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N,N-Bis(2-pyridylmethyl)-*tert*-butylamine

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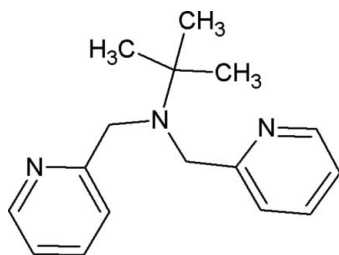
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 13.7.

In the title compound, $\text{C}_{16}\text{H}_{21}\text{N}_3$, the dihedral angle between the two pyridine rings is $88.11(9)^\circ$. In the crystal, molecules are linked through intermolecular $\text{C}-\text{H}\cdots\pi$ interactions, forming a layer expanding parallel to the $(10\bar{1})$ plane.

Related literature

For related compounds, see: Mambanda *et al.* (2007); Foxon *et al.* (2007); Fujihara *et al.* (2004); Munro & Camp (2003). For metal complexes with the title compound as a ligand, see: Fujii *et al.* (2003); Lee & Lippard (2002); Mok *et al.* (1997). For the metal complex with *N,N*-bis(2-pyridylmethyl)ethylamine as a ligand, see: Pal *et al.* (1992).



Experimental

Crystal data

$\text{C}_{16}\text{H}_{21}\text{N}_3$
 $M_r = 255.36$
 Monoclinic, Cc
 $a = 6.1808(3)$ Å
 $b = 17.9502(8)$ Å
 $c = 13.7079(6)$ Å
 $\beta = 100.239(4)^\circ$

$V = 1496.62(12)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 293(2)$ K
 $0.50 \times 0.50 \times 0.30$ mm

Data collection

Oxford Diffraction Xcalibur2 CCD diffractometer
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
 $T_{\min} = 0.967$, $T_{\max} = 0.980$
 7475 measured reflections
 2392 independent reflections
 2024 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.012$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.119$
 $S = 1.02$
 2392 reflections
 175 parameters
 2 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.22$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$Cg1$ and $Cg2$ are the centroids of the $\text{N}2/\text{C}3-\text{C}7$ and $\text{N}3/\text{C}9-\text{C}13$ rings, respectively.

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C}7-\text{H}1\cdots\text{C}g2^{\text{i}}$	0.93	2.97	3.819 (2)	153
$\text{C}15-\text{H}16\cdots\text{C}g1^{\text{ii}}$	0.96	2.94	3.836 (2)	156

Symmetry codes: (i) $x - \frac{1}{2}, y - \frac{1}{2}, z$; (ii) $x, -y, z - \frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors gratefully acknowledge financial support from the University of Kwazulu-Natal and the South African National Research Foundation. We thank Mr C. Grimmer for the NMR analysis of the samples. We also thank Professor O. Q. Munro and Professor J. Field for their guidance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2355).

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supplementary materials

Acta Cryst. (2009). E65, o402 [doi:10.1107/S1600536809001366]

N,N-Bis(2-pyridylmethyl)-*tert*-butylamine

A. Mambanda, D. Jaganyi and K. Stewart

Comment

The title compound is a versatile tridentate N-donor ligand, and it (Fujii *et al.*, 2003; Lee & Lippard, 2002; Mok *et al.*, 1997) and its analogue, *N,N*-bis(2-pyridylmethyl)ethylamine (Pal *et al.*, 1992) have been used extensively in metal coordination. The related crystal structures of symmetrical bis(tridentate) ligands have been reported (Mambanda *et al.*, 2007; Foxon *et al.*, 2007; Fujihara *et al.*, 2004).

The crystal structure of the title compound (Fig. 1) shows that the three nitrogen atoms (one sp^3 and two pyridine sp^2) are not suitably orientated for pincer-like coordination to a metal. Rotation about the C2—C3 and C8—C9 bonds are required for that to occur. The relative orientation of the two pyridine rings is reflected in a dihedral angle between their mean planes of 88.11 (9)°, clearly this angle would have to change were the ligand to bind to a metal centre. The steric influence of the bulky *tert*-butyl group is reflected in the C1—N1—C2 and C1—N1—C8 angles [113.90 (13) and 115.34 (13)°, respectively], being larger than the C2—N1—C8 angle of 110.08 (13)°. The methylene groups of the structure all adopt the expected staggered (lowest energy) conformation (Munro & Camp, 2003). The pyridyl ring containing atom N2 is orientated at 18 (1)° relative to the mean plane of the *N-tert*-butyl group (plane through C16—C1—N1), whilst that containing N3 is orientated at 74 (1)°.

There are no short van der Waals contacts less than the sum of the van der Waals radii in this system, reflected in the loose packing, however weak (possibly stabilizing) C—H \cdots π intermolecular interactions do occur. The metrics of such interactions reflect a T-shaped, edge-to-face geometry. Specifically, let us define Cg1 as the centre of gravity of the pyridyl N2/C3—C7 ring and Cg2 the centre of gravity of the pyridyl N3/C9—C13 ring. A C—H \cdots π interaction with a separation of 2.97 (1) Å exists between C7—H1 from the pyridyl ring containing atom N2 and Cg2 of neighbouring symmetry related molecule [symmetry code: (i) $x - 1/2, y - 1/2, z$] (Table 1). A similar C—H \cdots π interaction with a separation of 2.94 (1) Å exists between C15—H16 from one of the methyl groups of the *tert*-butyl moiety and Cg1 on the symmetry related neighbouring molecule with symmetry code: (ii) $x, -y, z - 1/2$. Figure 2 shows the packing within the unit cell for the title compound.

Experimental

The compound was synthesized following a literature method (Pal *et al.*, 1992). Under a high flow of nitrogen, 6 ml of 20% NaOH solution was added to an aqueous solution of 2-picoly chloridehydrochloride [(3.937 g (24 mmol) in 0.5 ml ultra pure water] to form a pink emulsion solution. 2-Amino-2-methyl propane (12 mmol) was added and the mixture stirred at 60°C. 40 ml of 20% NaOH solution was then added over a period of 1 h and the mixture left to stir for a further 12 h. The crude product was extracted with CHCl₃ washed with ultra pure water and dried over Na₂SO₄. Excess solvent was removed under reduced pressure and the oil residue purified on a short chromatographic column packed with 0.5 g charcoal and 5 g of neutral alumina using CHCl₃ as an eluent to afford a light yellow solution. Colourless single crystals suitable for X-ray diffraction were obtained from slow evaporation of the solvent from its solution made from a 5% chloroform in ethanol solution (yield: 1.73 g, 60%).

supplementary materials

Spectroscopic data: ^1H NMR (400 MHz, CDCl_3) δ / p.p.m.: 8.40 (d, 2H), 7.60 (t, 2H), 7.45 (d, 2H), 7.05 (t, 2H), 3.95 (s, 4H), 1.18 (s, 9H). ^{13}C NMR (125 MHz, CDCl_3) δ / p.p.m.: 27.0, 57.0, 122.0, 123.0, 136.0, 148.0, 160. Anal. Calc. for $\text{C}_{16}\text{H}_{21}\text{N}_3$: C 75.26, H 8.29, N 16.46; Found: C 74.89, H 7.97, N 17.37.

Refinement

All Hydrogen atoms were positioned in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$. In the absence of significant anomalous scattering effects, Friedel pairs have been merged.

Figures

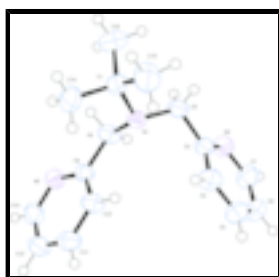


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and atomic numbering.

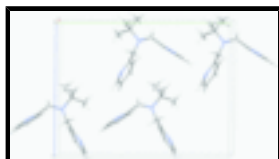


Fig. 2. Unit cell packing diagram of the title compound, viewed along the a axis.

N,N-Bis(2-pyridylmethyl)-*tert*-butylamine

Crystal data

$\text{C}_{16}\text{H}_{21}\text{N}_3$

$M_r = 255.36$

Monoclinic, Cc

Hall symbol: C -2yc

$a = 6.1808$ (3) Å

$b = 17.9502$ (8) Å

$c = 13.7079$ (6) Å

$\beta = 100.239$ (4)°

$V = 1496.62$ (12) Å³

$Z = 4$

$F_{000} = 552$

$D_x = 1.133$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4672 reflections

$\theta = 3.9$ – 32.0 °

$\mu = 0.07$ mm⁻¹

$T = 293$ (2) K

Plate, colourless

$0.50 \times 0.50 \times 0.30$ mm

Data collection

Oxford Diffraction Xcalibur2 CCD
diffractometer

2392 independent reflections

Radiation source: Enhance (Mo)X-Ray Source	2024 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.012$
Detector resolution: 8.4190 pixels mm^{-1}	$\theta_{\text{max}} = 31.9^\circ$
$T = 293(2)$ K	$\theta_{\text{min}} = 4.1^\circ$
ω -2 θ scans	$h = -8 \rightarrow 7$
Absorption correction: multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2008)	$k = -26 \rightarrow 26$
$T_{\text{min}} = 0.967$, $T_{\text{max}} = 0.980$	$l = -18 \rightarrow 20$
7475 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.119$	$w = 1/[\sigma^2(F_o^2) + (0.0873P)^2 + 0.017P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
2392 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
175 parameters	$\Delta\rho_{\text{max}} = 0.21 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$
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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C14	0.2251 (5)	0.16330 (11)	0.59751 (18)	0.0645 (6)
H20	0.1452	0.1875	0.6425	0.097*
H21	0.2314	0.1955	0.5421	0.097*
H19	0.3716	0.1525	0.6311	0.097*
C15	0.2342 (5)	0.05704 (14)	0.48509 (17)	0.0679 (6)
H18	0.3767	0.0409	0.5180	0.102*
H16	0.2508	0.0937	0.4359	0.102*
H17	0.1537	0.0152	0.4537	0.102*

supplementary materials

C16	-0.1269 (5)	0.10773 (16)	0.5103 (2)	0.0739 (7)
H15	-0.1940	0.0630	0.4806	0.111*
H14	-0.1260	0.1449	0.4600	0.111*
H13	-0.2090	0.1258	0.5586	0.111*
N3	0.1632 (2)	0.14031 (8)	0.88126 (11)	0.0448 (3)
C9	0.2329 (2)	0.09809 (8)	0.81277 (11)	0.0365 (3)
N1	0.1221 (2)	0.03781 (7)	0.64559 (9)	0.0382 (3)
C3	0.1172 (3)	-0.09657 (8)	0.68278 (12)	0.0384 (3)
C10	0.4530 (3)	0.08012 (10)	0.81845 (13)	0.0434 (3)
H8	0.4982	0.0513	0.7694	0.052*
C1	0.1094 (3)	0.09104 (10)	0.56073 (13)	0.0455 (4)
C2	0.0134 (3)	-0.03384 (10)	0.61861 (13)	0.0452 (4)
H11	0.0200	-0.0449	0.5499	0.054*
H12	-0.1403	-0.0300	0.6245	0.054*
N2	-0.0196 (2)	-0.14516 (8)	0.71406 (13)	0.0476 (3)
C8	0.0527 (3)	0.06774 (11)	0.73393 (12)	0.0442 (4)
H9	-0.0232	0.0287	0.7633	0.053*
H10	-0.0527	0.1073	0.7137	0.053*
C12	0.5344 (3)	0.14791 (10)	0.96934 (14)	0.0529 (4)
H6	0.6329	0.1652	1.0240	0.063*
C11	0.6047 (3)	0.10564 (11)	0.89812 (15)	0.0501 (4)
H7	0.7530	0.0941	0.9031	0.060*
C4	0.3437 (3)	-0.10609 (10)	0.70322 (14)	0.0466 (4)
H4	0.4352	-0.0713	0.6809	0.056*
C13	0.3140 (4)	0.16421 (10)	0.95790 (14)	0.0519 (4)
H5	0.2664	0.1935	1.0060	0.062*
C5	0.4322 (3)	-0.16716 (12)	0.75666 (16)	0.0553 (5)
H3	0.5836	-0.1743	0.7708	0.066*
C6	0.2920 (4)	-0.21757 (11)	0.78883 (17)	0.0567 (5)
H2	0.3460	-0.2594	0.8252	0.068*
C7	0.0701 (3)	-0.20409 (10)	0.76555 (17)	0.0554 (5)
H1	-0.0242	-0.2383	0.7871	0.066*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C14	0.0927 (17)	0.0403 (9)	0.0584 (12)	-0.0074 (10)	0.0077 (11)	0.0060 (8)
C15	0.0990 (18)	0.0620 (12)	0.0486 (11)	-0.0019 (12)	0.0296 (11)	0.0014 (9)
C16	0.0720 (14)	0.0773 (16)	0.0638 (13)	0.0155 (12)	-0.0114 (11)	0.0176 (11)
N3	0.0476 (8)	0.0460 (7)	0.0408 (7)	0.0030 (6)	0.0075 (6)	-0.0021 (5)
C9	0.0370 (7)	0.0395 (7)	0.0324 (6)	-0.0014 (5)	0.0047 (5)	0.0033 (5)
N1	0.0426 (7)	0.0397 (6)	0.0307 (6)	-0.0034 (5)	0.0021 (5)	0.0008 (4)
C3	0.0404 (8)	0.0389 (7)	0.0347 (7)	-0.0029 (6)	0.0033 (5)	-0.0005 (5)
C10	0.0369 (7)	0.0529 (9)	0.0396 (7)	0.0002 (6)	0.0044 (6)	-0.0019 (6)
C1	0.0559 (10)	0.0416 (8)	0.0371 (7)	0.0006 (6)	0.0034 (7)	0.0054 (6)
C2	0.0446 (8)	0.0451 (8)	0.0409 (8)	-0.0067 (6)	-0.0060 (6)	0.0039 (6)
N2	0.0412 (7)	0.0437 (7)	0.0568 (9)	-0.0058 (6)	0.0056 (6)	0.0045 (6)
C8	0.0342 (7)	0.0603 (10)	0.0369 (7)	-0.0018 (6)	0.0031 (6)	-0.0030 (6)

C12	0.0612 (11)	0.0493 (9)	0.0427 (9)	-0.0136 (8)	-0.0054 (8)	0.0022 (7)
C11	0.0403 (8)	0.0573 (10)	0.0493 (9)	-0.0036 (7)	-0.0013 (7)	0.0072 (7)
C4	0.0371 (8)	0.0526 (9)	0.0514 (9)	-0.0026 (6)	0.0114 (7)	0.0003 (7)
C13	0.0678 (11)	0.0456 (8)	0.0413 (9)	-0.0018 (8)	0.0071 (8)	-0.0066 (7)
C5	0.0433 (9)	0.0576 (10)	0.0637 (12)	0.0114 (8)	0.0061 (8)	-0.0027 (9)
C6	0.0618 (11)	0.0419 (8)	0.0640 (11)	0.0110 (7)	0.0043 (9)	0.0033 (8)
C7	0.0539 (10)	0.0426 (9)	0.0702 (12)	-0.0057 (7)	0.0127 (9)	0.0088 (8)

Geometric parameters (Å, °)

C14—C1	1.523 (3)	C3—C2	1.501 (2)
C14—H20	0.9600	C10—C11	1.385 (2)
C14—H21	0.9600	C10—H8	0.9300
C14—H19	0.9600	C2—H11	0.9700
C15—C1	1.525 (3)	C2—H12	0.9700
C15—H18	0.9600	N2—C7	1.336 (2)
C15—H16	0.9600	C8—H9	0.9700
C15—H17	0.9600	C8—H10	0.9700
C16—C1	1.531 (3)	C12—C11	1.367 (3)
C16—H15	0.9600	C12—C13	1.375 (3)
C16—H14	0.9600	C12—H6	0.9300
C16—H13	0.9600	C11—H7	0.9300
N3—C9	1.336 (2)	C4—C5	1.377 (3)
N3—C13	1.345 (2)	C4—H4	0.9300
C9—C10	1.387 (2)	C13—H5	0.9300
C9—C8	1.509 (2)	C5—C6	1.378 (3)
N1—C8	1.457 (2)	C5—H3	0.9300
N1—C2	1.468 (2)	C6—C7	1.374 (3)
N1—C1	1.497 (2)	C6—H2	0.9300
C3—N2	1.338 (2)	C7—H1	0.9300
C3—C4	1.388 (2)		
C1—C14—H20	109.5	C15—C1—C16	109.18 (19)
C1—C14—H21	109.5	N1—C2—C3	112.38 (12)
H20—C14—H21	109.5	N1—C2—H11	109.1
C1—C14—H19	109.5	C3—C2—H11	109.1
H20—C14—H19	109.5	N1—C2—H12	109.1
H21—C14—H19	109.5	C3—C2—H12	109.1
C1—C15—H18	109.5	H11—C2—H12	107.9
C1—C15—H16	109.5	C7—N2—C3	117.31 (16)
H18—C15—H16	109.5	N1—C8—C9	116.05 (14)
C1—C15—H17	109.5	N1—C8—H9	108.3
H18—C15—H17	109.5	C9—C8—H9	108.3
H16—C15—H17	109.5	N1—C8—H10	108.3
C1—C16—H15	109.5	C9—C8—H10	108.3
C1—C16—H14	109.5	H9—C8—H10	107.4
H15—C16—H14	109.5	C11—C12—C13	118.10 (17)
C1—C16—H13	109.5	C11—C12—H6	121.0
H15—C16—H13	109.5	C13—C12—H6	121.0
H14—C16—H13	109.5	C12—C11—C10	119.36 (17)

supplementary materials

C9—N3—C13	117.70 (16)	C12—C11—H7	120.3
N3—C9—C10	121.88 (15)	C10—C11—H7	120.3
N3—C9—C8	114.75 (14)	C5—C4—C3	119.78 (16)
C10—C9—C8	123.24 (14)	C5—C4—H4	120.1
C8—N1—C2	110.06 (14)	C3—C4—H4	120.1
C8—N1—C1	115.35 (14)	N3—C13—C12	123.79 (17)
C2—N1—C1	113.90 (12)	N3—C13—H5	118.1
N2—C3—C4	121.83 (15)	C12—C13—H5	118.1
N2—C3—C2	116.63 (15)	C4—C5—C6	118.68 (17)
C4—C3—C2	121.42 (15)	C4—C5—H3	120.7
C11—C10—C9	119.16 (17)	C6—C5—H3	120.7
C11—C10—H8	120.4	C7—C6—C5	117.95 (18)
C9—C10—H8	120.4	C7—C6—H2	121.0
N1—C1—C14	109.25 (14)	C5—C6—H2	121.0
N1—C1—C15	108.06 (15)	N2—C7—C6	124.45 (18)
C14—C1—C15	107.53 (19)	N2—C7—H1	117.8
N1—C1—C16	112.96 (17)	C6—C7—H1	117.8
C14—C1—C16	109.70 (18)		
C13—N3—C9—C10	-1.1 (2)	C2—C3—N2—C7	175.54 (17)
C13—N3—C9—C8	174.86 (16)	C2—N1—C8—C9	134.62 (15)
N3—C9—C10—C11	1.0 (2)	C1—N1—C8—C9	-94.82 (18)
C8—C9—C10—C11	-174.62 (17)	N3—C9—C8—N1	165.09 (14)
C8—N1—C1—C14	50.8 (2)	C10—C9—C8—N1	-19.0 (2)
C2—N1—C1—C14	179.45 (17)	C13—C12—C11—C10	-0.8 (3)
C8—N1—C1—C15	167.47 (17)	C9—C10—C11—C12	0.0 (3)
C2—N1—C1—C15	-63.8 (2)	N2—C3—C4—C5	0.3 (3)
C8—N1—C1—C16	-71.6 (2)	C2—C3—C4—C5	-175.51 (17)
C2—N1—C1—C16	57.1 (2)	C9—N3—C13—C12	0.3 (3)
C8—N1—C2—C3	-77.86 (18)	C11—C12—C13—N3	0.7 (3)
C1—N1—C2—C3	150.82 (15)	C3—C4—C5—C6	-0.1 (3)
N2—C3—C2—N1	137.29 (16)	C4—C5—C6—C7	0.1 (3)
C4—C3—C2—N1	-46.7 (2)	C3—N2—C7—C6	0.5 (3)
C4—C3—N2—C7	-0.5 (3)	C5—C6—C7—N2	-0.3 (3)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C7—H1 \cdots Cg2 ⁱ	0.93	2.97	3.819 (2)	153
C15—H16 \cdots Cg1 ⁱⁱ	0.96	2.94	3.836 (2)	156

Symmetry codes: (i) $x-1/2, y-1/2, z$; (ii) $x, -y, z-1/2$.

Fig. 1

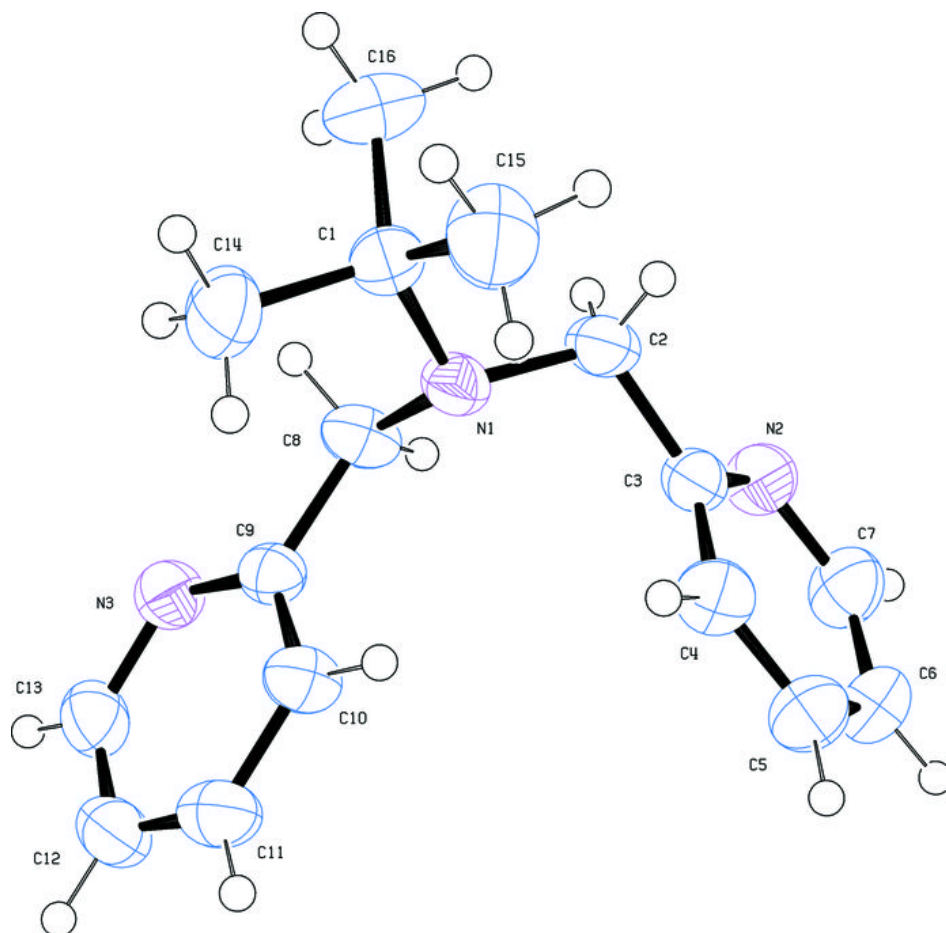


Fig. 2

