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(*E*)-*N*′-[3-Ethoxy-4-(4-nitrobenzyloxy)benzylidene]isonicotinohydrazide

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.161
Data-to-parameter ratio = 11.5

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

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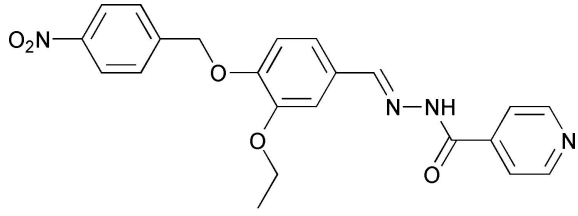
In the title compound, $C_{22}H_{20}N_4O_5$, the central vanillin group makes dihedral angles of 4.44 (11) and 60.33 (6)° with the pyridine and other benzene rings. The crystal packing is stabilized by N—H···N hydrogen bonds and C—H···O interactions, leading to an infinite network.

Comment

The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986; Klayman *et al.*, 1979). 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 here the synthesis and structure of the title compound, (I).



(I)

In the molecule of compound (I) (Fig. 1), the vanillin group (C8–C13/C16/O3) is planar, with an r.m.s. deviation for fitted atoms of 0.0223 Å. This plane makes dihedral angles of 4.44 (11) and 60.33 (6)° with the pyridine ring (C18–C22/N4) and the terminal benzene ring (C1–C6), respectively. The dihedral angle between the pyridine and benzene rings is 60.21 (7)°. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

The crystal packing of (I) is stabilized by intermolecular N—H···N hydrogen bonds and two C—H···O interactions, thus forming an infinite network (Table 1 and Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 4-(4-nitrobenzyloxy)-3-ethoxybenzaldehyde (3.01 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of isonicotinohydrazide (1.37 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a yellow precipitate. The product was isolated, recrystallized from ethanol and then dried in a vacuum to give the pure compound in 88% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{22}H_{20}N_4O_5$
M_r = 420.42
Monoclinic, $P2_1/c$
a = 12.454 (3) Å
b = 11.163 (2) Å
c = 14.923 (3) Å
β = 103.82 (3)°
V = 2014.6 (8) Å^3
Z = 4
D_x = 1.386 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, yellow
0.16 × 0.14 × 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} = 0.990
11991 measured reflections
3546 independent reflections
2525 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.161
S = 1.08
3546 reflections
308 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.09P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···N4^{i}	0.86	2.29	3.106 (3)	158
C4—H4A···O2^{ii}	0.93	2.52	3.336 (3)	146
C21—H21A···O5^{iii}	0.93	2.43	3.308 (3)	158

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{5}{2}$; (ii) $-x+1, -y+2, -z+1$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

The ethoxy group was refined with a disorder model over two different positions, O4/C14/C15 and O4′/C14′/C15′, both with site-occupation factors of 0.5. In the disordered components, restrained bond distances were 1.54 (1) Å for C—C bonds and 1.45 (1) Å for C—O bonds. H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene C—H, and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for imino N—H.

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*.

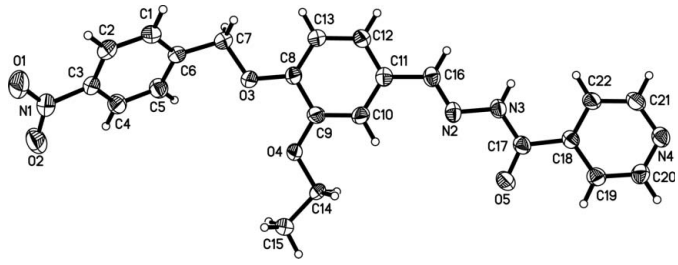


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. Only one component of the disordered ethoxy group is shown.

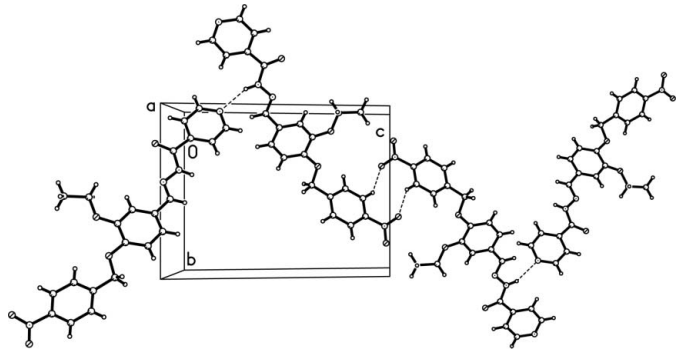


Figure 2
A packing diagram for (I), with hydrogen bonds drawn as dashed lines.

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