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(*E*)-1-(3-Ethoxy-4-hydroxybenzylidene)-2-(4-nitrophenyl)hydrazine

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The molecule of the title compound, $C_{15}H_{15}N_3O_4$, is non-planar. The ethylvanillin group makes a dihedral angle of 7.68 (7)° with the nitrophenylhydrazine mean plane. A trifurcated intra/intermolecular O—H···(O,O,O) hydrogen-bond system helps to establish the molecular conformation and consolidate the crystal packing.

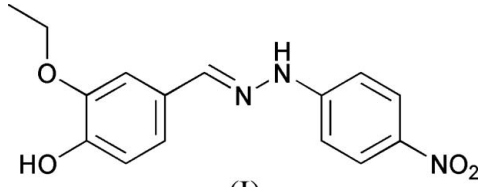
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.110
Data-to-parameter ratio = 13.9

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

Comment

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) (Fig. 1).



(I)

The ethylvanillin group (C1–C9/O1/O2) in (I) is planar, with an r.m.s. deviation, δ, from the mean plane of 0.044 Å. The nitrophenylhydrazine moiety (C10–C15/N1/N2/N3) is also planar, with δ = 0.030 Å. The dihedral angle between the two mean planes is 7.68 (7)°. The bond lengths and angles for (I) are unexceptional.

A trifurcated O—H···(O,O,O) intra/intermolecular O—H···O hydrogen-bond system is found in (I) (Table 1). The intramolecular bond stabilizes the conformation of the molecule, while the intermolecular bonds to the two O atoms of a nearby nitro group help to consolidate the crystal packing (Fig. 2). Conversely, the NH grouping does not participate in hydrogen bonds.

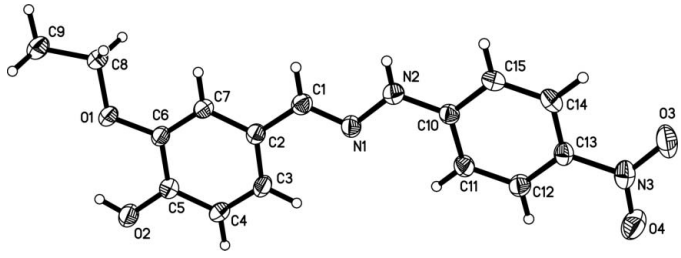


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

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Experimental

An anhydrous ethanol solution of 3-ethoxy-4-hydroxybenzaldehyde (1.66 g, 10 mmol) was added to an anhydrous ethanol solution of 1-(4-nitrophenyl)hydrazine (1.53 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen. A yellow precipitate appeared, which was isolated, recrystallized from ethanol, and then dried in a vacuum to give the pure compound in 87% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{15}H_{15}N_3O_4$
M_r = 301.30
Monoclinic, $P2_1/c$
a = 10.148 (2) Å
b = 9.0980 (19) Å
c = 15.967 (3) Å
β = 103.868 (3)°
V = 1431.2 (5) Å^3
Z = 4
D_x = 1.398 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2008 reflections
θ = 2.6–25.9°
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, yellow
0.34 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.975
7792 measured reflections
2904 independent reflections
1758 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 26.4°
$h = -12 \rightarrow 12$
$k = -9 \rightarrow 11$
$l = -19 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.00
2904 reflections
209 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.2257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0170 (18)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.83 (3)	2.27 (2)	2.6840 (19)	111 (2)
O2—H2···O4^{i}	0.83 (3)	2.26 (3)	2.987 (2)	146 (2)
O2—H2···O3^{i}	0.83 (3)	2.49 (3)	3.205 (2)	145 (2)

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

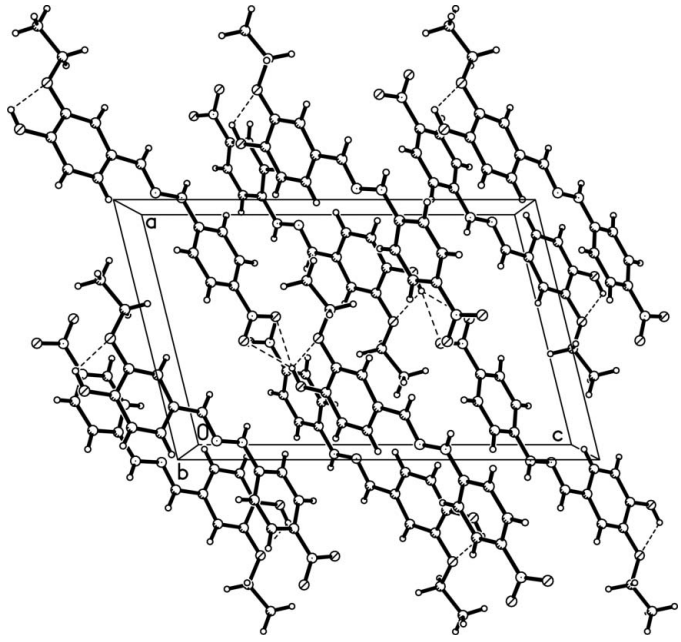

Figure 2
Hydrogen-bonding interactions (dashed lines) in (I).

The H atoms attached to O and N atoms were found in a difference map and their positions and U_{iso} values were freely refined. Other H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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