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1-Benzyl-1*H*-benzimidazole

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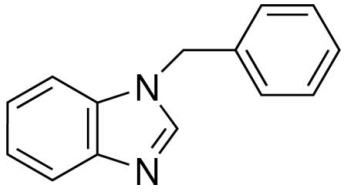
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.093; data-to-parameter ratio = 16.6.

In the title molecule, $C_{14}H_{12}N_2$, the benzimidazole ring system is essentially planar (r.m.s. deviation = 0.024 Å). The dihedral angle between the imidazole ring and the benzyl ring is 85.77 (4)°. In the crystal, molecules are linked into chains along the *a* axis by C—H···N hydrogen bonds. In addition, the packing is stabilized by C—H···π interactions involving both six-membered rings.

Related literature

For general background to benzimidazole derivatives, see: Ansari & Lal (2009). For the synthesis, see: Hayat *et al.* (2001).



Experimental

Crystal data

$C_{14}H_{12}N_2$
M_r = 208.26
Monoclinic, $P2_1/n$
a = 6.2265 (10) Å
b = 8.1740 (13) Å
c = 20.975 (4) Å
β = 97.839 (2)°
V = 1057.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 93 K
0.57 × 0.50 × 0.37 mm

Data collection

Rigaku SPIDER diffractometer
Absorption correction: none
8358 measured reflections
2412 independent reflections
2198 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.093
S = 1.00
2412 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···N2^{i}	0.99	2.50	3.4890 (14)	173
C7—H7···$Cg1^{ii}$	0.95	2.66	3.5220 (1)	151
C13—H13···$Cg2^{iii}$	0.95	2.80	3.5660 (3)	139

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y-1, -z+1$; (iii) $x, y+1, z$. $Cg1$ and $Cg2$ are the centroids of the C11–C16 and C4–C9 rings, respectively.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2926).

References

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supplementary materials

Acta Cryst. (2009). E**65**, o2613 [**doi:10.1107/S1600536809039051**]

1-Benzyl-1*H*-benzimidazole

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Comment

Benzimidazole derivatives are a class of important compounds which exhibit antimicrobial activity (Ansari & Lal, 2009). Here, we report the crystal structure of the title compound.

Bond lengths and angles in the title molecule are normal. The benzimidazole ring system is planar, with a maximum deviation of 0.035 (2)Å for atom C4. The imidazole ring and benzene ring in benzyl group are almost mutually perpendicular, with a dihedral angle of 85.77 (4)% (Fig. 1). The crystal packing is stabilized by C—H···N hydrogen bonds and C—H···π interactions (*Cg*1 is the centroid of the C11-C16 ring and *Cg*2 is the centroid of the C4—C9 ring) (Table 1).

Experimental

The title compound was synthesized according to the method reported in the literature (Hayat *et al.*, 2001). Colourless single crystals suitable for X-ray diffraction were obtained by slow evaporation of a methanol solution.

Refinement

All H atoms were placed in calculated positions, with C-H = 0.95 or 0.99 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

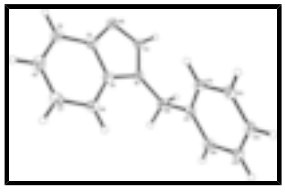

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

1-Benzyl-1*H*-benzimidazole

Crystal data

$C_{14}H_{12}N_2$	F_{000} = 440
M_r = 208.26	D_x = 1.308 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3307 reflections
a = 6.2265 (10) Å	θ = 3.2–27.5º
b = 8.1740 (13) Å	μ = 0.08 mm^{-1}

c = 20.975 (4) Å	T = 93 K
β = 97.839 (2)º	Block, colourless
V = 1057.5 (3) Å^3	0.57 × 0.50 × 0.37 mm
Z = 4	

Data collection

Rigaku SPIDER diffractometer	2198 reflections with $I > 2\sigma(I)$
Radiation source: Rotating Anode	R_{int} = 0.022
Monochromator: graphite	θ_{max} = 27.5º
T = 93 K	θ_{min} = 3.2º
ω scans	h = −8→8
Absorption correction: none	k = −10→10
8358 measured reflections	l = −27→27
2412 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H-atom parameters constrained
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.296P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
2412 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
145 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.41468 (13)	0.11825 (10)	0.58340 (4)	0.0151 (2)
N2	0.08985 (14)	0.00680 (11)	0.59213 (4)	0.0184 (2)

C2	0.21067 (16)	0.08189 (12)	0.55458 (5)	0.0164 (2)
H2	0.1602	0.1086	0.5110	0.020*
C4	0.22460 (16)	−0.00841 (12)	0.65071 (5)	0.0164 (2)
C5	0.18809 (18)	−0.08552 (13)	0.70781 (5)	0.0206 (2)
H5	0.0516	−0.1329	0.7122	0.025*
C6	0.35775 (19)	−0.09021 (14)	0.75762 (5)	0.0234 (3)
H6	0.3374	−0.1434	0.7966	0.028*
C7	0.55957 (19)	−0.01845 (14)	0.75220 (5)	0.0230 (3)
H7	0.6720	−0.0241	0.7876	0.028*
C8	0.59841 (17)	0.06012 (13)	0.69652 (5)	0.0190 (2)
H8	0.7338	0.1103	0.6929	0.023*
C9	0.42797 (16)	0.06166 (12)	0.64598 (5)	0.0153 (2)
C10	0.58686 (16)	0.19667 (13)	0.55403 (5)	0.0163 (2)
H10A	0.5488	0.1927	0.5067	0.020*
H10B	0.7223	0.1334	0.5653	0.020*
C11	0.62877 (16)	0.37280 (13)	0.57428 (5)	0.0148 (2)
C12	0.47606 (16)	0.46721 (13)	0.59998 (5)	0.0175 (2)
H12	0.3414	0.4201	0.6066	0.021*
C13	0.51869 (18)	0.63021 (13)	0.61606 (5)	0.0198 (2)
H13	0.4138	0.6936	0.6339	0.024*
C14	0.71437 (17)	0.70020 (13)	0.60598 (5)	0.0187 (2)
H14	0.7429	0.8119	0.6165	0.022*
C15	0.86811 (17)	0.60677 (13)	0.58054 (5)	0.0185 (2)
H15	1.0023	0.6544	0.5738	0.022*
C16	0.82598 (16)	0.44380 (13)	0.56497 (5)	0.0171 (2)
H16	0.9322	0.3801	0.5478	0.021*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0142 (4)	0.0141 (4)	0.0168 (4)	−0.0009 (3)	0.0017 (3)	−0.0012 (3)
N2	0.0160 (4)	0.0162 (4)	0.0226 (5)	−0.0005 (3)	0.0016 (3)	0.0004 (4)
C2	0.0155 (5)	0.0136 (5)	0.0195 (5)	0.0007 (4)	−0.0002 (4)	−0.0013 (4)
C4	0.0162 (5)	0.0131 (5)	0.0201 (5)	0.0014 (4)	0.0030 (4)	−0.0028 (4)
C5	0.0211 (5)	0.0181 (5)	0.0239 (5)	−0.0002 (4)	0.0084 (4)	−0.0008 (4)
C6	0.0305 (6)	0.0229 (6)	0.0178 (5)	0.0026 (5)	0.0074 (4)	0.0005 (4)
C7	0.0256 (6)	0.0248 (6)	0.0176 (5)	0.0029 (5)	−0.0006 (4)	−0.0033 (4)
C8	0.0171 (5)	0.0193 (5)	0.0205 (5)	−0.0003 (4)	0.0015 (4)	−0.0040 (4)
C9	0.0174 (5)	0.0119 (5)	0.0172 (5)	0.0017 (4)	0.0037 (4)	−0.0028 (4)
C10	0.0140 (5)	0.0167 (5)	0.0188 (5)	−0.0008 (4)	0.0043 (4)	−0.0016 (4)
C11	0.0154 (5)	0.0159 (5)	0.0129 (5)	0.0001 (4)	0.0009 (4)	0.0012 (4)
C12	0.0143 (5)	0.0187 (5)	0.0201 (5)	−0.0008 (4)	0.0039 (4)	0.0000 (4)
C13	0.0198 (5)	0.0173 (5)	0.0227 (5)	0.0031 (4)	0.0048 (4)	−0.0009 (4)
C14	0.0223 (5)	0.0143 (5)	0.0189 (5)	−0.0009 (4)	0.0010 (4)	0.0005 (4)
C15	0.0165 (5)	0.0198 (5)	0.0192 (5)	−0.0036 (4)	0.0027 (4)	0.0019 (4)
C16	0.0154 (5)	0.0196 (5)	0.0170 (5)	0.0009 (4)	0.0044 (4)	−0.0001 (4)

Geometric parameters (Å, °)

N1—C2	1.3630 (13)	C8—H8	0.95
N1—C9	1.3835 (13)	C10—C11	1.5137 (15)
N1—C10	1.4560 (13)	C10—H10A	0.99
N2—C2	1.3132 (14)	C10—H10B	0.99
N2—C4	1.3956 (13)	C11—C12	1.3892 (14)
C2—H2	0.95	C11—C16	1.3958 (14)
C4—C5	1.3992 (15)	C12—C13	1.3910 (15)
C4—C9	1.4055 (14)	C12—H12	0.95
C5—C6	1.3812 (16)	C13—C14	1.3881 (15)
C5—H5	0.95	C13—H13	0.95
C6—C7	1.4053 (17)	C14—C15	1.3870 (15)
C6—H6	0.95	C14—H14	0.95
C7—C8	1.3826 (16)	C15—C16	1.3881 (16)
C7—H7	0.95	C15—H15	0.95
C8—C9	1.3940 (14)	C16—H16	0.95
C2—N1—C9	106.23 (9)	N1—C10—C11	114.12 (8)
C2—N1—C10	127.14 (9)	N1—C10—H10A	108.7
C9—N1—C10	126.61 (8)	C11—C10—H10A	108.7
C2—N2—C4	104.17 (9)	N1—C10—H10B	108.7
N2—C2—N1	114.29 (9)	C11—C10—H10B	108.7
N2—C2—H2	122.9	H10A—C10—H10B	107.6
N1—C2—H2	122.9	C12—C11—C16	119.02 (10)
N2—C4—C5	130.19 (10)	C12—C11—C10	122.43 (9)
N2—C4—C9	109.93 (9)	C16—C11—C10	118.52 (9)
C5—C4—C9	119.80 (10)	C11—C12—C13	120.53 (10)
C6—C5—C4	117.59 (10)	C11—C12—H12	119.7
C6—C5—H5	121.2	C13—C12—H12	119.7
C4—C5—H5	121.2	C14—C13—C12	120.02 (10)
C5—C6—C7	121.82 (10)	C14—C13—H13	120.0
C5—C6—H6	119.1	C12—C13—H13	120.0
C7—C6—H6	119.1	C15—C14—C13	119.86 (10)
C8—C7—C6	121.57 (10)	C15—C14—H14	120.1
C8—C7—H7	119.2	C13—C14—H14	120.1
C6—C7—H7	119.2	C14—C15—C16	120.05 (10)
C7—C8—C9	116.34 (10)	C14—C15—H15	120.0
C7—C8—H8	121.8	C16—C15—H15	120.0
C9—C8—H8	121.8	C15—C16—C11	120.51 (10)
N1—C9—C8	131.71 (10)	C15—C16—H16	119.7
N1—C9—C4	105.38 (9)	C11—C16—H16	119.7
C8—C9—C4	122.85 (10)		
C4—N2—C2—N1	−0.14 (12)	N2—C4—C9—N1	−0.51 (11)
C9—N1—C2—N2	−0.17 (12)	C5—C4—C9—N1	176.66 (9)
C10—N1—C2—N2	178.24 (9)	N2—C4—C9—C8	−177.95 (9)
C2—N2—C4—C5	−176.38 (11)	C5—C4—C9—C8	−0.78 (15)
C2—N2—C4—C9	0.40 (11)	C2—N1—C10—C11	105.93 (11)
N2—C4—C5—C6	176.02 (10)	C9—N1—C10—C11	−75.97 (12)

C9—C4—C5—C6	−0.49 (15)	N1—C10—C11—C12	−20.55 (13)
C4—C5—C6—C7	0.97 (16)	N1—C10—C11—C16	161.34 (9)
C5—C6—C7—C8	−0.20 (17)	C16—C11—C12—C13	0.16 (15)
C6—C7—C8—C9	−1.03 (16)	C10—C11—C12—C13	−177.95 (10)
C2—N1—C9—C8	177.52 (11)	C11—C12—C13—C14	0.52 (16)
C10—N1—C9—C8	−0.91 (17)	C12—C13—C14—C15	−0.72 (16)
C2—N1—C9—C4	0.41 (11)	C13—C14—C15—C16	0.24 (16)
C10—N1—C9—C4	−178.02 (9)	C14—C15—C16—C11	0.45 (15)
C7—C8—C9—N1	−175.17 (10)	C12—C11—C16—C15	−0.64 (15)
C7—C8—C9—C4	1.52 (15)	C10—C11—C16—C15	177.54 (9)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10B···N2^{i}	0.99	2.50	3.4890 (14)	173
C7—H7···Cg1^{ii}	0.95	2.66	3.5220 (1)	151
C13—H13···Cg2^{iii}	0.95	2.80	3.5660 (3)	139

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) −*x*+1, −*y*−1, −*z*+1; (iii) *x*, *y*+1, *z*.

Fig. 1