4,6,12,14-Tetra-*tert*-butyl-17-*N*-(6-methyl-pyridin-2-yl)-8,16-dioxa-17-azatetracyclo-[7.7.1.0^{2,7}.0^{10,15}]heptadeca-2,4,6,10,12,14-hexaene methanol solvate

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The molecule of the title compoumd, $C_{37}H_{52}N_2O_3$, exhibits a propeller-like conformation, influenced by one intramolecular C—H$\cdots$N and four intramolecular C—H$\cdots$O hydrogen bonds. In the crystal structure, there are four weak C—H$\cdots\pi$ interactions.

Comment

Multidentate Schiff base ligands and their metal complexes have been extensively studied for many years (Daier *et al.*, 2004; Munro & Camp, 2003; Weber, 1967; Xu *et al.*, 2001). Schiff bases can be prepared by condensation of different types of amines and carbonyl compounds; one of the most popular methods has been the use of salicylideneamines, which can serve as efficient models for biologically important systems (Long, 1995) in addition to their diverse chelating ability (Kim *et al.*, 2001). The title compound, (I), was unexpectedly obtained in the reaction of 3,5-di-*tert*-butyl-salicylaldehyde with 6-amino-2-methylpyridine.

(I)
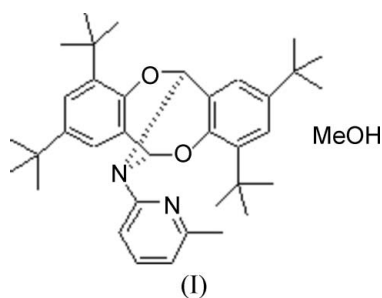
The title compound, (I), possesses three aryl rings, *viz.* benzene ring 1 (atoms C1–C6; denoted *R*1), benzene ring 2 (C10–C15; *R*2) and pyridyl ring 3 (N2/C19–C23; *R*3). These are connected to the central polyhedron (N1/C9/C18/O1/O2/C3/C4/C10/C11) to give a propeller-like conformation, which is influenced by one intramolecular C—H$\cdots$N and four intramolecular C—H$\cdots$O hydrogen bonds (Fig. 3 and Table 1). The dihedral angles for *R*1/*R*2, *R*1/*R*3 and *R*2/*R*3 are 79.4 (1), 27.8 (1) and 73.0 (1)°, respectively. The bond lengths and angles are unexceptional.

C—H$\cdots\pi$ interactions often play an important role in the formation of crystal structures (Low *et al.*, 2004; Sylvestre *et al.*, 2005). In the case of (I), an extended crystal structure (Fig. 4) is formed through weak intermolecular C—H$\cdots\pi$ interactions (Table 1).

Experimental

The title compound was synthesized by the reaction of 3,5-di-*tert*-butylsalicylaldehyde and 6-methyl-2-aminopyridine, under a nitrogen

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. Only one component of the disordered *tert*-butyl group is shown. The solvent molecule has been omitted for the sake of clarity.

Figure 3
The structure of (I), showing intramolecular hydrogen bonds (indicated by green lines).

Figure 2
The structure of (I), showing the propeller-like conformation.

Figure 4
The packing of (I), viewed along the *a* axis, showing the intermolecular C—H···π interactions as dashed lines.

atmosphere. A mixture of 3,5-di-*tert*-butylsalicylaldehyde (4 mmol) and 2-amino-6-methylpyridine (4.4 mmol) in ethanol (20 ml) was heated under reflux for 24 h, after adding formic acid as a catalyst. It was then allowed to stand at room temperature overnight. The solid product was isolated by filtration, and purified by thin-layer chromatography. Pale-yellow single crystals suitable for X-ray diffraction were obtained by evaporation of a methanol solution of the product.

Crystal data

$C_{36}H_{48}N_2O_2 \cdot CH_4O$	$Z = 2$
$M_r = 572.81$	$D_x = 1.091$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 10.282$ (2) Å	Cell parameters from 877
$b = 12.775$ (3) Å	reflections
$c = 15.601$ (3) Å	$\theta = 2.3–18.5°$
$\alpha = 66.313$ (4)°	$\mu = 0.07$ mm^{-1}
$\beta = 82.711$ (4)°	$T = 273$ (2) K
$\gamma = 68.295$ (4)°	Block, pale yellow
$V = 1743.0$ (7) Å^3	$0.30 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	1913 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.049$
Absorption correction: none	$\theta_{max} = 25.0°$
9105 measured reflections	$h = -12 \rightarrow 12$
6047 independent reflections	$k = -15 \rightarrow 13$
	$l = -18 \rightarrow 10$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0568P)^2]$
$wR(F^2) = 0.082$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.62$	$(\Delta/\sigma)_{max} = 0.015$
6047 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
408 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C18—H18$\cdots$N2	0.98	2.36	2.808 (3)	107
C161—H16$A\cdots$O2	0.96	2.37	3.013 (6)	124
C162—H16$F\cdots$O2	0.96	2.31	2.967 (8)	125
C82—H82$C\cdots$O1	0.96	2.40	3.033 (9)	124
C83—H83$A\cdots$O1	0.96	2.34	2.980 (9)	123
C163—H16$I\cdots$Cg1^i	0.96	2.91	3.565 (7)	127
C162—H16$D\cdots$Cg2^{ii}	0.96	3.06	3.893 (11)	146
C73—H73$A\cdots$Cg2^{iii}	0.96	2.95	3.725 (9)	138
C24—H24$B\cdots$Cg1^i	0.96	2.65	3.147 (7)	113

Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $x - 1, y + 1, z - 1$; (iii) $x - 1, y, z$. Cg1 is the centroid of R1 and Cg2 is the centroid of R2

After their location, all H atoms were placed in idealized positions and refined using a riding model; C—H = 0.93–0.98 Å, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). One of the *tert*-butyl groups is disordered over three sites; there are three sets of methyl groups (C171/C172/C173, C174/C175/C176 and C177/C178/C179) with site-occupancy factors of 0.5, 0.25 and 0.25 for groups 1, 2 and 3, respectively.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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