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2-(4-Chlorobenzyloxy)benzaldehyde

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In the title compound, $C_{14}H_{11}ClO_2$, the salicylaldehyde group makes a dihedral angle of 56.32 (7)° with the benzene ring.

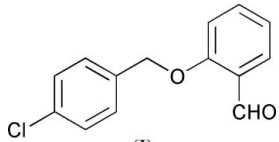
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.084
Data-to-parameter ratio = 13.6

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

Comment

The background to this study has been described in an earlier paper (Zhang *et al.*, 2006).



(I)

Bond lengths and angles in the title compound, (I), are within normal ranges (Allen *et al.*, 1987). The salicylaldehyde group (atoms C1–C7/O1) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.0071 Å. This group makes a dihedral angle of 56.32 (7)° with the C9–C14 benzene ring (Fig. 1).

Experimental

An anhydrous acetonitrile solution (100 ml) of 2-hydroxybenzaldehyde (1.22 g, 10 mmol) was added dropwise to an acetonitrile solution (50 ml) of 1-(bromomethyl)-4-chlorobenzene (2.05 g, 10 mmol) and pyridine (0.79 g, 10 mmol) and the mixture refluxed for 24 h under nitrogen. The solvent was removed and the resultant mixture poured into ice–water (100 ml). The white precipitate was isolated, recrystallized from acetonitrile and then dried in a vacuum to give pure compound (I) in 54% yield. Colorless single crystals suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

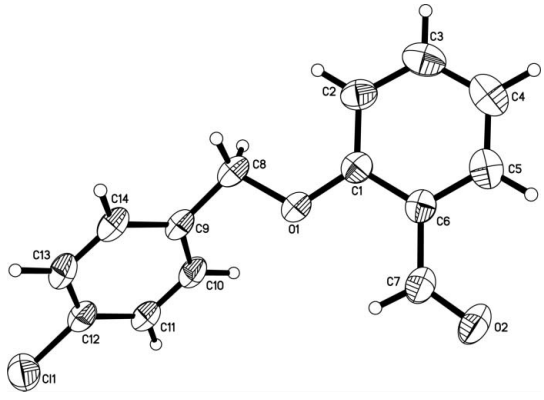


Figure 1
The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

Crystal data

$C_{14}H_{11}ClO_2$	$Z = 4$
$M_r = 246.68$	$D_x = 1.373$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 4.0635$ (11) Å	$\mu = 0.31$ mm^{-1}
$b = 14.894$ (4) Å	$T = 294$ (2) K
$c = 19.715$ (5) Å	Block, colorless
$V = 1193.2$ (5) Å^3	0.20 × 0.16 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	6035 measured reflections
φ and ω scans	2090 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1496 reflections with $I > 2\sigma(I)$
$T_{min} = 0.926$, $T_{max} = 0.982$	$R_{int} = 0.034$
	$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.063P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.036$	$(\Delta/\sigma)_{max} = 0.007$
$wR(F^2) = 0.084$	$\Delta\rho_{max} = 0.11$ e Å^{-3}
$S = 1.02$	$\Delta\rho_{min} = -0.10$ e Å^{-3}
2090 reflections	Absolute structure: Flack (1983), 817 Friedel pairs
154 parameters	Flack parameter: 0.08 (9)
H-atom parameters constrained	

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

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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