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4-(4-Fluorophenyl)-6-(3-nitrophenyl)-3,4-dihydropyridin-2(1*H*)-one

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Key indicators

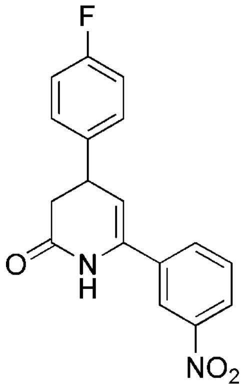
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 14.3

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

In the molecule of the title compound, $C_{17}H_{13}FN_2O_3$, the dihydropyridine ring is not planar and has a screw boat conformation, with a pseudo-twofold axis passing through the mid-points of the N—C(Ph—NO$_2$) and C—C(Ph—F) bonds. The dihedral angle between the benzene rings is 76.98 (3)°. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into centrosymmetric dimers; these may be effective in the stabilization of the crystal structure.

Comment

2-Pyridone derivatives are well known compounds because of their considerable biological importance as cardiotonic agents, such as milirinone (Krohnke & Dittmar, 1988), and as potential HIV-1 specific transcriptase inhibitors (Philip DeShong *et al.*, 1988; Boeckman *et al.*, 1987). Many derivatives of 2-pyridone are frequently used as intermediates for the construction of alkaloids (Curran & Liu, 1992; Liu *et al.*, 1995; Kozikowski *et al.*, 1996; Carles *et al.*, 2002). On the basis of previous work in decorating the 2-pyridone ring, we report here the crystal structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). Ring *A* (N2/C7–C11) is not planar, having a total puckering amplitude Q_T of 0.439 (2) Å and a screw boat conformation [φ = 33.36 (3)° and θ = 115.90 (4)°] (Cremer & Pople, 1975), with a pseudo-twofold axis passing through the mid-points of the N2—C7 and C9—C10 bonds, as can be deduced from the torsion angles (Table 1). Rings *B* (C1–C6) and *C* (C12–C17) are, of course, planar and the dihedral angle between them is 76.98 (3)°.

As can be seen from Fig. 2, the intermolecular N—H···O hydrogen bonds (Table 2) link the molecules into centro-

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symmetric dimers, which may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

Experimental

Compound (I) was prepared by the reaction of the condensation product of 4-fluorobenzaldehyde (0.25 g, 2 mmol) with Meldrum's acid (0.29 g, 2 mmol), 3-nitroacetophenone (0.33 g, 2 mmol) and ammonium acetate (1.0 g, 12 mmol) using acetic acid (98%, 1.4 ml) as an energy-transfer agent under microwave irradiation (yield 0.56 g, 90%; m.p. 505–506 K). Single crystals of (I) suitable for X-ray analysis were obtained in 4 days by slow evaporation of a dimethylformamide (DMF) solution (95%, 10 ml).

Crystal data

$C_{17}H_{13}FN_2O_3$
$M_r = 312.29$
Monoclinic, $P2_1/c$
$a = 13.960$ (3) Å
$b = 8.5633$ (18) Å
$c = 12.523$ (3) Å
$\beta = 103.789$ (4)°

$V = 1453.9$ (6) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 294$ (2) K
0.24 × 0.22 × 0.18 mm

Data collection

Bruker CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.962$, $T_{\max} = 0.981$

7954 measured reflections
2977 independent reflections
1475 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.053$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.126$
$S = 0.99$
2977 reflections

208 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.16$ e Å^{-3}
$\Delta\rho_{\min} = -0.19$ e Å^{-3}

Table 1
Selected torsion angles (°).

C11—N2—C7—C8	−16.1 (3)	C8—C9—C10—C11	−49.2 (3)
N2—C7—C8—C9	−0.8 (3)	C7—N2—C11—C10	−3.4 (3)
C7—C8—C9—C10	32.4 (3)	C9—C10—C11—N2	37.3 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3$^{\rm i}$	0.86	2.06	2.913 (2)	172

Symmetry code: (i) $-x+1, -y, -z+1$.

H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H, respectively, and constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

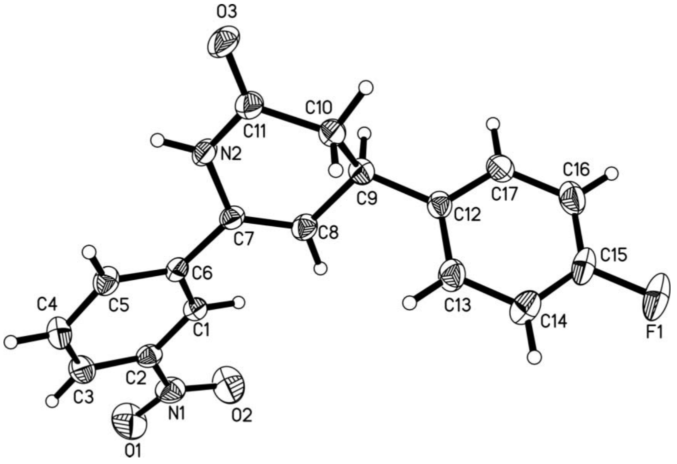

Figure 1
The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

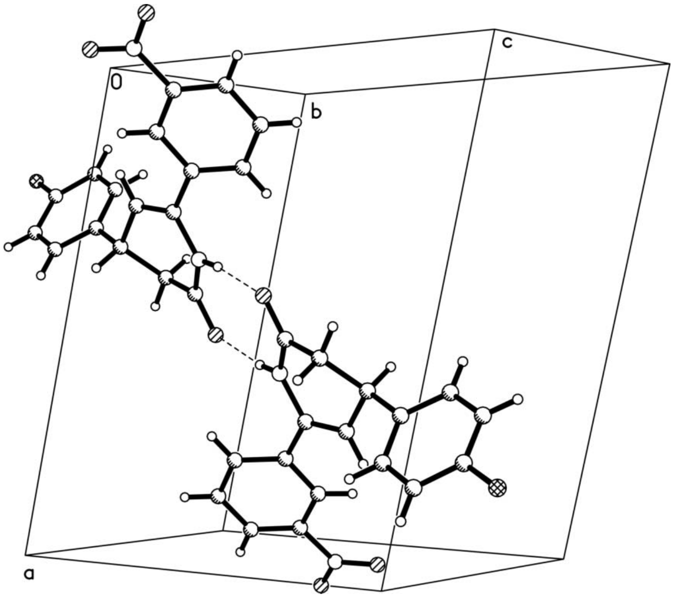

Figure 2
A partial packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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