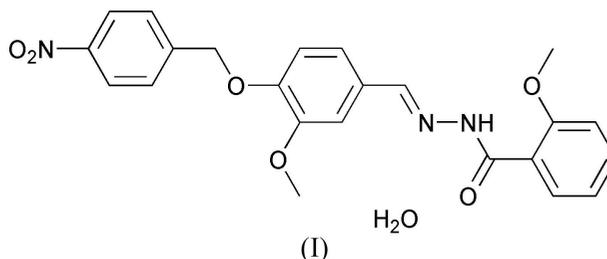


(E)-2-Methoxy-N'-[3-methoxy-4-(4-nitrobenzyloxy)-benzylidene]benzohydrazide monohydrate**Chun-Hua Diao* and Ming Yu**College of Sciences, Tianjin University of
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In the title compound, $C_{23}H_{23}N_3O_7$, the vanillin group makes dihedral angles of 15.55 (12) and 10.89 (14)° with the nitrobenzene ring and the benzohydrazide mean plane, respectively. Intramolecular N—H···O hydrogen bonds help to stabilize the molecular conformation, while intermolecular and intramolecular O—H···O hydrogen bonds link molecules, forming an infinite network.

Received 25 October 2006
Accepted 6 November 2006**Key indicators**Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.060
 wR factor = 0.181
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Comment**

There has been steady growth of interest in the structure and reactivity of Schiff bases due to their potential biological activities such as antibacterial and antitumor (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 the synthesis and structure of the title compound, (I).



In (I) (Fig. 1), the vanillin group (C8–C13/C15/O3/O4) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.0084 Å. This plane makes dihedral angles of 10.89 (14) and 15.55 (12)° with the benzohydrazide residue (C17–C22) and the nitrobenzene ring (C1–C6), respectively. The dihedral angle between the benzohydrazide residue and the nitrobenzene ring is 4.67 (16)°. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

An intramolecular hydrogen bond links the NH group to O6, thereby influencing the molecular conformation. The crystal structure contains two intermolecular O—H···O hydrogen bonds (Table 1) linking the main molecule and the solvent molecule. These O—H···O hydrogen bonds link molecules into an infinite network (Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 3-methoxy-4-(4-nitrobenzyloxy)benzaldehyde (2.87 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 2-methoxybenzohydrazide (1.66 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 78% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a 95% ethanol–water solution.

Crystal data

$C_{23}H_{21}N_3O_6 \cdot H_2O$ $Z = 8$
 $M_r = 453.44$ $D_x = 1.374 \text{ Mg m}^{-3}$
 Monoclinic, $C2/c$ Mo $K\alpha$ radiation
 $a = 37.270 (6) \text{ \AA}$ $\mu = 0.10 \text{ mm}^{-1}$
 $b = 8.5936 (13) \text{ \AA}$ $T = 294 (2) \text{ K}$
 $c = 14.431 (2) \text{ \AA}$ Block, yellow
 $\beta = 108.436 (5)^\circ$ $0.26 \times 0.22 \times 0.18 \text{ mm}$
 $V = 4384.8 (12) \text{ \AA}^3$

Data collection

Bruker SMART APEX CCD area-detector diffractometer 11971 measured reflections
 φ and ω scans 4444 independent reflections
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996) 2548 reflections with $I > 2\sigma(I)$
 $T_{\min} = 0.952$, $T_{\max} = 0.982$ $R_{\text{int}} = 0.036$
 $\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.074P)^2 + 5.1033P]$
 $R[F^2 > 2\sigma(F^2)] = 0.060$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.181$ $(\Delta/\sigma)_{\text{max}} = 0.001$
 $S = 1.01$ $\Delta\rho_{\text{max}} = 0.52 \text{ e \AA}^{-3}$
 4444 reflections $\Delta\rho_{\text{min}} = -0.58 \text{ e \AA}^{-3}$
 301 parameters
 H-atom parameters constrained

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N3-H3 \cdots O6$	0.86	1.96	2.635 (3)	135
$O7-H7C \cdots O5$	0.85	2.14	2.913 (4)	149
$O7-H7D \cdots O4^i$	0.85	2.43	2.986 (3)	123

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

The H atoms were included in calculated positions and refined using a riding-model approximation. Constrained C–H and N–H bond lengths and isotropic U parameters: 0.93 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for Csp^2 , 0.97 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylene, 0.96 \AA and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl, 0.85 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$ for water, and 0.86 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ for imino H atoms.

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

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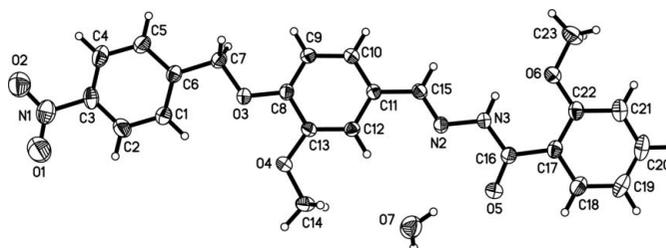


Figure 1

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

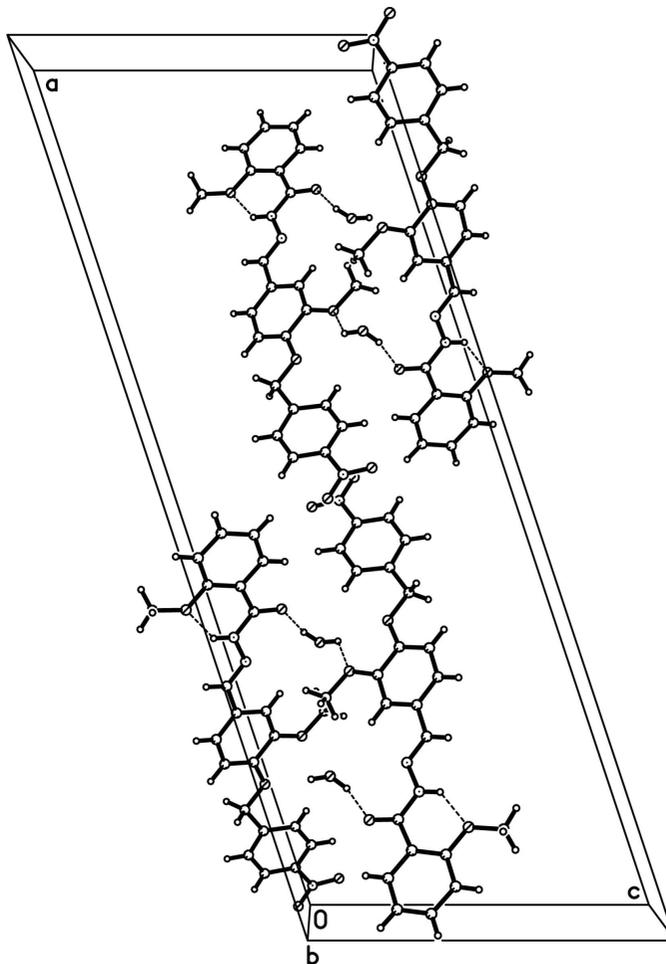


Figure 2

A packing diagram for (I), with hydrogen bonds shown as dashed lines.

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