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# 2-[4-(Dimethylamino)phenyl]-1-{[4-(dimethylamino)phenyl]methyl}-1*H*-benzimidazole

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.045
*wR* factor = 0.073
Data-to-parameter ratio = 14.1

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



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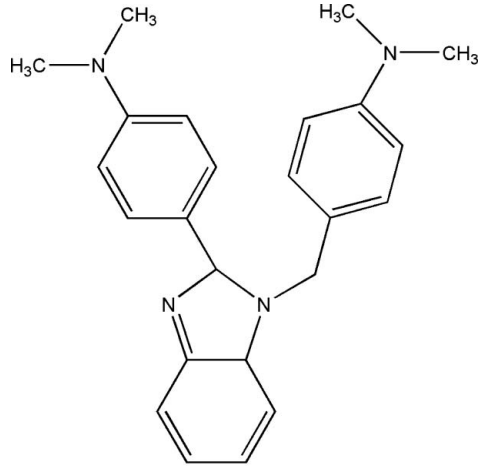
Molecules of the title compound, $C_{24}H_{26}N_4$, are linked by C—H···N hydrogen bonds, forming a *C*(5) chain along the [010] direction. Neighboring chains are connected by four C—H···π interactions, resulting in the formation of a three-dimensional network.

## Comment

The title compound, (I), was obtained unexpectedly in the condensation reaction between 4-dimethylaminobenzaldehyde and *o*-phenylenediamine. Benzimidazole derivatives display wide-ranging biological activities, for example as inhibitors of hepatitis C virus NS5B polymerase (Ishida *et al.*, 2006) and heparanase (Xu *et al.*, 2006), and antimicrobial activities (Özden *et al.*, 2005). Here we report the crystal structure of (I).



(I)

In the molecule of compound (I) (Fig. 1), the dihedral angles between the benzimidazole ring system and benzene rings C9–C14 and C17–C22 are 88.02 (6)° and 26.44 (8)°, respectively. The geometric parameters for (I) are normal.

In the crystal structure of (I), the molecules are linked through C—H···N hydrogen bonds, forming a *C*(5) chain (Bernstein *et al.*, 1995) along the [010] direction (Fig. 2 and Table 1). Neighboring chains are connected by four C—H···π interactions [C6···$Cg2^{i}$ = 3.641 (5) Å, C6—H6···$Cg2^{i}$ = 173°; C15···$Cg2^{ii}$ = 3.942 (5) Å, C15—H15*a*···$Cg2^{ii}$ = 159°; C16···$Cg1^{iii}$ = 3.912 (3) Å, C16—H16*b*···$Cg1^{iii}$ = 164°; C19···$Cg1^{iv}$ = 3.840 (3) Å, C19—H19···$Cg1^{iv}$ = 155°, where *Cg*1 is the centroid of the ring C2–C7 and *Cg*2 is the centroid of the ring C9–C14. Symmetry codes: (i) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (ii) $1-x, -1-y, -z$; (iii) $1-x, -y, -z$; (iv) $x, \frac{3}{2}-y, -\frac{1}{2}+z$] (Fig.3),

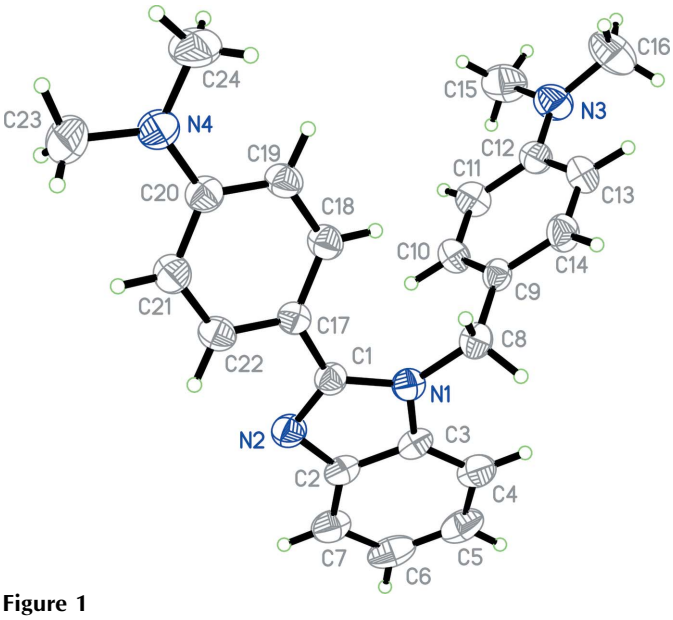



**Figure 1**
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

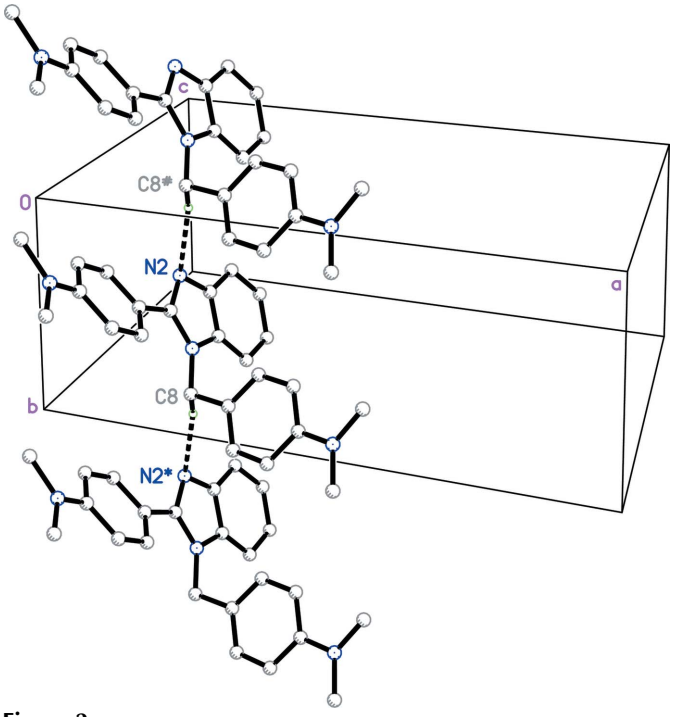



**Figure 2**
Part of the crystal structure of (I), showing the formation of a $C(5)$ chain in the [010] direction. For clarity, H atoms not involved in the motif shown have been omitted. [Symmetry codes: (*) $x, y+1, z$; (#) $x, -1+y, z$]. Dashed lines indicate hydrogen bonds.

resulting in the formation of a three-dimensional network structure.

## Experimental

The reaction mixture containing 4-dimethylaminobenzaldehyde (2.98 g, 20 mmol) and *o*-phenylenediamine (1.08 g, 10 mmol) was refluxed for about 4 h in ethanol (30 ml), then cooled and the product filtered off, washed with ethanol and dried. Yellow crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p.465–467 K).

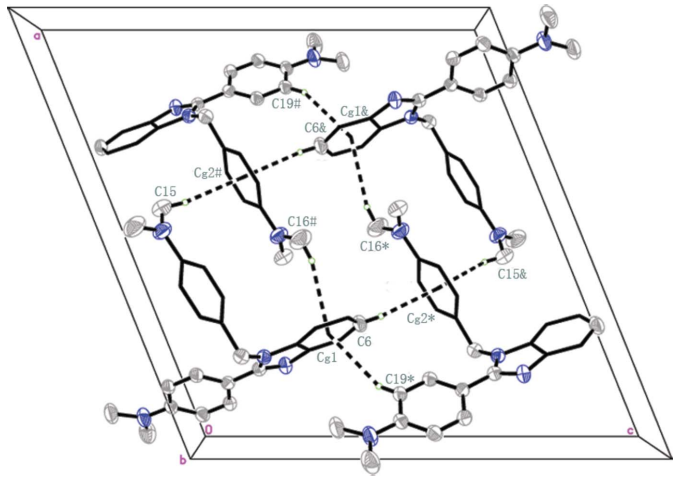



**Figure 3**
Part of the crystal structure of (I), viewed down the *b* axis, showing molecular chains linked by four C—H···$\pi$ interactions. Displacement ellipsoids are drawn at the 30% probability level. *Cg*1 and *Cg*2 are the centroids of rings C2–C7 and C9–C14, respectively. For clarity, bonds on rings C2–C7 and C9–C14 are shown as thin lines and H atoms not involved in the motif have been omitted. [Symmetry codes: (*) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (#) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (&) $1-x, 1-y, 1-z$]. Dashed lines indicate C—H···$\pi$ interactions.

### *Crystal data*

$C_{24}H_{26}N_4$
$M_r$ = 370.49
Monoclinic, $P2_1/c$
$a$ = 18.754 (3) Å
$b$ = 6.294 (2) Å
$c$ = 18.522 (3) Å
$\beta$ = 111.973 (3)°
$V$ = 2027.4 (8) Å$^3$
$Z$ = 4
$D_x$ = 1.214 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 298 (2) K
Needle, yellow
0.56 × 0.28 × 0.27 mm

### *Data collection*

Siemens SMART 1000 CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.960, $T_{max}$ = 0.981
10086 measured reflections
3565 independent reflections
1550 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 25.0°

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.073
$S$ = 1.00
3565 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0071P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.15 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8a···N2$^{i}$ | 0.97 | 2.55 | 3.499 (3) | 165 |

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

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms, and C—H = 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ 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*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*.

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