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

In the title compound, C_{27}H_{25}FN_{2}, the dihedral angle between the 4-fluorophenyl ring and the adjacent phenyl ring is 62.3\(^\circ\). The crystal structure is stabilized by C-H-\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 (Aakeroy, 1997; Desiraju, 2000). Weak intermolecular forces of the type C-H-\pi play an important role in various systems of biological and chemical interest (Nishio et al., 2004). Intramolecular C-H-\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-labeling scheme, is shown in Fig. 1. Relevant bond distances and torsion angles are given in Table 1. Atom N1 deviates by 0.604 (2) \AA from
the least-squares plane passing through atoms C5/C3/C4/C7/C6. The crystal structure is stabilized by C—H⋯π 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

\[ \text{C}_{26} \text{H}_{23} \text{F}_2 \text{N}_{2} \]

\[ M = 382.46 \]

Monoclinic, \( P2_1/c \)

\( a = 13.220\ (8) \text{ Å} \)

\( b = 18.431\ (11) \text{ Å} \)

\( c = 8.475\ (5) \text{ Å} \)

\( \beta = 103.223\ (11) \)°

\( V = 2016.0\ (2) \text{ Å}^3 \)

\( Z = 4 \)

Data collection

Bruker SMART APEX CCD area detector diffractometer

\( \phi \) and \( \omega \) scans

Absorption correction: multi-scan

(SADABS: Sheldrick, 1996)

\( T_{	ext{min}} = 0.939, T_{	ext{max}} = 0.988 \)

15238 measured reflections

3975 independent reflections

2935 reflections with \( I > 2\sigma(I) \)

Refinement

Refinement on \( F^2 \)

\( R(F^2 > 2\sigma(F^2)) = 0.082 \)

\( wR(F^2) = 0.137 \)

\( S = 1.23 \)

3975 reflections

354 parameters

All H-atom parameters refined

Table 1

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Bond</th>
<th>Length (Å)</th>
<th>Bond</th>
<th>Length (Å)</th>
<th>Bond</th>
<th>Length (Å)</th>
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<tbody>
<tr>
<td>N2—C4</td>
<td>1.392 (3)</td>
<td>N1—C20</td>
<td>1.461 (3)</td>
<td>N1—C20</td>
<td>1.461 (3)</td>
<td>N2—C6</td>
<td>1.343 (3)</td>
</tr>
<tr>
<td>N3—C7</td>
<td>1.393 (3)</td>
<td>N1—C5</td>
<td>1.467 (3)</td>
<td>N1—C5</td>
<td>1.467 (3)</td>
<td>N1—C8</td>
<td>1.473 (3)</td>
</tr>
<tr>
<td>N2—C6</td>
<td>1.343 (3)</td>
<td>N1—C8</td>
<td>1.473 (3)</td>
<td>N1—C8</td>
<td>1.473 (3)</td>
<td>N1—C8</td>
<td>1.473 (3)</td>
</tr>
<tr>
<td>F1—C11</td>
<td>1.356 (3)</td>
<td>C5—N1—C20—C26</td>
<td>60.4 (3)</td>
<td>C20—N1—C6—C9</td>
<td>169.2 (2)</td>
<td>C6—N1—C20—C26</td>
<td>176.4 (3)</td>
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<tr>
<td>C9—C14—C1—C2</td>
<td>-144.7 (3)</td>
<td>D—H⋯A</td>
<td>1.02 (2)</td>
<td>D—H⋯A</td>
<td>1.02 (2)</td>
<td>D—H⋯A</td>
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</table>

Table 2

Hydrogen-bond geometry (Å, °).

<table>
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<tr>
<th>D—H⋯A</th>
<th>D—H</th>
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<th>D—A</th>
<th>D—H⋯A</th>
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<tr>
<td>C9—H9⋯C11</td>
<td>0.95 (3)</td>
<td>2.79 (3)</td>
<td>3.648 (4)</td>
<td>150 (2)</td>
</tr>
</tbody>
</table>

Symmetry code: (i) \(-x, -y + 1, -z + 1\). C11 is the centroid of the five-membered ring C1—C4N1.

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

We thank the Department of Science and Technology, India for data collection on the CCD facility set up under the IRFADST programme. DC thanks CSIR, India for a JRF.

References


