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3-(2,4-Dichlorobenzyloxy)-4-methoxybenzaldehyde

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.062
wR factor = 0.132
Data-to-parameter ratio = 13.4

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

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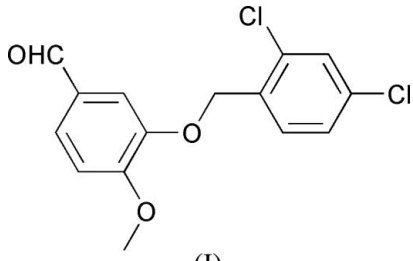
In the title compound, $C_{15}H_{12}Cl_2O_3$, the isovanillin group makes a dihedral angle of 3.12 (12)° with the dichlorobenzene ring. Intermolecular C—H···O hydrogen bonds help to consolidate the crystal packing.

Comment

As part of our interest in the coordination properties of Schiff bases functioning as ligands, we investigated the title compound, (I), used as a precursor in the preparation of Schiff bases.



(I)

In the crystal structure of (I) (Fig. 1), the bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The isovanillin group (atoms C1–C6/C8/O1/O2) is essentially planar, with an r.m.s. deviation for the fitted atoms of 0.016 Å. This plane makes a dihedral angle of 3.12 (12)° with the mean plane of the C10–C15 benzene ring.

The crystal packing of (I) is stabilized by weak C—H···O interactions that link adjacent molecules into zigzag chains running along the *c* axis (Table 1 and Fig. 2).

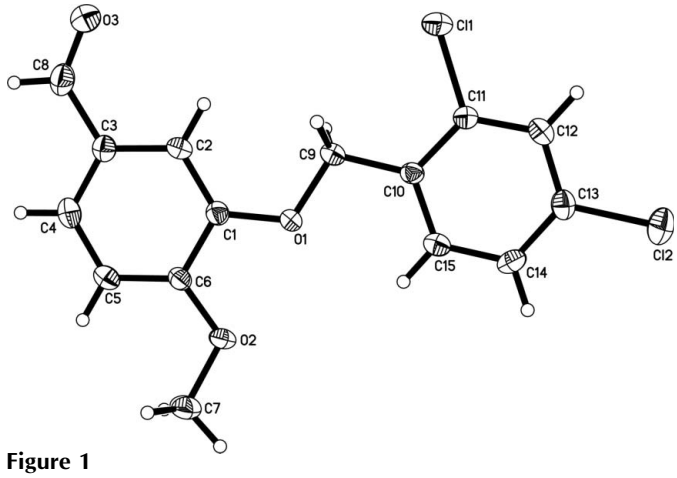


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

Experimental

An anhydrous acetonitrile solution (50 ml) of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a solution (100 ml) of 1-(bromomethyl)-2,4-dichlorobenzene (2.40 g, 10 mmol) and potassium carbonate (1.38 g, 10 mmol) in acetonitrile, over a period of 30 min, and the mixture refluxed for 24 h under a nitrogen atmosphere. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The white precipitate was then isolated and recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 50% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{15}H_{12}Cl_2O_3$
M_r = 311.15
Monoclinic, $P2_1/n$
a = 7.456 (3) Å
b = 24.850 (9) Å
c = 8.370 (3) Å
β = 114.616 (6)°
V = 1409.9 (9) Å^3
Z = 4
D_x = 1.466 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.46 mm^{-1}
T = 294 (2) K
Block, colorless
0.24 × 0.20 × 0.16 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.878, T_{max} = 0.929
6657 measured reflections
2436 independent reflections
1493 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.132
S = 1.03
2436 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 2.615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O3^{i}	0.93	2.60	3.526 (5)	175

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

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

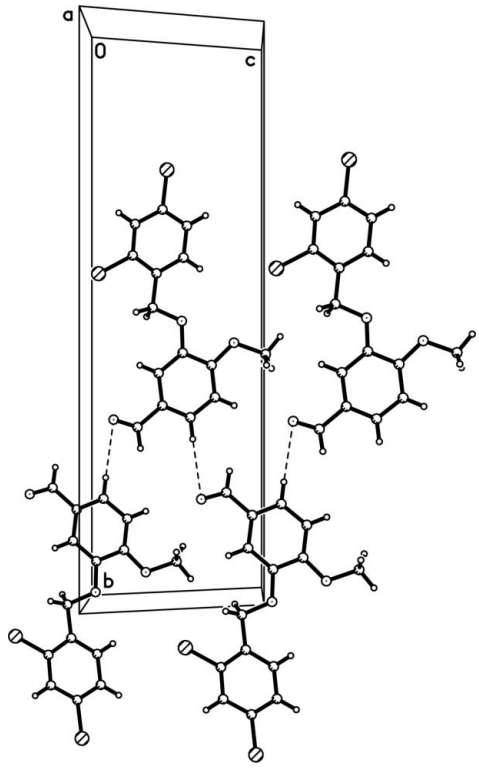


Figure 2
A partial packing diagram for (I), with hydrogen bonds shown as dashed lines.

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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