

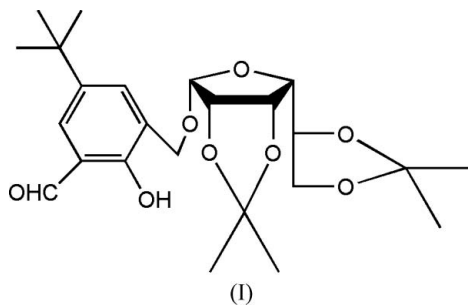
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Key indicators

Single-crystal X-ray study
 $T = 113$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.041
 wR factor = 0.104
Data-to-parameter ratio = 9.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.5-*tert*-Butyl-3-[[6-(2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-*d*][1,3]-dioxol-4-yloxy]methyl]-2-hydroxybenzaldehydeThere are two independent molecules in the asymmetric unit of the title compound, $\text{C}_{24}\text{H}_{34}\text{O}_8$. The crystal packing is mainly determined by weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and van der Waals interactions.Received 12 June 2006
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Comment

Chiral manganese–salen complexes [salen is bis(salicylidene)ethylenediamine] are effective catalysts owing to their ability for highly stereoselective epoxidation of unfunctionalized alkenes (Lane & Burgess, 2003). In order to test the effects of carbohydrates on the asymmetric epoxidation of olefins, we have designed and synthesized a series of chiral salicylaldehyde derivatives, ligands and complexes. The structure of 3-*tert*-butyl-5-[[5-(2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yloxy]methyl]-2-hydroxybenzaldehyde has been reported previously (Zhao *et al.*, 2006). In this paper, we present the results of our study of another derivative of salicylaldehyde, (I), obtained by the condensation of 5-*tert*-butyl-3-(chloromethyl)-2-hydroxybenzaldehyde and 2,3:5,6-di-*O*-isopropylidene- α -D-mannofuranose.The asymmetric unit of (I) contains two independent molecules (Fig. 1), which show normal bond distances and angles (Allen *et al.*, 1987). The distances between the newly bonded atoms $\text{C}13-\text{O}6$ and $\text{C}37-\text{O}14$ are 1.442 (3) and 1.433 (3) Å, respectively. In the crystal structure, weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1) contribute to the stabilization of the crystal packing (Fig. 2), along with van der Waals interactions.

Experimental

The title compound was prepared according to the procedure of Zhao *et al.* (2006). Colourless single crystals of (I) were grown by slow evaporation of a petroleum ether–EtOAc (5:1 *v/v*) solution. The structure of (I) (m.p. 353–354 K) was confirmed by optical rotation $[\alpha]_D^{20} = +85.0^\circ$ (EtOH), elemental analysis, NMR and IR data.

Crystal data

$C_{24}H_{34}O_8$
 $M_r = 450.51$
 Monoclinic, $P2_1$
 $a = 12.7880$ (19) Å
 $b = 6.7749$ (10) Å
 $c = 26.859$ (4) Å
 $\beta = 92.118$ (2)°
 $V = 2325.4$ (6) Å³

$Z = 4$
 $D_x = 1.287$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 113$ (2) K
 Block, colourless
 $0.32 \times 0.20 \times 0.16$ mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.970$, $T_{\max} = 0.985$

20584 measured reflections
 5939 independent reflections
 4809 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $\theta_{\text{max}} = 27.9^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.104$
 $S = 1.00$
 5939 reflections
 598 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0633P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.36$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.23$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O15-H15\cdots O16$	0.83 (3)	1.87 (3)	2.617 (2)	150 (3)
$O7-H7\cdots O8$	0.84 (3)	1.84 (3)	2.618 (2)	152 (3)
$C13-H13B\cdots O4^i$	0.99	2.35	3.330 (3)	172
$C37-H37B\cdots O12^i$	0.99	2.44	3.398 (3)	163

Symmetry code: (i) $x, y - 1, z$.

The H atom of the hydroxy group was located in a difference Fourier map and refined, with an O—H distance restraint of 0.84 (3) Å. All other H atoms were included in calculated positions, with C—H = 0.95–1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement; the absolute configuration is known from that of the mannofuranose reagent.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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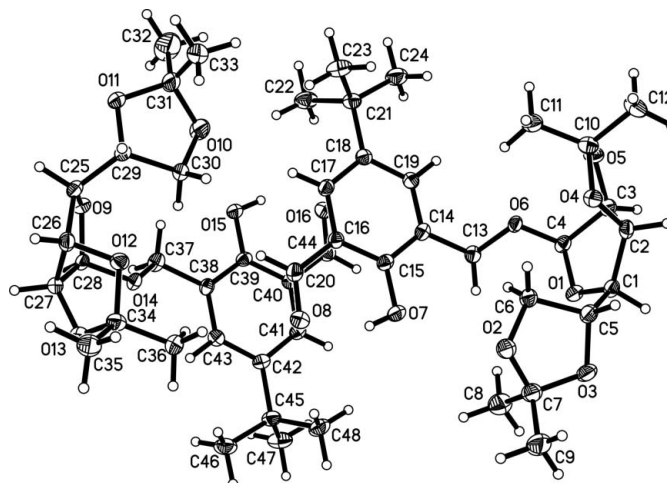


Figure 1

The asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms are shown as small spheres of arbitrary radii.

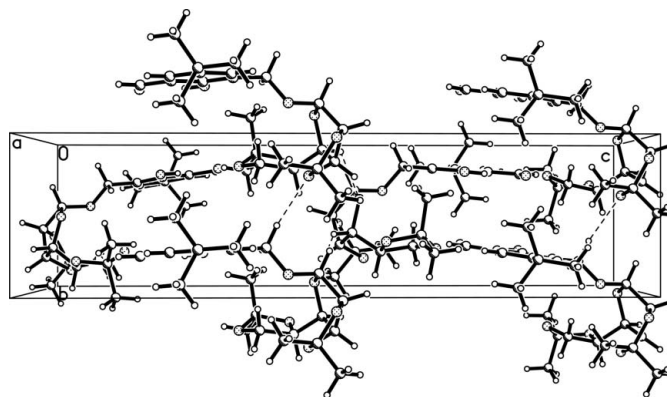


Figure 2

A packing diagram of (I), viewed along the a axis. Dashed lines denote intermolecular hydrogen bonds

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