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(*Z*)-1-[2-(2-Chlorobenzyloxy)benzylidene]-2-(2,4-dinitrophenyl)hydrazine *N*,*N*-dimethylformamide solvate

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In the title compound, $C_{23}H_{22}ClN_5O_6$, the central benzene ring makes dihedral angles of 4.68 (15) and 4.79 (9)° with the terminal benzene 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 five weak intermolecular hydrogen-bonding interactions, one N—H···O and four C—H···O.

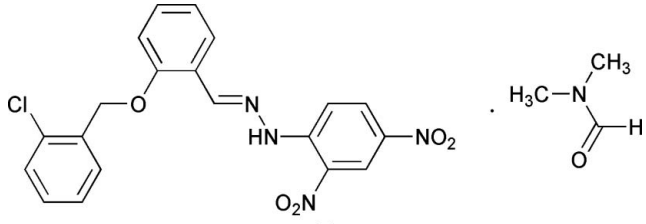
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.132
Data-to-parameter ratio = 13.2

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

Comment

The synthesis and structure of Schiff bases have attracted much attention in biology and chemistry (Klayman *et al.*, 1979). Consequently, a large number of Schiff base derivatives have been synthesized. 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 their crystal structures, which will provide useful information for the coordination properties of Schiff bases functioning as ligands, we report here the synthesis and molecular and crystal structure of the title compound, (I) (Fig. 1).



(I)

All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The phenylhydrazine residue (C15–C20/N1/N2) is nearly planar, with an r.m.s. deviation for the fitted atoms of 0.0305 Å. This plane makes dihedral angles of 8.41 (14) and 4.79 (9)° with the terminal benzene ring (C1–C6) and the central benzene ring (C8–C14/O1), respectively. In addition, the dihedral angle between the terminal benzene ring (C1–C6) and the central benzene ring (C8–C14/O1) is 4.68 (15)°. The two nitro groups (O2/N3/O3 and O4/N4/O5) and their attached aromatic ring (C15–C20) are not coplanar. The dihedral angles are 7.94 (3)° for O2/N3/O3 and 6.23 (6)° for O4/N4/O5.

An intramolecular hydrogen bond links the NH group to O2, thereby influencing the molecular conformation. The main molecule and the solvent molecule are linked by four weak intermolecular hydrogen bonds, one N—H···O and three C—H···O. An O2···O6($1-x, y-\frac{1}{2}, -z+\frac{1}{2}$) short contact of 2.896 (3) Å is observed in (I). Intermolecular C9—H9···O4($1+x, y-1, z$) hydrogen bonds link adjacent molecules into one-dimensional extended chains (Fig. 2).

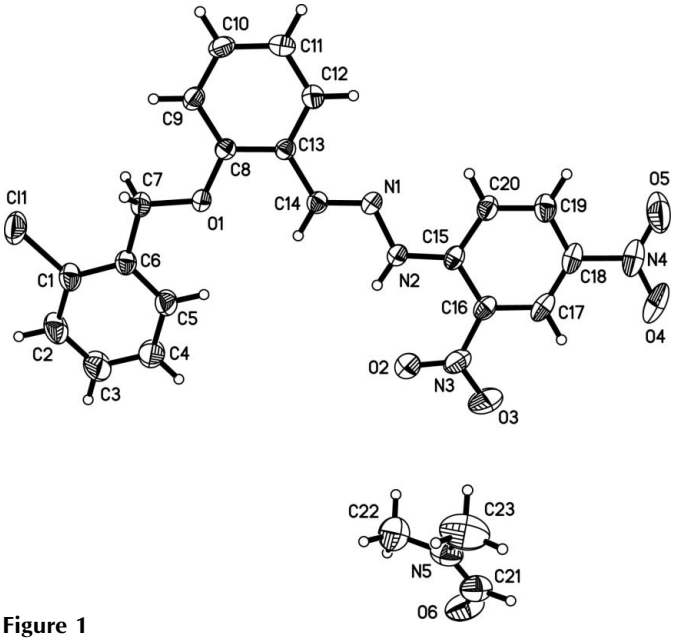


Figure 1
The asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level.

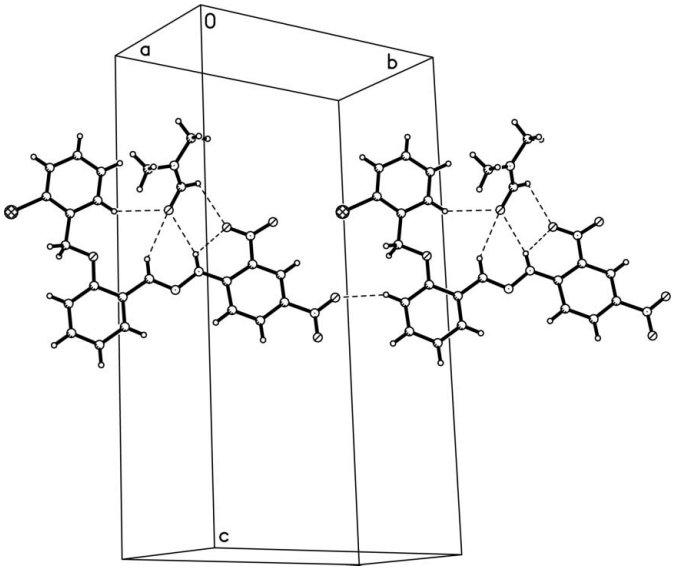


Figure 2
A partial packing diagram for (I), with hydrogen bonds drawn as dashed lines.

Experimental

An anhydrous ethanol solution (50 ml) of 2-(2-chlorobenzyloxy)benzaldehyde (2.47 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 stirred at 350 K for 5 h under nitrogen, giving a red precipitate. The product was isolated, recrystallized from acetonitrile and then dried in a vacuum, to give the pure compound in 84% yield. Red single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an *N*,*N*-dimethylformamide solution.

Crystal data

$C_{20}H_{15}ClN_4O_5\cdot C_3H_7NO$
M_r = 499.91
Monoclinic, $P2_1/c$
a = 7.844 (4) Å
b = 12.887 (7) Å
c = 23.631 (13) Å
β = 92.455 (9)°
V = 2387 (2) Å^3
Z = 4
D_x = 1.391 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 294 (2) K
Block, red
0.30 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.935, T_{max} = 0.967
11916 measured reflections
4199 independent reflections
2393 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.132
S = 1.05
4199 reflections
318 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 0.5074P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2	0.86	2.05	2.647 (3)	126
N2—H2···O6^{i}	0.86	2.33	3.085 (3)	147
C5—H5···O6^{i}	0.93	2.54	3.349 (4)	146
C14—H14···O6^{i}	0.93	2.42	3.240 (4)	147
C9—H9···O4^{ii}	0.93	2.35	3.185 (4)	150
C21—H21···O2^{iii}	0.93	2.46	2.979 (4)	115

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

H atoms were included in calculated positions and refined using a riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl, and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(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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