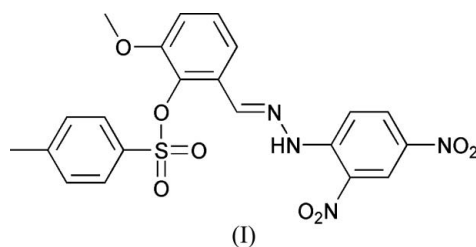


**(E)-1-(2,4-Dinitrophenyl)-2-[3-methoxy-2-(*p*-tolyl-sulfonyloxy)benzylidene]hydrazine****Xin Chen\* and Ming Yu**College of Sciences, Tianjin University of  
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People's Republic of ChinaCorrespondence e-mail:  
chen\_xin9999@163.com**Key indicators**Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.113  
Data-to-parameter ratio = 14.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

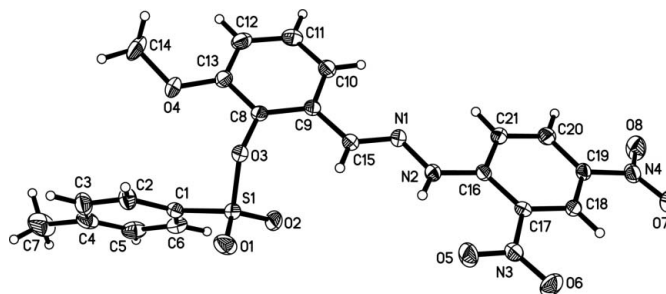
In the title compound,  $\text{C}_{21}\text{H}_{18}\text{N}_4\text{O}_8\text{S}$ , the *o*-vanillin group makes dihedral angles of  $73.80(6)$  and  $6.46(8)^\circ$  with the terminal 4-methylbenzene ring and the phenylhydrazine mean plane, respectively. An intramolecular hydrogen bond links the NH group to an O atom of the nearest nitro group. The crystal structure contains four weak intermolecular hydrogen bonds, namely one  $\text{N}-\text{H}\cdots\text{O}$  and three  $\text{C}-\text{H}\cdots\text{O}$ .

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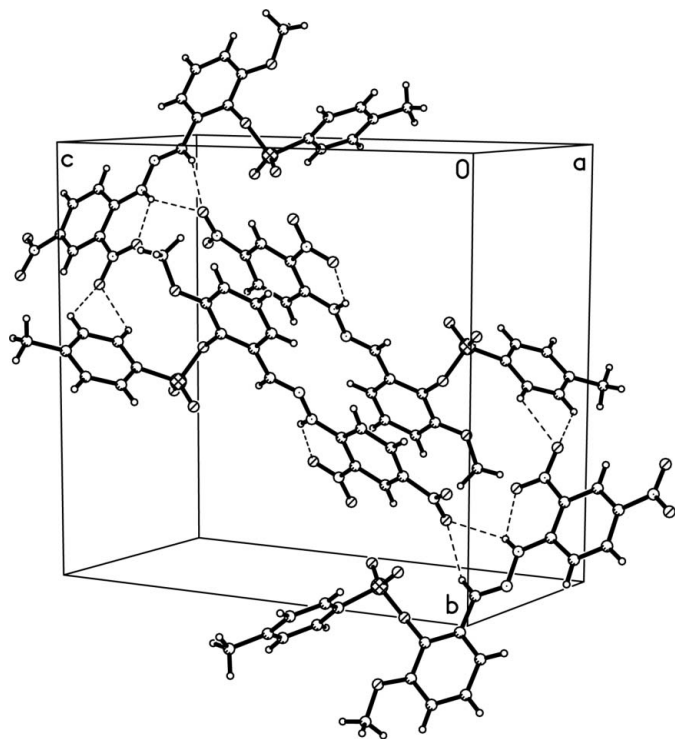
The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Kahwa *et al.*, 1986; Klayman *et al.*, 1979). One of the aims of investigating the structural chemistry of Schiff bases is to develop protein and enzyme mimics (Santos *et al.*, 2001). Structural information is useful when investigating the coordination properties of Schiff bases functioning as ligands. We report here the synthesis and molecular structure of the title Schiff base compound, (I), (Fig. 1).



The phenylhydrazine residue (atoms C16–C21/N1/N2) is planar, with an r.m.s. deviation for fitted atoms of  $0.0280$  Å. This plane makes dihedral angles of  $69.11(7)$  and  $6.46(8)^\circ$  with the terminal benzene ring (C1–C6) and the *o*-vanillin group (C8–C13/C15/O3/O4), respectively. The dihedral angle between the terminal benzene ring (C1–C6) and the *o*-vanillin group is  $73.80(6)^\circ$ .



**Figure 1**  
The molecular 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.

An intramolecular hydrogen bond links the NH group to O5, thereby influencing the molecular conformation. The crystal structure contains four weak intermolecular hydrogen bonds, namely one N—H···O and three C—H···O (Table 1). These intermolecular hydrogen bonds help to consolidate the crystal packing (Fig. 2). In addition, a  $\pi$ – $\pi$  stacking interaction is observed between the C8–C13 benzene ring and the C16–C21 benzene ring of the molecule at the symmetry position  $(1-x, 2-y, -z)$ ; the centroid–centroid distance between the two rings is 3.709 (2) Å.

## Experimental

An anhydrous ethanol solution (50 ml) of 3-benzyloxy-4-methoxybenzaldehyde (2.42 g, 10 mmol) was added to an anhydrous ethanol solution (100 ml) of 1-(2,4-dinitrophenyl)hydrazine (1.98 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, recrystallized from acetonitrile and dried in a vacuum to give the pure compound in 89% yield. Yellow single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution.

### Crystal data

$C_{21}H_{18}N_4O_8S$   
 $M_r = 486.46$   
 Monoclinic,  $P2_1/c$   
 $a = 7.9826$  (14) Å  
 $b = 16.545$  (3) Å  
 $c = 16.664$  (3) Å  
 $\beta = 101.556$  (3)°  
 $V = 2156.2$  (7) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.499$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.21$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 Block, yellow  
 $0.30 \times 0.26 \times 0.22$  mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.921$ ,  $T_{\max} = 0.956$   
 12063 measured reflections  
 4410 independent reflections  
 2614 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.046$   
 $\theta_{\max} = 26.5^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.114$   
 $S = 1.00$   
 4410 reflections  
 308 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 0.2099P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.25$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.29$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

S1—O3	1.6035 (16)	N1—N2	1.372 (2)
O3—C8	1.418 (3)	N2—C16	1.356 (3)
N1—C15	1.272 (3)		
C8—O3—S1	119.87 (14)	N1—C15—C9	120.2 (2)
C15—N1—N2	116.00 (19)	N2—C16—C21	119.9 (2)
C16—N2—N1	119.48 (18)	N2—C16—C17	123.9 (2)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2···O5	0.86	2.04	2.648 (3)	127
C2—H2A···O6 <sup>i</sup>	0.93	2.58	3.219 (3)	126
C3—H3···O6 <sup>i</sup>	0.93	2.70	3.284 (4)	122
C15—H15···O7 <sup>ii</sup>	0.93	2.53	3.394 (3)	155
N2—H2···O7 <sup>ii</sup>	0.86	2.55	3.345 (2)	153

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

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  $U_{\text{iso}}(\text{H})$  parameters: C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic, C—H = 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl, and N—H = 0.86 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$  for NH 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.

## References

- Bruker (1999). SMART (Version 5.0) and SAINT (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Kahwa, I. A., Selbin, J., Hsieh, T. C.-Y. & Laine, R. A. (1986). *Inorg. Chim. Acta*, **118**, 179–185.
- Klayman, D. L., Bartosevich, J. F., Griffin, T. S., Mason, C. J. & Scovill, J. P. (1979). *J. Med. Chem.* **22**, 855–862.
- 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. (1997a). SHELXS97 and SHELXL97. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). SHELXTL. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.