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2-(4-Methoxybenzoylamino)benzimidazole

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Key indicators

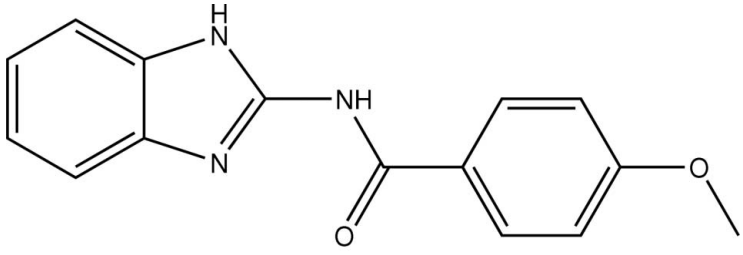
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.121
Data-to-parameter ratio = 14.2

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

The asymmetric unit of the title compound, $C_{15}H_{13}N_3O_2$, contains two molecules. In the crystal structure, intermolecular N—H···O and N—H···N hydrogen bonds link the molecules, forming infinite chains along the *a* axis The packing is further stabilized by C—H···π interactions.

Comment

Benzimidazoles have wide applications because of their structural characteristics (Liao *et al.*, 1996; Bag *et al.*, 1996). As medicine intermediates, they have broad biological activity (Lunn *et al.*, 1996; Xu *et al.*, 1996). Thus, they have been intensely studied over several decades. As part of our ongoing research on benzimidazole derivatives, the title compound, (I), was synthesized.



(I)

The asymmetric unit of (I) contains two molecules (Fig. 1). The bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The benzimidazole units, C1–C7/N1/N2 and C16–C22/N4/N5, are essentially planar. The dihedral angles between rings *A* (C1–C6), *B* (C1/C6/C7/N1/N2), *D* (C16–C21) and *E* (C16/C21/C22/N4/N5) are *A*/*B* = 0.66 (1)°

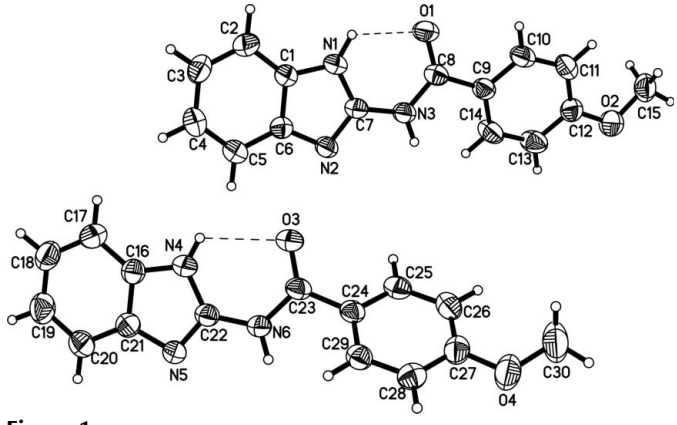


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

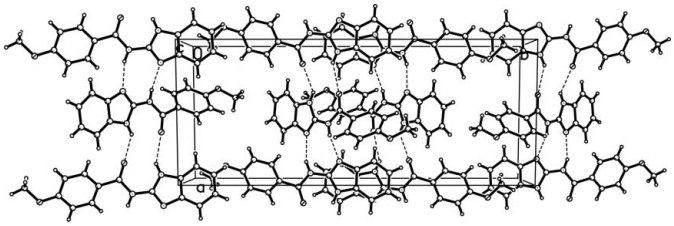


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines. Dashed lines indicate hydrogen bonds.

and D/E = 1.53 (1)°. The dihedral angles between the benzimidazole units C1–C7,N1,N2 and C16–C22,N4,N5 and the benzene rings *C* (C9–C14) and *F* (C24–C29) are 16.73 (1) and 51.04 (1)°, respectively. Intramolecular N—H···O interactions (Table 2) result in the formation of six-membered rings (Fig. 1).

In the crystal structure, intermolecular N—H···O and N—H···N hydrogen bonds (Table 2) link the molecules, forming infinite chains along the *a* axis (Fig. 2). The packing is further stabilized by C—H···π interactions (Table 2). The short distances $Cg1\cdots Cg1^{iv}$ (3.708 Å) and $Cg1\cdots Cg3^{iv}$ (3.596 Å) [symmetry code: (iv) $-x, 1-y, 1-z$], where *Cg*1 and *Cg*3 denote the centroids of rings *B* and *A*, respectively, indicate π–π interactions between the benzimidazole units.

Experimental

2-Aminobenzimidazole (6.65 g, 73 mmol) and 4-methoxybenzoyl chloride (8.55 g, 50 mmol) were added to a solution of dry pyridine (50 ml). The solution was filtered after stirring for 6 h at 373 K. A white solid was obtained and dried (yield 85%, m.p. 512–515 K). The product was dissolved in methanol/ethyl acetate (1:2). After filtration, the colorless filtrate was left at room temperature. Single crystals suitable for X-ray crystallographic analysis were obtained.

Crystal data

$C_{15}H_{13}N_3O_2$
M_r = 267.28
Monoclinic, $P2_1/c$
a = 10.158 (2) Å
b = 24.784 (5) Å
c = 10.474 (2) Å
β = 98.626 (3)°
V = 2607.0 (9) Å^3
Z = 8
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, colorless
0.41 × 0.16 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.989
14506 measured reflections
5111 independent reflections
3791 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.121
S = 1.04
5111 reflections
361 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.5412P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.229 (2)	N3—C8	1.367 (2)
O2—C12	1.359 (2)	N3—C7	1.383 (2)
O3—C23	1.227 (2)	N6—C23	1.367 (2)
O4—C30	1.422 (3)	N6—C22	1.375 (2)
C12—O2—C15	117.70 (17)	C23—N6—C22	125.47 (16)
C27—O4—C30	118.6 (2)	N3—C8—C9	115.96 (17)
C8—N3—C7	125.68 (16)	N6—C23—C24	114.70 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5B···$Cg6^{i}$	0.93	2.80	3.515	135
C15—H15B···$Cg1^{ii}$	0.96	2.71	3.319	121
C19—H19A···$Cg2^{iii}$	0.93	2.89	3.728	151
C25—H25A···$Cg2^{i}$	0.93	2.99	3.558	120
N1—H1A···O1	0.86	2.21	2.716 (2)	117
N1—H1A···O3^{iv}	0.86	2.32	3.072 (2)	145
N3—H3A···N5^{i}	0.86	2.19	2.979 (2)	152
N4—H4A···O3	0.86	2.25	2.733 (2)	116
N4—H4A···O1^{iv}	0.86	2.52	3.240 (2)	142
N6—H6A···N2^{i}	0.86	2.08	2.845 (2)	147

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x, -y-\frac{1}{2}, z-\frac{3}{2}$; (iv) $-x, -y+1, -z+1$. *Cg*1, *Cg*2 and *Cg*6 denote the centroids of rings *B*, *E* and *F*, respectively.

H atoms were positioned geometrically, with N—H = 0.86 Å and C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,N), where x = 1.5 for methyl and x = 1.2 for all other H atoms.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1997); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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