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(*E*)-1-(4-Nitrophenyl)-2-[4-(2-phenoxyethoxy)-benzylidene]hydrazine

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In the title compound, $C_{21}H_{19}N_3O_4$, the central benzene ring makes dihedral angles of 75.46 (6) and 4.07 (6)° with the terminal benzene ring and the phenylhydrazine mean plane, respectively. The packing is stabilized by intermolecular N—H···O hydrogen bonds and weak non-classical intermolecular C—H···O hydrogen-bonding interactions.

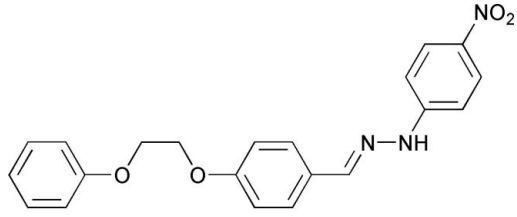
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.105
Data-to-parameter ratio = 15.0

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

Comment

Metal complexes based on Schiff bases have attracted much attention because of their biological activity (Kahwa *et al.*, 1986; Klayman *et al.*, 1979). Consequently, a large number of Schiff base derivatives have been synthesized and employed to develop protein and enzyme mimics, such as models to mimic hydrolase in the hydrolysis of *p*-nitrophenyl picolinate (Li *et al.*, 2005). 1-(4-Nitrophenyl)hydrazine forms a variety of Schiff bases with aldehydes, and the synthesis and crystal structures of some of them, such as (*E*)-1-(4-methoxy-3-propoxy-benzylidene)-2-(4-nitrophenyl)hydrazine (Shi, 2005) and (*E*)-1-[4-(benzyloxy)benzylidene]-2-(4-nitrophenyl)hydrazine (Jun, 2005), have been reported.



(I)

In the present study we report the synthesis and molecular structure of the nitrophenylhydrazine Schiff base derivative (I) (Fig. 1).

The phenylhydrazine residue (C16–C21/N1/N2) is planar, with an r.m.s. deviation for fitted atoms of 0.0279 Å. This plane makes dihedral angles of 71.60 (6) and 4.07 (6)° with the terminal phenyl ring (C1–C6) and the central benzene fragment (C9–C15/O2), respectively. In addition, the dihedral angle between the terminal phenyl ring (C1–C6) and the central benzene fragment (C9–C15/O2) is 75.46 (6)°. The nitro group (O3/N3/O4) and its attached aromatic ring are not coplanar, with a dihedral angle of 3.70 (17)°. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds and weak C—H···O intermolecular hydrogen-bonding interactions that link molecules into one-dimensional extended chains (Table 1 and Fig. 2).

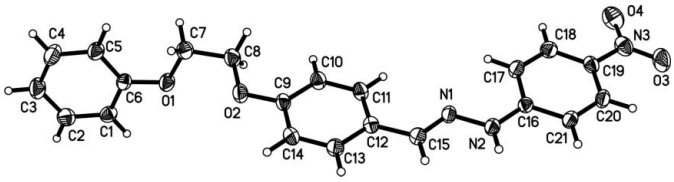


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

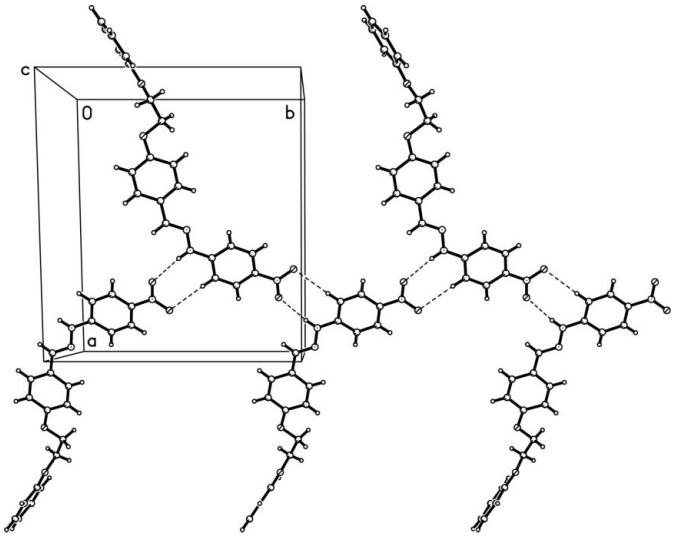


Figure 2
Packing diagram for (I), with hydrogen bonds drawn as dashed lines.

Experimental

An anhydrous ethanol solution (50 ml) of 4-(2-phenoxyethoxy)-benzaldehyde (2.42 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 1-(4-nitrophenyl)hydrazine (1.53 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a red precipitate. The product was isolated and recrystallized from acetonitrile. Red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{21}H_{19}N_3O_4$
M_r = 377.39
Monoclinic, $C2/c$
a = 16.850 (5) Å
b = 14.868 (4) Å
c = 15.190 (4) Å
β = 100.120 (5)°
V = 3746.3 (18) Å^3
Z = 8
D_x = 1.338 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 294 (2) K
Block, red
0.34 × 0.28 × 0.22 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.948, T_{max} = 0.980
10330 measured reflections
3794 independent reflections
2184 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 0.99
3794 reflections
253 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0478P)^2 + 0.2798P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O3^{i}	0.86	2.23	3.087 (2)	173
C21—H21···O4^{i}	0.93	2.56	3.485 (2)	176

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

The H atoms were included in calculated positions and refined using a riding model, with C—H = 0.93 Å for Csp^2 and 0.97 Å for methylene, N—H = 0.86 Å, and U_{iso}(H) = 1.2U_{eq}(C,N).

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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