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

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In the title compound, $C_{20}H_{17}ClN_2O_3S$, the vanillin group makes dihedral angles of 73.65 (11) and 2.16 (16)° with the chloro-substituted benzene ring and the thiophene mean plane, respectively. The crystal packing is stabilized by an intermolecular N—H···O hydrogen bond that forms a centrosymmetric dimer.

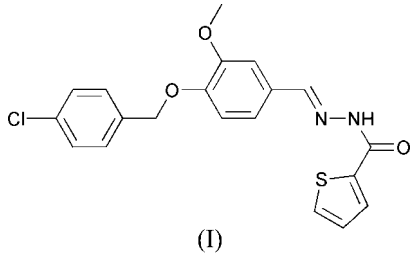
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.007 Å
R factor = 0.056
wR factor = 0.176
Data-to-parameter ratio = 13.3

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

Comment

For the background to this study, see the first paper in this series of three (Zhang *et al.*, 2006). We report here the synthesis and structure of the title compound, (I) (Fig. 1).



(I)

All bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). The vanillin group (C8–C13/C15/O1/O2) is nearly planar, with an r.m.s. deviation for fitted atoms of 0.0280 Å. This plane makes dihedral angles of 2.16 (16) and 73.65 (11)° with the thiophene ring (C17–C20/S1) and the terminal benzene ring (C1–C6), respectively. The dihedral angle between the thiophene and benzene rings is 72.24 (14)°.

The crystal packing is stabilized by an intermolecular N—H···O=C hydrogen bond (Table 1) that forms a centrosymmetric dimer (Fig. 2).

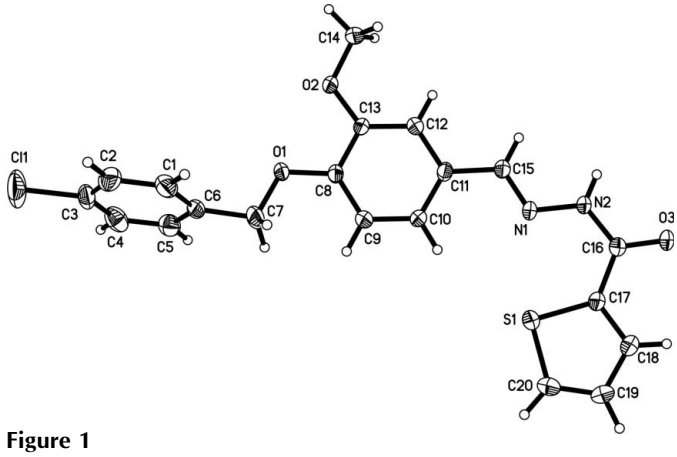


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level.

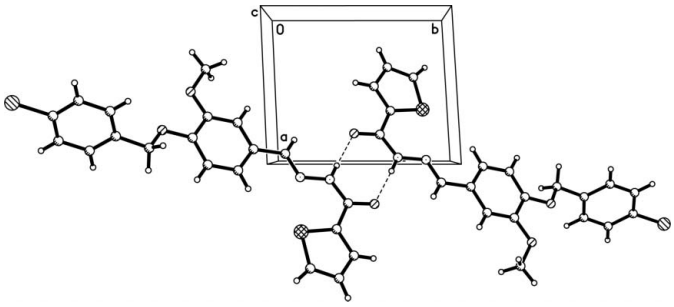


Figure 2
A packing diagram of (I), viewed along the *c* axis, showing hydrogen bonds as dashed lines.

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 thiophene-2-carbohydrazide (1.42 g, 10 mmol) and the mixture was stirred at 350 K for 5 h under nitrogen, giving a white precipitate. The product was isolated, recrystallized from ethanol and dried in a vacuum to give (I) in 82% yield. Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{20}H_{17}ClN_2O_3S$
M_r = 400.88
Triclinic, $P\overline{1}$
a = 8.275 (3) Å
b = 9.884 (3) Å
c = 11.584 (3) Å
α = 89.503 (5)°
β = 81.062 (5)°
γ = 86.951 (5)°
V = 934.6 (5) Å^3
Z = 2
D_x = 1.424 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 294 (2) K
Block, colourless
0.14 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.931, T_{max} = 0.973
4778 measured reflections
3264 independent reflections
1803 reflections with $I > 2\sigma(I)$
R_{int} = 0.035
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.176
S = 1.06
3264 reflections
246 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0663P)^2 + 0.5087P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 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	1.95	2.811 (5)	175

Symmetry code: (i) $-x+2, -y+3, -z$.

H atoms were included in calculated positions, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C).

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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