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

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Key indicators

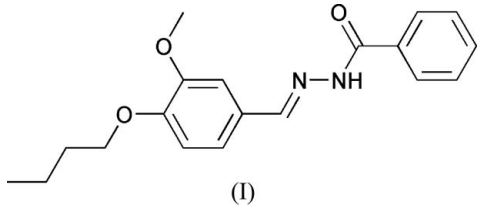
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.125
Data-to-parameter ratio = 16.3

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

The molecule of the title compound, $C_{19}H_{22}N_2O_3$, is not planar. The vanillin residue makes dihedral angles of 4.84 (18) and 11.96 (7)° with the planes of the butyl group and the terminal benzene ring, respectively. Intermolecular N—H···O and C—H···O hydrogen bonds help to consolidate the crystal packing.

Comment

Macrocyclic and macroacyclic ligands, such as Schiff bases and crown ethers, have attracted much attention in biology and chemistry (Kahwa *et al.* 1986). Consequently, a large array of metal complexes of Schiff bases have been prepared as mimics of active centres in different proteins and enzymes (Santos *et al.* 2001). Structural investigations can provide useful information on the coordination properties of Schiff bases functioning as ligands. In the present study, we report the synthesis and molecular structure of the benzohydrazide Schiff base derivative (I) (Fig. 1).



(I)

In (I) the vanillin residue (C8–C14/O2/O3) is planar, with an r.m.s. deviation of fitted atoms of 0.0053 Å. This plane makes a dihedral angle of 11.96 (7)° with the terminal benzene ring (C1–C6), in contrast 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). The butyl group (C15–C18) is also reasonably planar, with an r.m.s. deviation for fitted atoms of 0.0077 Å. It makes dihedral angles of 4.84 (18)° and 16.29 (14)° with the

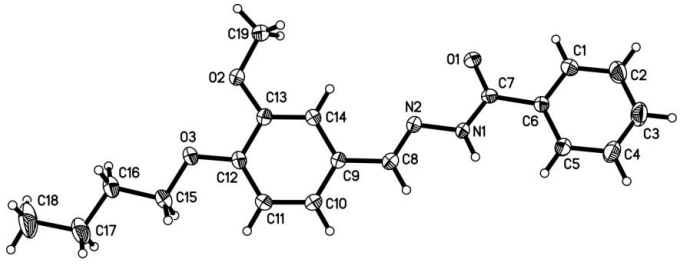


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

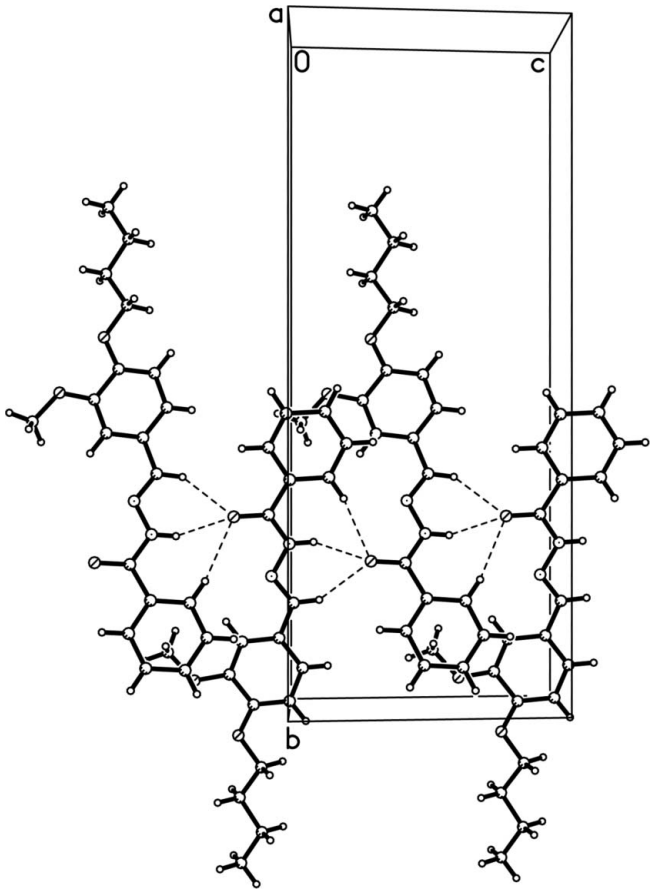


Figure 2
Packing diagram for (I), with hydrogen bonds drawn as dashed lines.

vanillin residue and the terminal benzene ring, respectively.

All bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). Packing is stabilized by intermolecular N1—H1···O1 hydrogen bonds, forming infinite chains along the *c* axis, together with weak, non-classical intermolecular C5—H5···O1 and C8—H8···O1 hydrogen bonds (Fig. 2, Table 2).

Experimental

An anhydrous ethanol solution of 4-butoxy-3-methoxybenzaldehyde (2.08 g, 10 mmol) was added to an anhydrous ethanol solution of benzohydrazide (1.36 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, whereupon a yellow precipitate appeared. The product was isolated, recrystallized from ethanol and dried in a vacuum to give the pure compound in 88% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{19}H_{22}N_2O_3$
M_r = 326.39
Monoclinic, $P2_1/c$
a = 7.583 (4) Å
b = 24.124 (11) Å
c = 9.761 (5) Å
β = 97.180 (8)°
V = 1771.7 (14) Å^3
Z = 4
D_x = 1.224 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1568 reflections
θ = 2.3–21.7°
μ = 0.08 mm^{-1}
T = 294 (2) K
Block, colourless
0.28 × 0.22 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.961, T_{max} = 0.988
9822 measured reflections
3582 independent reflections
1699 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 26.3°
$h = -9 \rightarrow 9$
$k = -16 \rightarrow 30$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.125
S = 0.98
3582 reflections
220 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0095 (12)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.232 (2)	O3—C15	1.432 (2)
O2—C13	1.364 (2)	N1—C7	1.344 (2)
O2—C19	1.430 (2)	N1—N2	1.383 (2)
O3—C12	1.362 (2)	N2—C8	1.273 (3)
C13—O2—C19	117.84 (16)	N2—C8—C9	121.4 (2)
C12—O3—C15	117.01 (17)	O3—C12—C11	125.3 (2)
C7—N1—N2	119.56 (17)	O3—C12—C13	115.29 (19)
C8—N2—N1	114.77 (18)	O2—C13—C14	125.13 (19)
O1—C7—N1	121.89 (19)	O2—C13—C12	115.27 (18)
O1—C7—C6	121.3 (2)	O3—C15—C16	108.58 (19)
N1—C7—C6	116.79 (18)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.15	2.961 (3)	157
C5—H5···O1^{i}	0.93	2.53	3.451 (3)	169
C8—H8···O1^{i}	0.93	2.37	3.208 (3)	149

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

H atoms were included in calculated positions and refined using the riding-model approximation. Constrained C—H and N—H bond lengths and isotropic U parameters: 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic CH; 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene CH_2; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl CH_3; 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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