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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.130
Data-to-parameter ratio = 13.0

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

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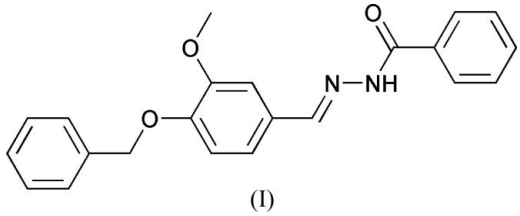
The title compound, $C_{22}H_{20}N_2O_3$, was prepared by the reaction of 4-benzyloxy-3-methoxybenzaldehyde and benzohydrazide. The central vanillin system makes dihedral angles of 18.2 (1) and 14.3 (1)° with the planes of the benzohydrazide and benzyl groups, respectively. The crystal structure is stabilized by intermolecular N—H···O hydrogen bonding.

Comment

Macrocyclic and macroacyclic ligands, such as Schiff bases and crown ethers, have played an important role in our understanding of the nature of metal–metal ion interactions in systems of biological interest (Kahwa *et al.*, 1986). The homodinuclear complexes of ligands and lanthanide cations (Ln^{3+}) could provide information regarding $Ln^{3+}\cdots Ln^{3+}$ interactions that is critical for our scientific understanding and technological applications of rare earths (Lehn, 1980). Consequently, a large array of metal complexes of Schiff bases have been prepared as mimics of active centres in various proteins and enzymes (Santos *et al.*, 2001). As part of our investigation, we now report the synthesis and molecular structure of the title compound, (I).



(I)

As shown in Fig. 1, the central vanillin system (C8–C13/C15/O1/O2) is planar, with an r.m.s. deviation of fitted atoms of 0.016 Å. The benzyl group (C1–C7) is planar, with an r.m.s. deviation of fitted atoms of 0.007 Å. The dihedral angle between the two planes is 14.3 (1)°. The benzohydrazide group (C16–C22) is planar, with an r.m.s. deviation of fitted atoms of 0.008 Å and makes a dihedral angle of 18.2 (1)° with the central system. This angle is somewhat larger than the value of 9.3 (1)° found in (*E*)-*N*′-{1-[4-(2-hydroxyethoxy)-3-methoxyphenyl]ethylidene}benzohydrazide monohydrate (Diao *et al.*, 2005).

It should be noted that intermolecular N—H···O hydrogen bonding is found in the crystal structure (Table 1), and this stabilizes the zigzag supramolecular structure (Fig. 2).

Experimental

An anhydrous ethanol solution of 4-benzyloxy-3-methoxybenzaldehyde (2.42 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 pale-yellow precipitate appeared. The product was then isolated, recrystallized from ethanol and then dried in a vacuum to give the pure compound in 85% yield. Colourless single crystals of (I), suitable for X-ray analysis, were obtained by slow evaporation of an ethanol solution.

Crystal data

$C_{22}H_{20}N_2O_3$
M_r = 360.40
Monoclinic, $P2_1/c$
a = 7.528 (3) Å
b = 25.027 (10) Å
c = 9.938 (4) Å
β = 97.293 (8)°
V = 1857.3 (13) Å^3
Z = 4
D_x = 1.289 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1673 reflections
θ = 2.6–23.1°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.30 × 0.24 × 0.20 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} = 0.983
8409 measured reflections
3225 independent reflections
1786 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 25.0°
$h = -7 \rightarrow 8$
$k = -26 \rightarrow 29$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.130
S = 1.00
3225 reflections
249 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.89 (1)	2.11 (1)	2.958 (2)	158 (2)

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

The H atom attached to N2 was found in a difference Fourier map and refined freely to give N—H = 0.89 (1) Å. Carbon-bound H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined using a riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C) or 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*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*.

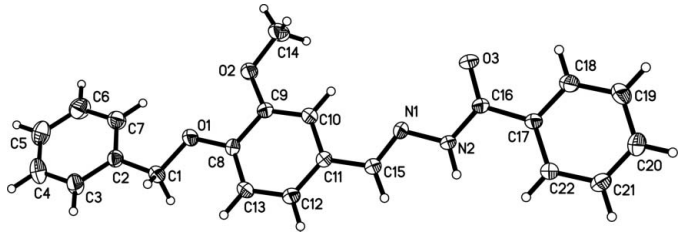


Figure 1
The structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

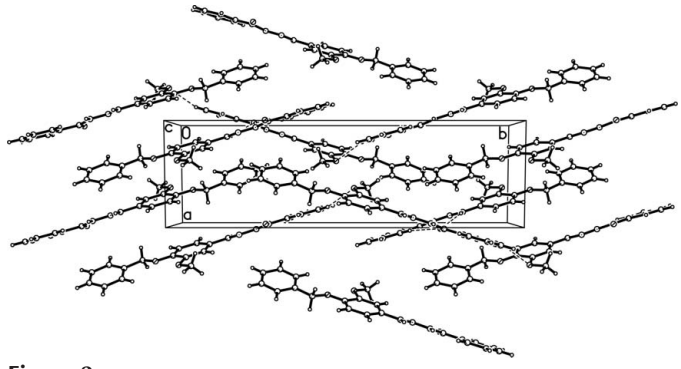


Figure 2
Intermolecular hydrogen-bonding interactions (dashed lines) in (I).

References

Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
Diao, C.-H., Yu, M., Chen, X., Jing, Z.-L & Deng, Q.-L. (2005). *Acta Cryst.* E**61**, o3500–o3501.
Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.
Lehn, J. M. (1980). *J. Pure Appl. Chem.* **52**, 2441.
Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.