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(*E*)-*N*′-[4-(4-Chlorobenzyloxy)-3-methoxybenzylidene]furan-2-carbohydrazide

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Key indicators

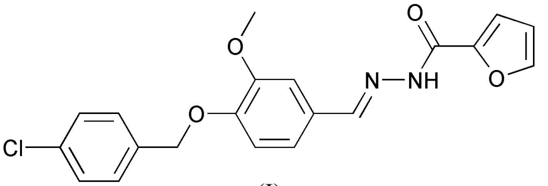
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.046
wR factor = 0.117
Data-to-parameter ratio = 11.5

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

In the title compound, $C_{20}H_{17}ClN_2O_4$, the vanillin group makes dihedral angles of 54.50 (10) and 23.85 (15)° with the chlorobenzene ring and the furan mean plane, respectively. Packing is stabilized by intermolecular N—H···O hydrogen bonds and weak non-classical intermolecular C—H···O hydrogen-bonding interactions that link adjacent molecules into one-dimensional extended chains.

Comment

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). As part of an investigation of the coordination properties of Schiff bases functioning as ligands, we report the synthesis and structure of the title compound, (I).



(I)

In compound (I) (Fig. 1), the vanillin group (C8–C13/C15/O1/O2) is nearly planar, with an r.m.s. deviation for the fitted atoms of 0.0244 Å. This plane makes dihedral angles of 23.85 (15) and 54.50 (10)° with the furan ring (C17–C20/O4) and the chlorobenzene ring (C1–C6), respectively. The dihedral angle between the furan ring and the benzene ring is 78.18 (13)°. All bond lengths are within normal ranges (Allen *et al.*, 1987).

The crystal packing of (I) is stabilized by N—H···O and weak C—H···O intermolecular hydrogen-bonding interactions that link adjacent molecules into one-dimensional extended chains (Table 1, Fig. 2).

Experimental

An anhydrous ethanol solution (50 ml) of 4-(4-chlorobenzyloxy)-3-methoxybenzaldehyde (2.77 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of furan-2-carbohydrazide (1.26 g, 10 mmol) and the mixture stirred at 350 K for 5 h under nitrogen, giving a white precipitate. The product was isolated, recrystallized from ethanol and then dried in a vacuum to give the pure compound in 88% yield. Colourless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

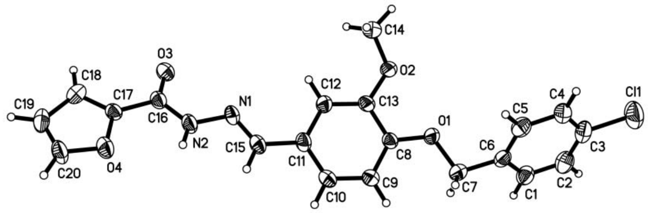


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

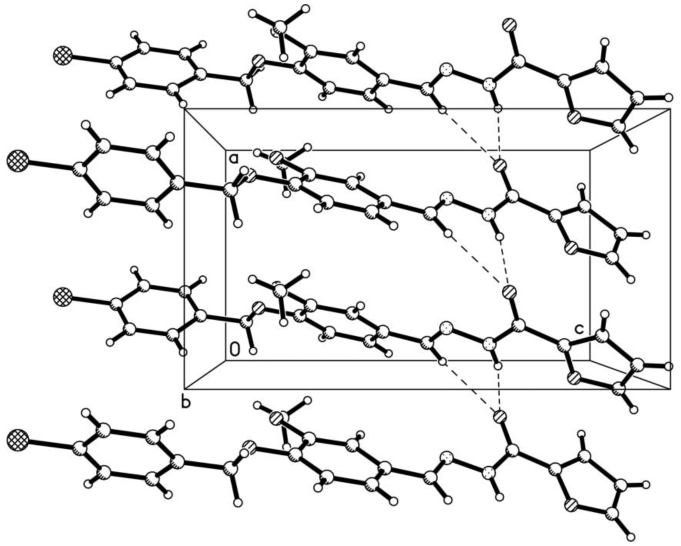


Figure 2
A packing diagram for (I), with hydrogen bonds drawn as dashed lines.

Crystal data

$C_{20}H_{17}ClN_2O_4$	$V = 1837.4$ (8) Å^3
$M_r = 384.81$	$Z = 4$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 7.797$ (2) Å	$\mu = 0.24$ mm^{-1}
$b = 17.456$ (4) Å	$T = 294$ (2) K
$c = 13.500$ (3) Å	$0.20 \times 0.18 \times 0.18$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	7263 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2838 independent reflections
$T_{min} = 0.923$, $T_{max} = 0.958$	1743 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.047$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$	H-atom parameters constrained
$wR(F^2) = 0.117$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 0.98$	$\Delta\rho_{min} = -0.17$ e Å^{-3}
2838 reflections	Absolute structure: Flack (1983), with 1134 Friedel pairs
246 parameters	Flack parameter: 0.13 (13)
7 restraints	

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2$\cdots$O3^{i}	0.86	2.18	3.014 (4)	163
C15—H15$\cdots$O3^{i}	0.93	2.48	3.306 (5)	148

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

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 H, C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene H, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H, and N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N) for imino H.

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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