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(*E*)-*N*′-(3-Ethoxy-4-methoxybenzylidene)-benzohydrazide

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Key indicators

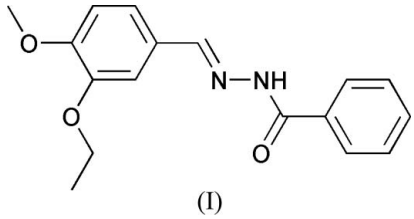
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.115
Data-to-parameter ratio = 15.6

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

In the title compound, $C_{17}H_{18}N_2O_3$, the isovanillin group makes a dihedral angle of 9.63 (11)° with the plane of the terminal phenyl ring. Intermolecular N—H···O hydrogen bonds help to consolidate the crystal packing.

Comment

There has been a steady growth of interest in the synthesis, structure, and reactivity of Schiff bases due to their potential applications in biological modeling, catalysis, design of molecular magnets and materials chemistry (Jones *et al.*, 1979; Larson & Pecoraro, 1991). Consequently, a significant effort has been devoted to the synthesis of Schiff base derivatives (Santos *et al.*, 2001). Structural information is useful when investigating the coordination properties of Schiff bases functioning as ligands. We report here the synthesis and molecular structure of the benzohydrazide Schiff base compound (I) (Fig. 1).



(I)

In (I), the isovanillin group (C8–C14/O2/O3) is essentially planar, with an r.m.s. deviation of fitted atoms of 0.0179 Å. This plane makes a dihedral angle of 9.63 (11)° with the terminal phenyl ring (C1–C6), which is similar to the value of 9.31 (11)° found in the closely related structure of (*E*)-*N*′-{1-[4-(2-hydroxyethoxy)-3-methoxyphenyl]ethylidene}benzohydrazide hydrate (Diao *et al.*, 2005).

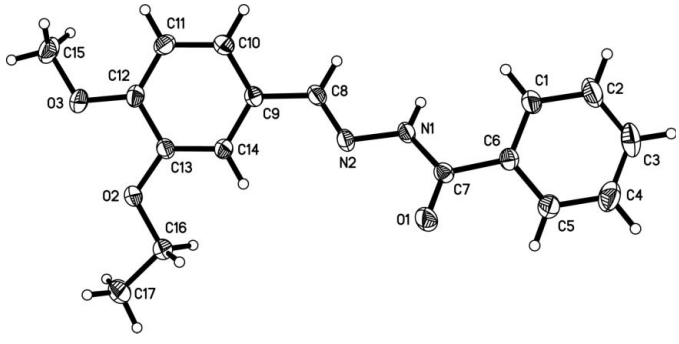


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

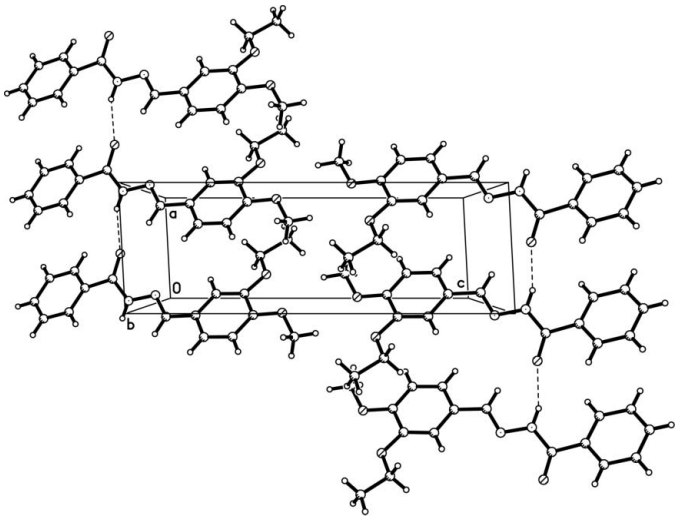


Figure 2
Packing diagram for (I), with hydrogen bonds drawn as dashed lines.

Furthermore, the plane of the functional group (C7/O1/N1/N2) of the benzohydrazide makes dihedral angles of 28.45 (10) and 32.21 (8)° with its attached phenyl ring and the isovanillin group, respectively.

All bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987).

The packing is stabilized by intermolecular N1–H1···O1^{i} (symmetry code as in Table 2) hydrogen bonds, that form infinite chains along the *a* axis (Fig. 2 and Table 2).

Experimental

An anhydrous ethanol solution of 3-ethoxy-4-methoxybenzaldehyde (1.80 g, 10 mmol) was added to an anhydrous ethanol solution of benzohydrazide (1.36 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, whereupon a yellowish precipitate appeared. The product was isolated, recrystallized from ethanol and then dried in a vacuum to give the pure compound in 88% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{17}H_{18}N_2O_3$
M_r = 298.33
Monoclinic, $P2_1/n$
a = 5.0465 (8) Å
b = 20.264 (3) Å
c = 14.956 (2) Å
β = 92.938 (3)°
V = 1527.4 (4) Å^3
Z = 4
D_x = 1.297 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2371 reflections
θ = 2.9–26.3°
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, colorless
0.18 × 0.16 × 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
8556 measured reflections
3134 independent reflections
1985 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.4°
$h = -6 \rightarrow 6$
$k = -25 \rightarrow 25$
$l = -9 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.01
3134 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0466P)^2 + 0.3517P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.2279 (19)	N1—C7	1.344 (2)
O2—C13	1.367 (2)	N1—N2	1.3892 (19)
O2—C16	1.434 (2)	N2—C8	1.273 (2)
C13—O2—C16	117.52 (14)	N1—C7—C6	115.36 (15)
C7—N1—N2	120.55 (14)	N2—C8—C9	121.88 (17)
C8—N2—N1	114.35 (15)	O2—C13—C14	125.21 (17)
O1—C7—N1	122.84 (16)	O2—C13—C12	114.65 (15)
O1—C7—C6	121.80 (16)	O2—C16—C17	106.75 (16)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.11	2.9131 (19)	155

Symmetry code: (i) $x-1, y, z$.

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 methylene CH_2; C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl CH_3; N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for imino 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*.

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