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1-*n*-Butyl-2-(4′-fluorophenyl)-1*H*-benzimidazole-6-carbonitrile

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The structure of the title compound, $C_{18}H_{16}FN_3$, consists of neutral molecules. The asymmetric unit contains two independent molecules with similar conformations: the dihedral angles between the benzimidazole moiety and the benzene rings are 34.99 (9) and 36.08 (8)°. The crystal structure is stabilized by dipole–dipole and van der Waals interactions.

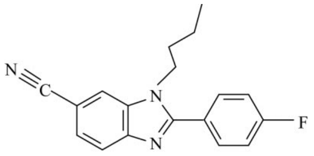
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.083
Data-to-parameter ratio = 8.1

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

Comment

Benzimidazoles have pharmacological effects and are incorporated in many commercially available drugs (Sakai *et al.*, 1989; Dubertret *et al.*, 1999; Netland *et al.*, 2000; Caro *et al.*, 2001; Matsumori, 2003). Because of their antiparasitic and antiviral activities, new benzimidazoles have been synthesized and investigated for medical applications. Some of us have studied the syntheses and potent antifungal activities of a series of 5-cyanobenzimidazoles with substituted phenyl groups, and found that some of these compounds displayed wide antifungal activity against *Candida sp*., comparable to that of the commonly used antifungal, fluconazole (Goker *et al.*, 2002). In this paper, we present the structure and stereochemical properties of a new cyanobenzimidazole, namely 1-*n*-butyl-2-(4′-fluorophenyl)-1*H*-benzimidazole-6-carbonitrile, (I) (Fig. 1).



(I)

The structure of (I) consists of neutral molecules. There are two independent molecules with similar conformations in the asymmetric unit of (I). The imidazole and benzene rings are coplanar; the bicyclic benzimidazole moiety is essentially planar with an r.m.s. deviation from the least-squares plane of 0.004 Å. The dihedral angles between the benzimidazole ring systems and the fluoro-substituted benzene rings are 34.99 (9) and 36.08 (8)°, for the F1- and F2-containing molecules, respectively. For the F1-containing molecule, the fluorine and cyano substituents are also coplanar with their parent benzene rings, but the first and last C atoms (C15 and C18) of the *n*-butyl group deviate from the mean plane of the benzimidazole system by 0.64 (4) Å. Corresponding deviations of 0.75 (2) Å arise for C33 and C36 in the F2-containing molecule. The C—N distances and N—C—N and C—N—C angles of (I) are similar and comparable to the data reported for

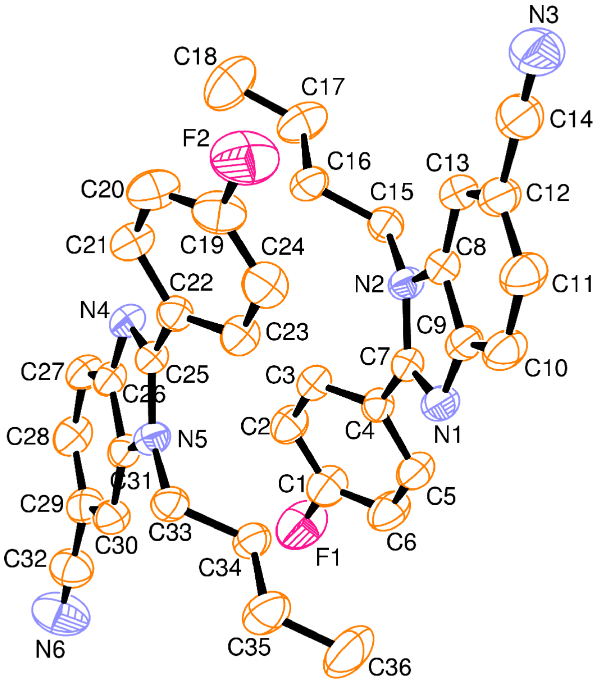


Figure 1
A view of the asymmetric unit of (I) (40% displacement ellipsoids). H atoms have been omitted.

related compounds (Bruno *et al.*, 1996, 1997; Kendi *et al.*, 1998, 1999; Özcan *et al.*, 2000; Stibrany *et al.* 2003).

A packing diagram of (I) is shown in Fig. 2. There are no conventional hydrogen bonds and the crystal packing is dominated by van der Waals and dipole–dipole interactions between fluorine and the nitrogen of the CN group, resulting in the packing of the molecules in layers.

Experimental

The sodium metabisulfite adduct of 4-fluorobenzaldehyde (0.265 g, 1.25 mmol) was added to a suspension of 4-amino-3-*n*-butylaminobenzonitrile (0.19 g, 1 mmol) in DMF (5 ml), and heated at 383 K for 4 h. The reaction mixture was cooled and poured into water. The solid product was collected by filtration, washed with water and chromatographed with EtOAc–*n*-hexane (1:3). The final product was dissolved in ethanol and colourless crystals of (I) were grown by slow evaporation at room temperature.

Crystal data

$C_{18}H_{16}FN_3$
$M_r = 293.34$
Orthorhombic, $Pca2_1$
$a = 18.0843$ (5) Å
$b = 8.1980$ (14) Å
$c = 21.4690$ (12) Å
$V = 3182.9$ (6) Å^3
$Z = 8$
$D_x = 1.224$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 15 369 reflections
$\theta = 0.0$–24.7°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.40 × 0.32 × 0.06 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: none
43 476 measured reflections
3216 independent reflections
1791 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.117$
$\theta_{\rm max} = 26.0°$
$h = -22 \rightarrow 22$
$k = -10 \rightarrow 9$
$l = -26 \rightarrow 26$

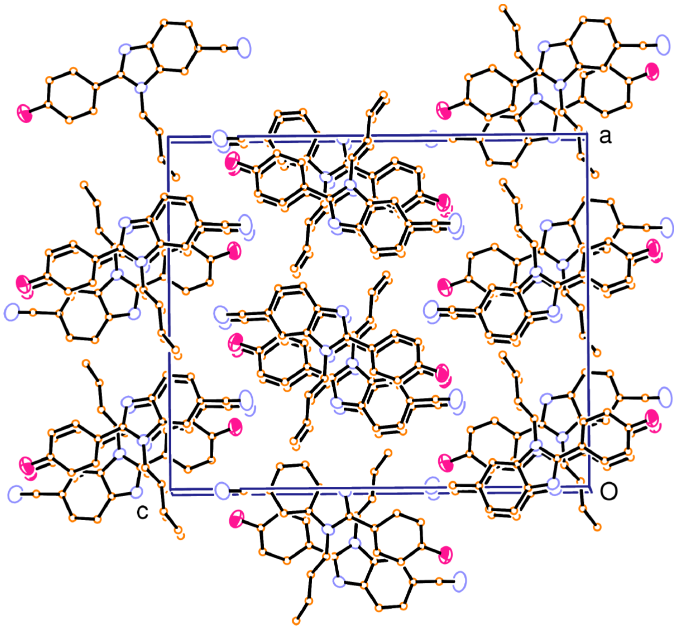


Figure 2
Packing diagram of (I).

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.083$
$S = 0.80$
3216 reflections
398 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.12$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.13$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0088 (7)

Table 1
Selected geometric parameters (Å, °).

C7—N1	1.315 (4)	C25—N4	1.316 (3)
C7—N2	1.382 (4)	C25—N5	1.376 (4)
C8—N2	1.389 (4)	C26—N4	1.381 (4)
C9—N1	1.385 (4)	C31—N5	1.391 (4)
C14—N3	1.145 (5)	C32—N6	1.129 (5)
N1—C7—N2	112.9 (3)	N6—C32—C29	178.0 (6)
N1—C7—C4	122.0 (3)	C7—N1—C9	105.2 (3)
N2—C8—C9	105.4 (3)	C7—N2—C8	106.2 (2)
N3—C14—C12	178.6 (6)	C25—N4—C26	104.9 (3)
N4—C25—N5	113.4 (3)	C31—N5—C33	123.3 (3)
N5—C31—C26	105.4 (3)		

H atoms were included using a riding model, with C—H = 0.93–0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}$(methyl C). The Flack (1983) absolute structure parameter refined to an indeterminate value, and for the final cycles of refinement, Friedel pairs were merged.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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