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(*E*)-*N*′-(4-Benzyloxy-3-methoxybenzylidene)isonicotinohydrazide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.118
Data-to-parameter ratio = 15.4

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

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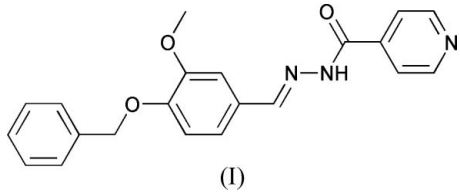
The title compound, $C_{21}H_{19}N_3O_3$, was prepared by the reaction of 4-benzyloxy-3-methoxybenzaldehyde and isonicotinohydrazide. The vanillin group makes dihedral angles of 27.88 (7) and 58.94 (6)° with the planes of the pyridine and phenyl rings, respectively. A weak intermolecular C—H···N hydrogen bond helps to consolidate the crystal packing.

Comment

Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986). One of the aims of investigating the structural chemistry of Schiff bases is to develop protein and enzyme mimics (Santos *et al.*, 2001). As part of an investigation of the coordination properties of Schiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I). In (I) (Fig. 1), the vanillin group (C8–C13/C15/O1/O2) is planar, with an r.m.s. deviation from the mean plane of 0.0325 Å. It makes dihedral angles of 27.88 (7) and 58.94 (6)° with the pyridine ring (C17–C21/N3) and the phenyl ring (C1–C6), respectively. The dihedral angle between the pyridine ring and the phenyl ring is 32.58 (10)°. All bond lengths and angles for (I) (Table 1) are within normal ranges. A weak intermolecular C—H···N hydrogen bond is found in (I) (Table 2), which helps to consolidate the crystal packing (Fig. 2).



(I)

Experimental

An anhydrous ethanol solution of 4-(benzyloxy)-3-methoxybenzaldehyde (2.42 g, 10 mmol) was added to an anhydrous ethanol solution of isonicotinohydrazide (1.37 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen. A pale-yellow product precipitated, and was then isolated, recrystallized from ethanol and dried in a vacuum to give the pure compound in 83% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{21}H_{19}N_3O_3$
M_r = 361.39
Orthorhombic, *Pbca*
a = 11.0418 (17) Å
b = 8.0714 (12) Å
c = 41.313 (7) Å
V = 3682.0 (10) Å^3
Z = 8
D_x = 1.304 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3439 reflections
θ = 2.7–25.5°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, colorless
0.24 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.968, T_{max} = 0.991
19513 measured reflections
3765 independent reflections
2281 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 26.5°
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 10$
$l = -42 \rightarrow 51$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.118
S = 1.01
3765 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 0.519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C8	1.357 (2)	N1—C15	1.279 (2)
O1—C7	1.439 (2)	N1—N2	1.3821 (19)
O2—C13	1.369 (2)	N2—C16	1.350 (2)
O2—C14	1.415 (2)	N3—C19	1.321 (2)
O3—C16	1.220 (2)	N3—C20	1.329 (3)
C8—O1—C7	117.75 (14)	C16—N2—N1	119.59 (15)
C13—O2—C14	117.54 (14)	C19—N3—C20	115.63 (17)
C15—N1—N2	115.32 (15)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C18—H18···N3^{i}	0.93	2.55	3.475 (3)	174

Symmetry code: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

The H atoms were included in calculated positions and refined using a riding model approximation [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH; C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for CH_2; C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for CH_3; and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for NH].

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); 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*.

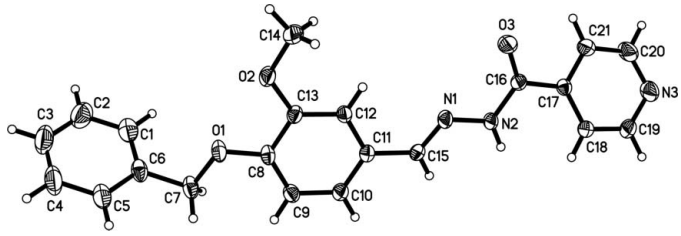


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

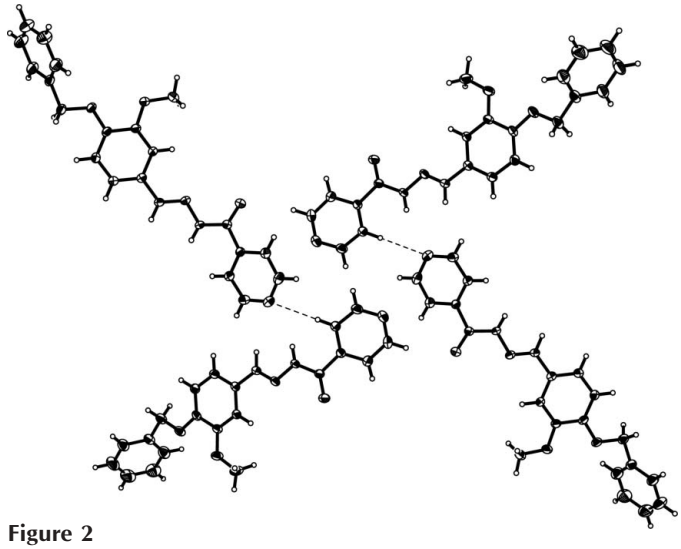


Figure 2
Intermolecular hydrogen bonding interactions (dashed lines) in (I).

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