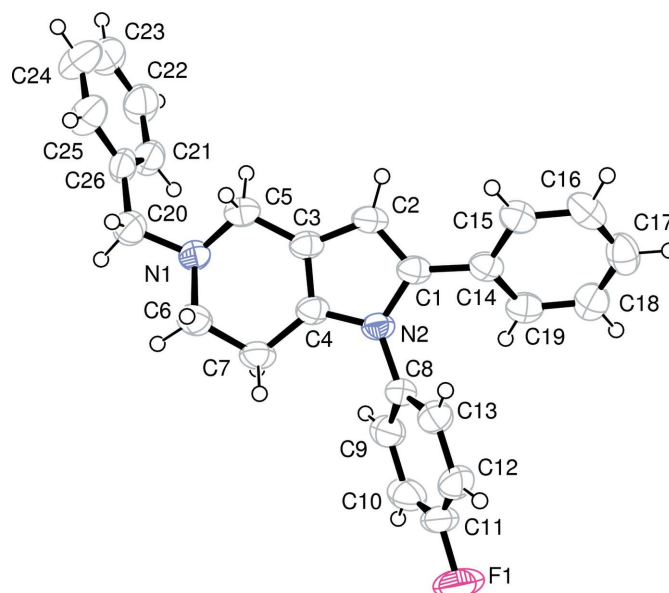
**Table 2**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
C9—H9 $\cdots$ Cg1 <sup>i</sup>	0.95 (3)	2.79 (3)	3.648 (4)	150 (2)

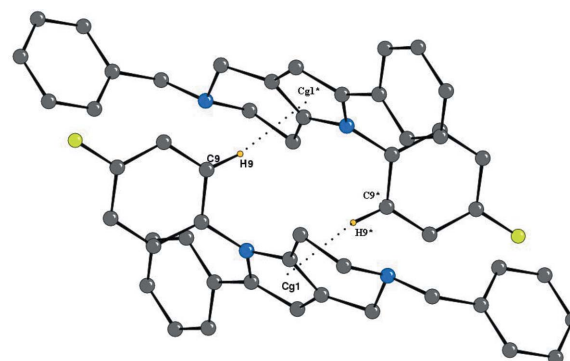
Symmetry code: (i)  $-x, -y + 1, -z + 1$ . Cg1 is the centroid of the five-membered ring C1—C4/N2.

All H atoms were located in difference Fourier maps and refined isotropically. The C—H bond distances are in the range 0.92 (3)  $\text{\AA}$  to 1.02 (2)  $\text{\AA}$ .



**Figure 1**

Molecular structure of (I), showing 50% probability displacement ellipsoids.



**Figure 2**

A molecular dimer. Dashed lines indicate C—H $\cdots\pi$  interactions. Atoms labelled with an asterisk (\*) are at the symmetry position ( $-x, 1 - y, 1 - z$ ).

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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