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1-(4-Methylphenylsulfonyl)-5-nitro-1*H*-benzimidazole

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In the title compound, $C_{17}H_{15}N_3O_4S$, the mean plane of the benzimidazole fragment and the benzene ring of the *p*-tosyl group make a dihedral angle of 86.72 (14)°. The molecules are linked by weak C—H···O intermolecular hydrogen bonds into chains parallel to the *b* axis. The crystal packing is further stabilized by π–π stacking interactions.

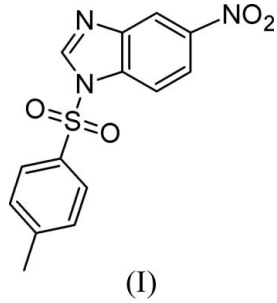
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.059
wR factor = 0.158
Data-to-parameter ratio = 12.2

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

Comment

The title compound, (I), is analogous to 1-(4-methylphenylsulfonyl)5-nitro-2-[(*E*)-prop-1-enyl]-1*H*-benzimidazole, (II) (Rashid *et al.*, 2006).



(I)

In (I) (Fig. 1), all bond lengths and angles are in normal ranges (Allen *et al.*, 1987) and comparable to those observed in (II). The mean plane of the benzimidazole fragment and the benzene ring of the *p*-tosyl group make a dihedral angle of 86.72 (14)°. The crystal packing (Fig. 2) exhibits weak intermolecular C—H···O hydrogen bonds (Table 2), which link the molecules into chains parallel to the *b* axis, and $\pi\cdots\pi$ stacking interactions with a shortest distance of 3.645 (2) Å between the centroids of the N1/N2/C1/C6/C7 and (C1—C6)^{ii} rings [symmetry code: (ii) $1-x, -y, -z$].

Experimental

Equimolar quantities of 4-nitro-1,2-phenylenediamine and methanoic acid were refluxed in 4 *N* HCl to synthesize 5-nitrobenzimidazole. The title compound was then synthesized by a known method (Hasan *et al.*, 1992) and recrystallized from ethanol (yield 38%, m.p. 446 K).

Crystal data

$C_{14}H_{11}N_3O_4S$
M_r = 317.32
Monoclinic, $P2_1/n$
a = 10.630 (3) Å
b = 9.950 (3) Å
c = 13.662 (4) Å
β = 104.577 (4)°
V = 1398.5 (7) Å^3
Z = 4
D_x = 1.507 Mg m^{-3}
Mo *K*α radiation
μ = 0.25 mm^{-1}
T = 298 (2) K
Block, colourless
0.29 × 0.24 × 0.19 mm

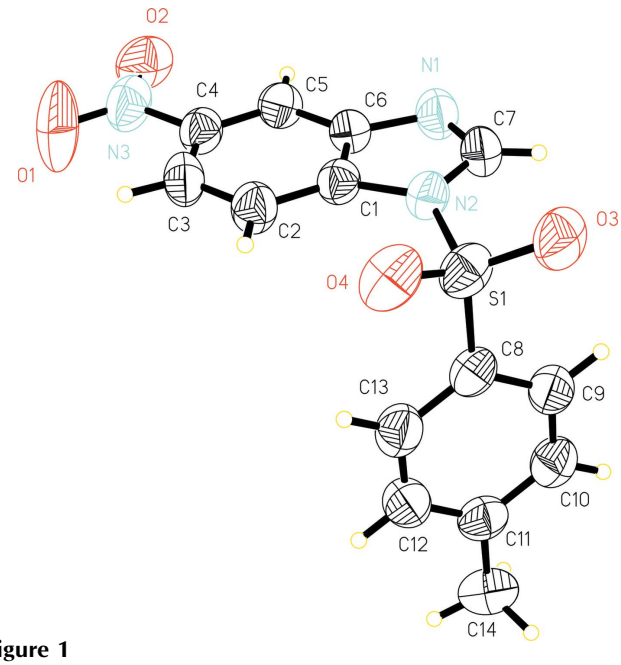


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probablity level.

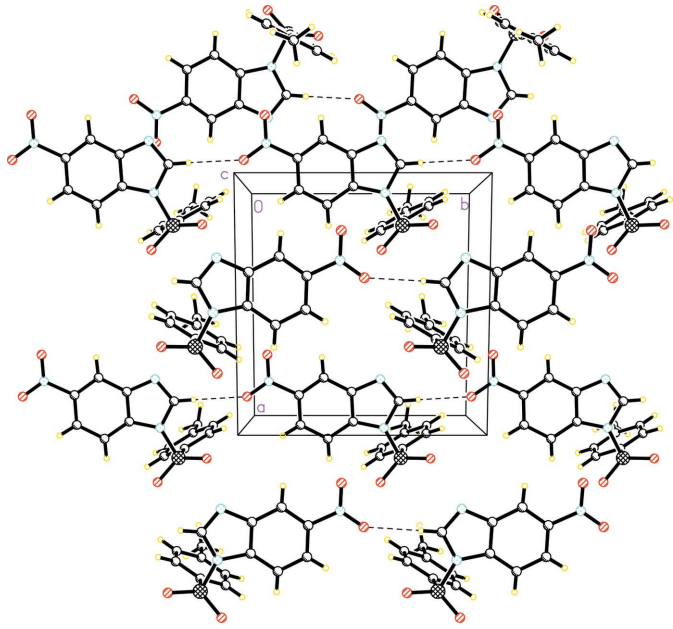


Figure 2
The crystal packing, viewed down the *c* axis. Dashed lines denote C—H···O hydrogen bonds.

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.929, T_{max} = 0.953
6561 measured reflections
2453 independent reflections
1871 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.158
S = 1.09
2453 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 1.2495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0012 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O1^{i}	0.93	2.31	3.239 (5)	173

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

All H atoms were postioned geometrically [C—H 0.93–0.96 Å] and constrained to ride on their parent atoms with U_{iso}(H)= 1.2–1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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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