2-Phenyl-1,3-bis(2-pyridylmethyl)-imidazolidine

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Key indicators

Single-crystal X-ray study
$T = 120$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.111
Data-to-parameter ratio = 17.7

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

In the title compound, $C_{21}H_{22}N_4$, all three substituents are
found in equatorial positions. Intermolecular C—H···N and
C—H···π interactions seem to be responsible for the packing.

Comment

Subsequent to the publication of reports on some coordin-
ation compounds with the ligand *N*-benzyl-*N'*-carboxymethyl-
N,N'-bis(2-pyridylmethyl)-1,2-ethanediamine (Baffert *et al.*,
2003), we have succeeded in crystallizing the ligand precursor
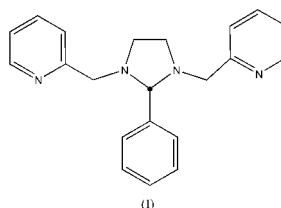2-phenyl-1,3-bis(2-pyridylmethyl)imidazolidine, (I).

(I)

Fig. 1 shows the molecular structure of (I) with the atom-
numbering scheme. The five-membered ring is in an envelope
conformation, with C3 as the apex [$\varphi_2 = 5.6\ (2)°$, total ring
puckering amplitude $Q_2 = 0.3974\ (16)$ Å; Cremer & Pople
(1975)]. The ring has a pseudo-mirror, which includes the
phenyl ring through C3 and is orthogonal to the C1—C2 bond.
All three substituents are in equatorial positions, and the
pyridine rings are oriented in a *syn* fashion *i.e.* the two N
atoms are both pointing in the same direction as the axial H
atom on C2. The exact orientations of the central ring and
substituents are summarized in Table 2, which gives the
dihedral angles formed by least-squares planes through the
individual rings.

Extensive C—H···π interactions (closest H···Centroid
contact = 2.79 Å) exist between the aromatic rings. Other

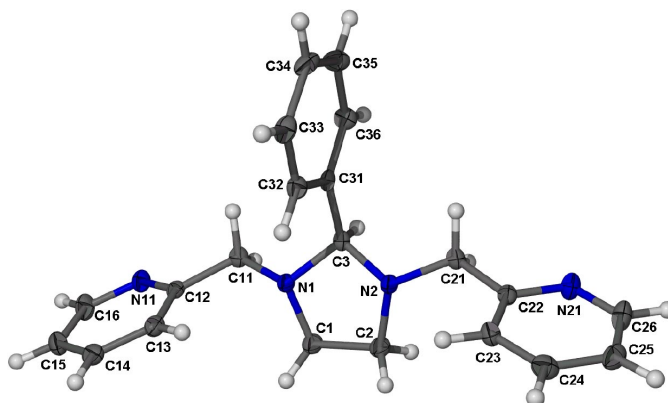**Figure 1**
View of (I), with 50% probability displacement ellipsoids.

short contacts include N1···H36^i 3.48 Å, N2···H36^i 3.07 Å, N11···H34^{ii} 2.90 Å and N21···H2B^{iii} 2.76 Å [symmetry codes: (i) $x + 1, y, z$; (ii) $x - \frac{1}{2}, y - \frac{1}{2}, \frac{1}{2} - z$; (iii) $-x, -y, -z$]. The first two result in stacking along the a axis of the unit cell.

Experimental

2-Phenyl-1,3-bis(2-pyridylmethyl)imidazolidine was prepared according to a literature method (Baffert *et al.*, 2003). Colourless block-shaped single crystals were grown by slow evaporation of a dichloromethane solution.

Crystal data

$C_{21}H_{22}N_4$	$D_x = 1.253$ Mg m^{-3}
$M_r = 330.43$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 22931
$a = 6.003$ (5) Å	reflections
$b = 15.175$ (5) Å	$\theta = 2.7–26.2°$
$c = 19.237$ (5) Å	$\mu = 0.08$ mm^{-1}
$\beta = 91.794$ (5)°	$T = 120$ (2) K
$V = 1751.5$ (16) Å^3	Block, colourless
$Z = 4$	$0.45 \times 0.25 \times 0.10$ mm

Data collection

Bruker SMART CCD diffractometer	4019 independent reflections
ω rotation scans	2464 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.083$
$T_{min} = 0.883$, $T_{max} = 0.992$	$\theta_{max} = 27.5°$
20244 measured reflections	$h = -7 \rightarrow 7$
	$k = -19 \rightarrow 19$
	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.1083P]$
$R[F^2 > 2\sigma(F^2)] = 0.049$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{max} = 0$
$S = 1.02$	$\Delta\rho_{max} = 0.24$ e Å^{-3}
4019 reflections	$\Delta\rho_{min} = -0.2$ e Å^{-3}
227 parameters	Extinction correction: *SHELXL*97
H-atom parameters constrained	Extinction coefficient: 0.0053 (8)

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.467 (2)	C2—N2	1.476 (2)
C1—C2	1.523 (2)	C3—N1	1.456 (2)
N1—C1—C2	104.64 (13)	C3—N1—C1	105.09 (12)
N2—C2—C1	104.28 (13)	C3—N2—C2	106.04 (12)
N1—C3—N2	101.65 (13)		

Table 2
Dihedral angles formed by least-squares planes (°).

	B	C	D
A	21.97 (8)	73.97 (8)	70.71 (9)
B		84.34 (8)	71.65 (9)
C			85.44 (9)

Least-squares planes: A N11/C12–C16, B N21/C22–C26, C C31–C36 and D N1/C1/C2/N2/C3

All H natoms could be located from a Fourier difference map, but were refined with ideal coordinates and riding displacement parameters, U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *X-Seed* (Barbour, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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