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## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.044  
 $wR$  factor = 0.129  
Data-to-parameter ratio = 15.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*N'*-[(*E*)-4-(2-Hydroxyethoxy)-3-methoxy-  
benzylidene]benzohydrazide monohydrate

The title compound,  $\text{C}_{17}\text{H}_{18}\text{N}_2\text{O}_4 \cdot \text{H}_2\text{O}$ , was prepared by the reaction of 4-(2-hydroxyethoxy)-3-methoxybenzaldehyde and benzohydrazide. The crystal structure determination was undertaken in order to study the effect of intramolecular hydrogen bonding ( $\text{C}-\text{H} \cdots \text{O}$  and  $\text{N}-\text{H} \cdots \text{O}$ ) on the molecular conformation, and the effect of intermolecular hydrogen bonding ( $\text{O}-\text{H} \cdots \text{O}$ ,  $\text{O}-\text{H} \cdots \text{N}$  and  $\text{C}-\text{H} \cdots \text{O}$ ) on the stability of the structure in the solid state.

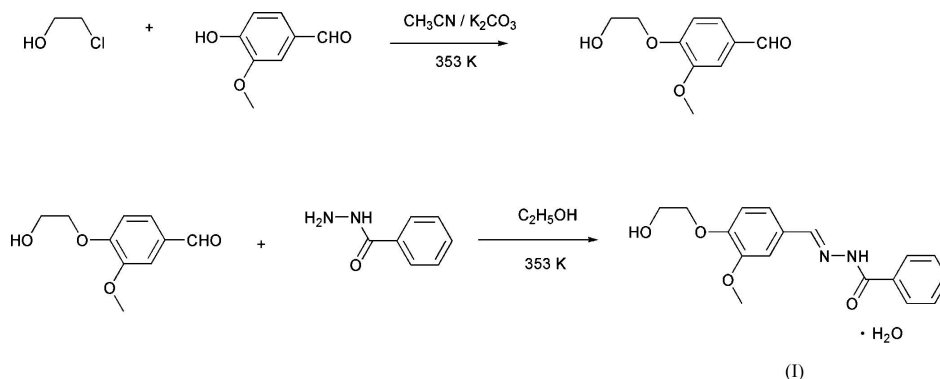
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## Comment

The synthesis of new and designed crystal structures has attracted attention in medicine and chemistry. One of the aims of crystal engineering is to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Tynan *et al.*, 2005; Parashar *et al.*, 1988). In the present study, we report the synthesis and molecular structure of the title compound, (I).



The bond lengths of  $\text{O1}-\text{C8}$  and  $\text{O2}-\text{C7}$  are 1.412 (2) and 1.430 (2) Å, respectively, and are normal. The bond length of  $\text{N1}-\text{C10}$  is 1.269 (2) Å and is similar to the value of 1.279 (3) Å in isonicotinic acid (2-hydroxy-3-methoxybenzylidene)hydrazide (Yu *et al.*, 2005). The vanillin group ( $\text{C1}-\text{C7}/\text{O2}/\text{O3}$ ) and the benzohydrazide group ( $\text{C11}-\text{C17}$ ) are each

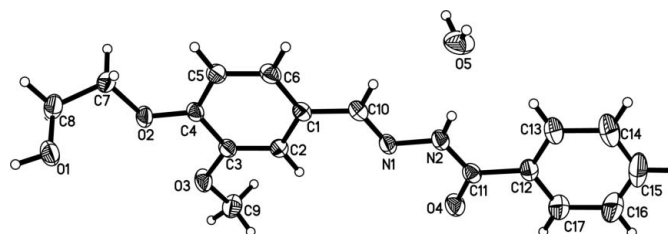


Figure 1

A view of the title compound with 30% probability displacement ellipsoids.

planar, with r.m.s. deviations of the fitted atoms of 0.0342 and 0.0085 Å, respectively. The dihedral angle between these two planes is 9.31 (11)°. It should be noted that strong intra- and intermolecular hydrogen bonds are found in the crystal structure (Table 1). The intramolecular hydrogen bonds stabilize the conformation of the molecule, while the intermolecular hydrogen bonds contribute to the stabilization of the solid state. At the same time, the solvent water molecule participates in interactions with the organic molecules through hydrogen bonds, further stabilizing the zigzag suprastructure, as shown in Fig. 2.

## Experimental

To a solution of 4-hydroxy-3-methoxybenzaldehyde (15.2 g, 10 mmol) and potassium carbonate (13.8 g, 10 mmol) in acetonitrile (500 ml), 2-chloroethanol (8.5 g, 10 mmol) was added over a period of 30 min, and the mixture was refluxed for 24 h under nitrogen. The solvent was removed and the resultant oil was poured into ice-water (500 ml). The white precipitate was then isolated and recrystallized from ethanol to give 4-(2-hydroxyethoxy)-3-methoxybenzaldehyde in 43% yield. An anhydrous ethanol solution of 4-(2-hydroxyethoxy)-3-methoxybenzaldehyde (1.96 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 yellow precipitate appeared. The product was isolated and recrystallized from ethanol, and then dried *in vacuo* to give the pure compound in 83% yield. Colourless single crystals of (1) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.

### Crystal data

$C_{17}H_{18}N_2O_4 \cdot H_2O$   
 $M_r = 332.35$   
 Monoclinic,  $P2_1/n$   
 $a = 9.924$  (2) Å  
 $b = 11.936$  (3) Å  
 $c = 14.890$  (4) Å  
 $\beta = 104.003$  (4)°  
 $V = 1711.5$  (7) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.290$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 2599 reflections  
 $\theta = 2.2$ – $25.8$ °  
 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 Block, colourless  
 $0.46 \times 0.40 \times 0.30$  mm

### Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 1999)  
 $T_{\min} = 0.948$ ,  $T_{\max} = 0.972$   
 9477 measured reflections

3508 independent reflections  
 2112 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 26.5$ °  
 $h = -9 \rightarrow 12$   
 $k = -14 \rightarrow 14$   
 $l = -18 \rightarrow 9$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.129$   
 $S = 1.00$   
 3508 reflections  
 234 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0588P)^2 + 0.3524P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.23$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.20$  e Å<sup>-3</sup>

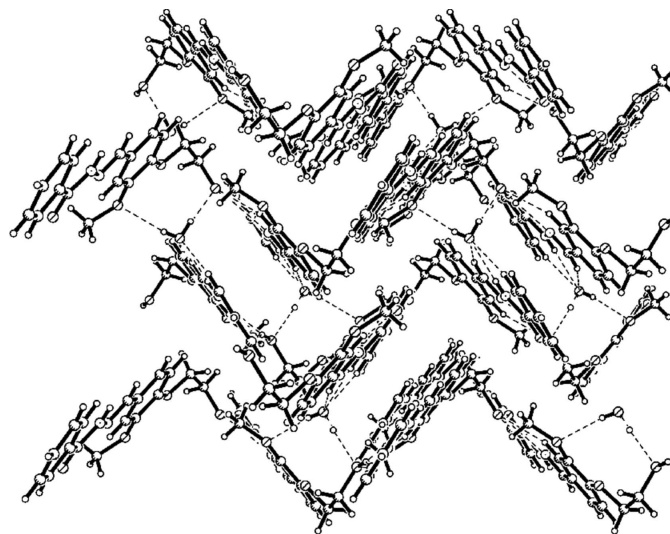


Figure 2  
 Intermolecular hydrogen-bonding interactions (dashed lines).

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O5-H5B \cdots O1^i$	0.92 (4)	1.89 (4)	2.805 (3)	176 (4)
$O5-H5A \cdots O3^i$	0.74 (4)	2.30 (4)	3.033 (3)	172 (4)
$N2-H2 \cdots O5$	0.84 (2)	2.14 (2)	2.962 (3)	164 (2)
$O1-H1 \cdots N1^{ii}$	0.88 (3)	2.42 (3)	3.091 (2)	133 (2)
$O1-H1 \cdots O4^{ii}$	0.88 (3)	1.95 (3)	2.768 (2)	153 (3)
$C17-H17 \cdots O4$	0.93	2.44	2.757 (3)	100
$C13-H13 \cdots O5$	0.93	2.56	3.476 (3)	167
$C10-H10 \cdots O5$	0.93	2.50	3.312 (3)	146
$C2-H2A \cdots O1^{iii}$	0.93	2.54	3.443 (2)	163

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

H atoms bonded to C atoms were included in calculated positions ( $C-H = 0.93$ – $0.96$  Å) and refined using a riding-model approximation, with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$  or  $1.5U_{\text{eq}}(\text{methyl } C)$ . The H atoms attached to O and N atoms were located in a difference Fourier map and refined freely.

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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