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3-(1*H*-Benzotriazol-1-yl)-1-(2-fluorophenyl)-propan-1-one

Wu-Lan Zeng,[a] Sai Bi,[b] Fan Zhang[b] and Jun Wan[b]*

[a]Department of Chemistry and Chemical Engineering, Weifang University, 261061 Weifang, Shandong, People's Republic of China, and [b]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, 266042 Qingdao, Shandong, People's Republic of China

Correspondence e-mail: shushzhang@126.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.143
Data-to-parameter ratio = 13.9

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

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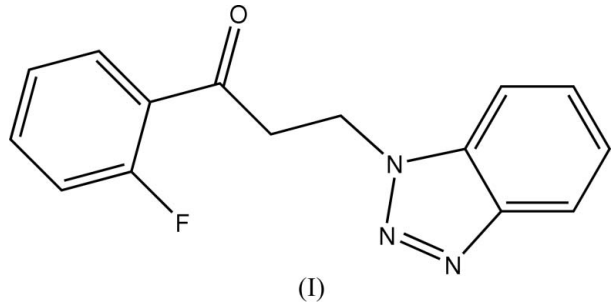
In the title compound, $C_{15}H_{12}FN_3O$, an intramolecular C—H···F hydrogen bond forms a six-membered ring. Molecules are linked into a tape along the *b* axis by an intermolecular C—H···N hydrogen bond. The crystal packing is further stabilized by C—H···π and π–π interactions.

Comment

We have recently reported the crystal structure of 3-(1*H*-benzotriazol-1-yl)-1-(4-fluorophenyl)propan-1-one, (II) (Yu *et al.*, 2006). As part of a search for new benzotriazole derivatives with higher bioactivity, the title compound, (I), has been synthesized and its structure is reported here.



(I)

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are comparable to those of (II). The benzotriazole ring system is essentially planar, with a dihedral angle of 1.18 (1)° between the C10–C15 and N1–N3/C10/C11 rings. The mean plane of the benzotriazole unit makes a dihedral angle of 82.49 (1)° with the C1–C6 benzene ring. An intramolecular C—H···F hydrogen bond (Table 1) forms a six-membered ring (Fig. 1).

In the crystal structure, molecules are linked into a tape along the *b* axis by an intermolecular C—H···N hydrogen bond (Table 1 and Fig. 2). The crystal packing is further stabilized by a C—H···π (Table 2) and two π–π interactions between the N1–N3/C10/C11 and C10–C15 rings and between C10–C15 rings; the centroid–centroid distances of $Cg1\cdots Cg3(2-x, 1-y, 2-z)$ and $Cg3\cdots Cg3(2-x, 1-y, 2-z)$ are 3.784 and 3.707 Å, respectively (*Cg*1 and *Cg*3 denote the centroids of the N1–N3/C10/C11 and C10–C15 rings, respectively).

Experimental

The title compound was prepared according to the literature method of Yu *et al.* (2006). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol–petroleum ether (1:2 *v*/*v*) solution at room temperature over a period of one week.

Crystal data

$C_{15}H_{12}FN_3O$
$M_r = 269.28$
Monoclinic, $P2_1/c$
$a = 15.551$ (6) Å
$b = 5.971$ (2) Å
$c = 14.221$ (6) Å
$\beta = 104.339$ (6)°
$V = 1279.4$ (8) Å^3
$Z = 4$
$D_x = 1.398$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293$ (2) K
Column, colourless
0.47 × 0.17 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.954$, $T_{max} = 0.991$
6710 measured reflections
2520 independent reflections
1923 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 26.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.143$
$S = 0.97$
2520 reflections
181 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8B···F1	0.97	2.40	2.760 (2)	101
C8—H8B···N3^{i}	0.97	2.53	3.336 (3)	140
C15—H15A···$Cg3^{ii}$	0.93	2.80	3.446 (2)	127

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+2, y-\frac{1}{2}, -z+\frac{5}{2}$.

H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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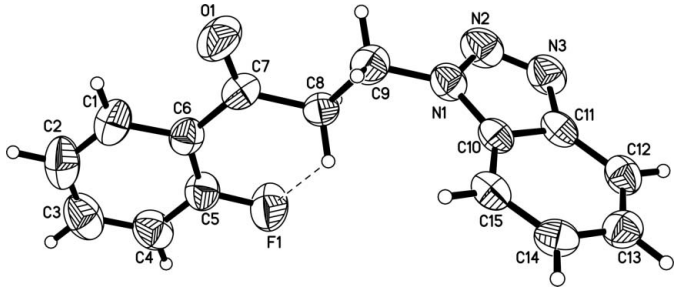

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates a hydrogen bond.

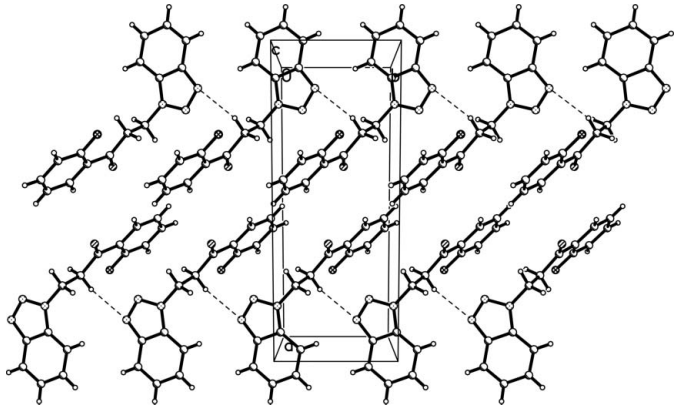

Figure 2
Packing diagram of (I), viewed along the *c* axis, showing the intermolecular hydrogen bonds (dashed lines).

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