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(*E*)-1-(4-Benzoyloxy-3-methoxybenzylidene)-2-(4-nitrophenyl)hydrazine

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In the title compound, $C_{21}H_{17}N_3O_5$, the central planar group makes dihedral angles of 83.55 (11) and 5.54 (8)° with the terminal phenyl ring and the phenylhydrazine mean planes, respectively. The molecular packing is stabilized by intermolecular N—H···O hydrogen bonds that link adjacent molecules into one-dimensional chains.

Key indicators

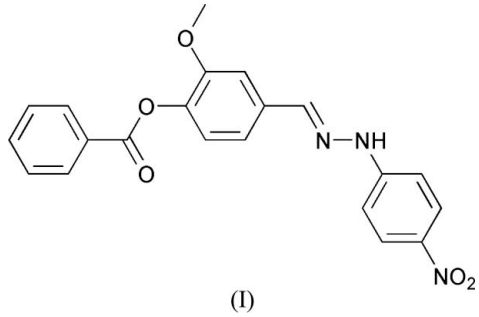
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.069
wR factor = 0.159
Data-to-parameter ratio = 12.6

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

Comment

A large number of Schiff base derivatives have been synthesized and employed in the development of protein and enzyme mimics, for example as a model to mimic hydrolase in the hydrolysis of *p*-nitrophenyl picolinate (Li *et al.*, 2005).

In the title compound, (I) (Fig. 1), a nitrophenylhydrazine Schiff base derivative, the central group (C8–C13/C15/O2/O3) is essentially planar, with an r.m.s. deviation of the fitted atoms of 0.01 Å. It makes dihedral angles of 5.54 (8) and 83.55 (11)° with the phenylhydrazine residue and with the terminal phenyl ring, respectively. The nitro group is twisted around the C—N bond; the dihedral angle between the nitro group and the C16–C21 ring is 15.73 (16)°.



(I)

The crystal packing of (I) is stabilized by intermolecular N2—H2···O5^{i} [symmetry code (i): $\frac{5}{2}-x,\frac{1}{2}+y,\frac{5}{2}-z$] hydrogen

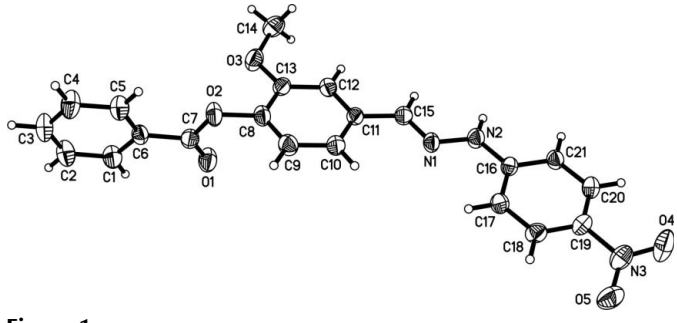


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

bonds that link adjacent molecules into one-dimensional chains running along the *b* axis (Table 1 and Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 4-formyl-2-methoxyphenyl benzoate (2.56 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 an orange precipitate. The product was isolated, recrystallized from acetonitrile and then dried in a vacuum to give the pure compound in 78% yield. Orange single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{21}H_{17}N_3O_5$
M_r = 391.38
Monoclinic, $P2_1/n$
a = 8.1110 (16) Å
b = 14.965 (3) Å
c = 16.220 (3) Å
β = 104.07 (3)°
V = 1909.7 (7) Å^3
Z = 4
D_x = 1.361 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, orange
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.973, T_{max} = 0.990
11378 measured reflections
3322 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.159
S = 1.02
3322 reflections
263 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 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···O5^{i}	0.86	2.06	2.907 (4)	169

Symmetry code: (i) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{5}{2}$.

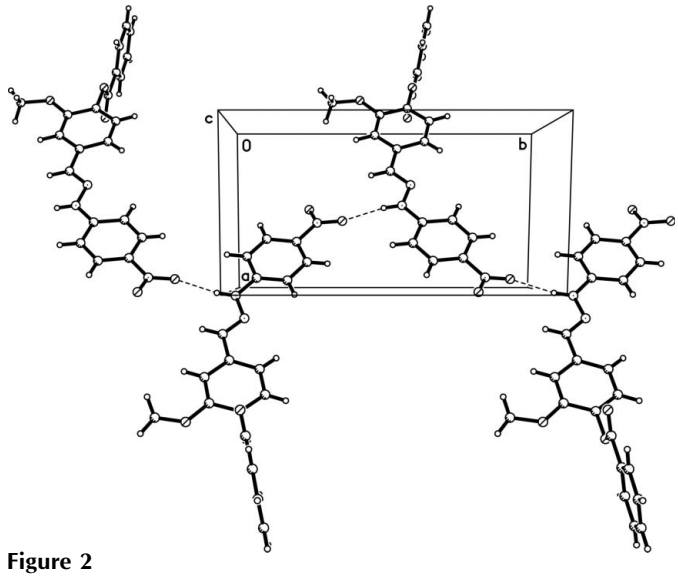


Figure 2
Part of the crystal structure of compound (I), showing the formation of a hydrogen-bonded chain. Hydrogen bonds are drawn as dashed lines.

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_{iso}(H) parameters: 0.93 Å and 1.2U_{eq}(C) for Csp^2, 0.96 Å and 1.5U_{eq}(C) for methyl, and 0.86 Å and 1.2U_{eq}(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, 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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