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#### Key indicators

Single-crystal X-ray study  
 $T = 150$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.102  
Data-to-parameter ratio = 7.1

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

## (3*S*)-3-Benzyloxymethyl-1,4-dioxane-2,5-dione

The lactide ring in the title compound,  $\text{C}_{12}\text{H}_{12}\text{O}_5$ , adopts a screw-boat conformation.  $\text{C}-\text{H}\cdots\text{O}$  interactions link the molecules into a chain in the  $[100]$  direction.

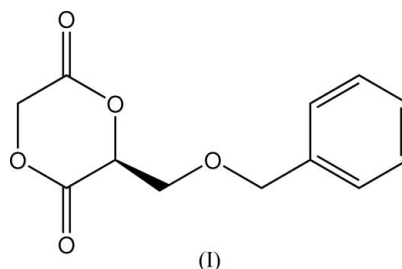
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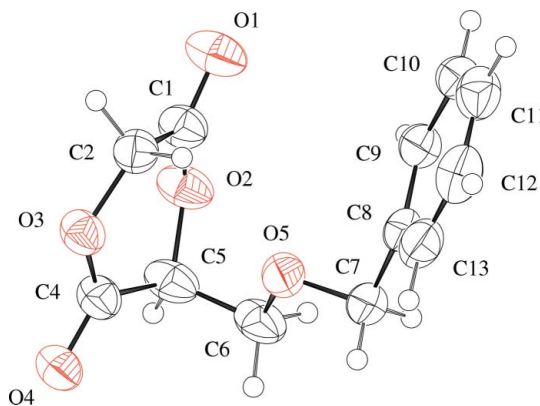
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#### Comment

The structure of the title compound, (I), was determined in the course of our investigations towards a better understanding of the regioselectivity observed in the ring-opening polymerization of various substituted (3*S*)-3-benzyloxymethyl-1,4-dioxane-2,5-dione derivatives (Leemhuis *et al.*, 2005). Earlier, we reported the crystal structures of the 6(*R*)-methyl (Kooijman *et al.*, 2005*a*) and the 6(*S*)-methyl derivatives (Kooijman *et al.*, 2005*b*). The molecular structure of (I) is displayed in Fig. 1 and selected geometric parameters are given in Table 1.



The lactide ring has taken a somewhat deformed screw-boat conformation. The asymmetry parameter (Duax & Norton, 1975)  $\Delta C_2(\text{C}2-\text{O}3) = 6.4$  (5) $^\circ$ ; all other asymmetry parameters have values of 18 $^\circ$  or higher. The Cremer & Pople puckering parameters (Cremer & Pople, 1975) are  $\theta =$



**Figure 1**

Atomic displacement plot (Spek, 2003) of the title compound, showing the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level.

77.1 (6)° and  $\varphi = 320.3$  (6)°; the ideal values for the observed screw-boat conformation are  $\theta = 67.5^\circ$  and  $\varphi = 330^\circ$ . The benzyloxymethyl substituent of the lactide ring occupies the axial position, as illustrated by the angle between the least-squares plane through the non-planar lactide ring and the C5—C6 bond, which amounts to 77.9 (3)°. In the 6(*R*)-methyl derivative, the benzyloxymethyl group also occupies the axial position [plane–bond angle = 67.20 (13)°]. The 6(*S*)-methyl derivative, however, has the benzyloxymethyl group in the equatorial position [plane–bond angle is 13.13 (13)°], most likely due to steric hindrance between the substituents of the lactide ring. The link between the two ring systems is not in an all-*trans* conformation, the torsion angles C4—C5—C6—O4 and O5—C7—C8—C9 having the *-gauche* conformation.

The packing displays short C—H...O contacts, geometric details of which are given in Table 2. These contacts link the molecules into an infinite chain in the [100] direction (see Fig. 2).

## Experimental

The synthesis of the title compound is described elsewhere (Leemhuis *et al.*, 2003). Crystals were grown from a solution in methyl *tert*-butyl ether.

### Crystal data

C <sub>12</sub> H <sub>12</sub> O <sub>5</sub>	$D_x = 1.413 \text{ Mg m}^{-3}$
$M_r = 236.22$	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 219 reflections
$a = 6.925$ (4) Å	$\theta = 2.0\text{--}25.0^\circ$
$b = 7.025$ (4) Å	$\mu = 0.11 \text{ mm}^{-1}$
$c = 11.733$ (8) Å	$T = 150 \text{ K}$
$\beta = 103.44$ (3)°	Prism, colourless
$V = 555.2$ (6) Å <sup>3</sup>	0.15 × 0.05 × 0.05 mm
$Z = 2$	

### Data collection

Nonius KappaCCD area-detector diffractometer	899 reflections with $I > 2\sigma(I)$
$\varphi$ scans and $\omega$ scans with $\kappa$ offsets	$R_{\text{int}} = 0.087$
Absorption correction: none	$\theta_{\text{max}} = 25.3^\circ$
12280 measured reflections	$h = -8 \rightarrow 8$
1098 independent reflections	$k = -8 \rightarrow 8$
	$l = -14 \rightarrow 14$

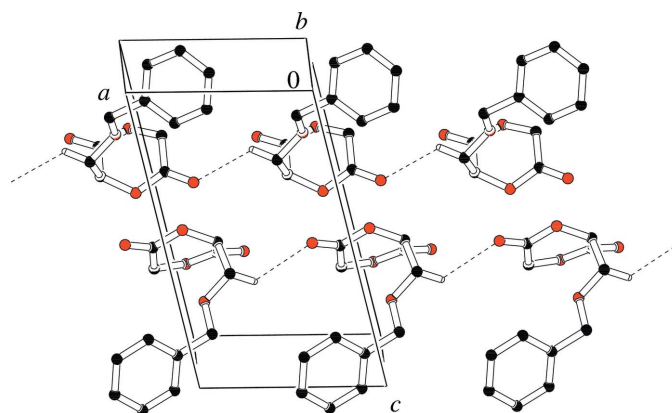
### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.1P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.102$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.11$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
1098 reflections	$\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$
154 parameters	
H-atom parameters constrained	

**Table 1**

Selected geometric parameters (Å, °).

O2—C1	1.339 (4)	O3—C2	1.437 (5)
O2—C5	1.446 (4)	O3—C4	1.333 (4)
C1—O2—C5	118.3 (3)	C2—O3—C4	120.7 (3)
C7—O5—C6—C5	−179.6 (3)	C4—C5—C6—O5	−61.9 (4)
C6—O5—C7—C8	158.0 (3)	O5—C7—C8—C9	−59.7 (4)



**Figure 2**

Short contacts C6—H6A...O1( $x - 1, y, z$ ) link the molecules into an infinite chain in the [100] direction.

**Table 2**

Hydrogen-bond geometry (Å, °).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
C6—H6A...O1 <sup>i</sup>	0.99	2.58	3.274 (5)	127

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

In the absence of significant anomalous scatterers, Friedel's law still holds. Friedel pairs were therefore averaged. The absolute configuration of C5 was chosen in accordance with the enantiopure starting material. H atoms were introduced in calculated positions, with C—H = 0.95–1.00 Å, and refined as riding on their carrier atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997); data reduction: DENZO; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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