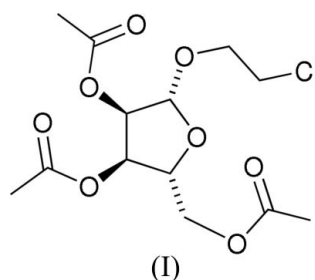
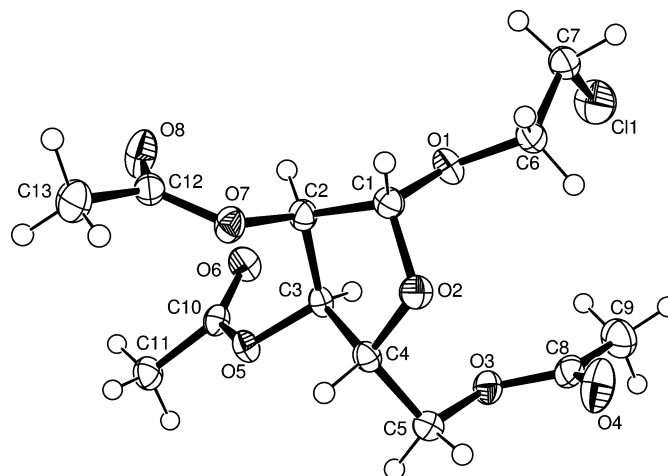
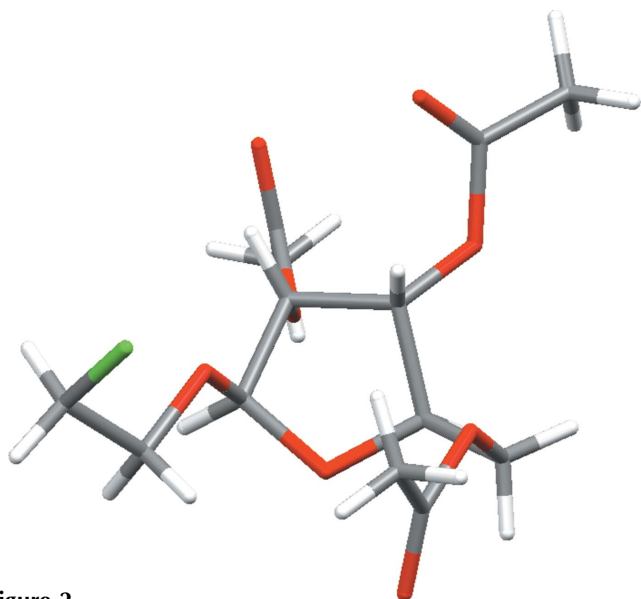


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Department of Chemistry, University of Basel,  
Spitalstrasse 51, CH 4056 Basel, SwitzerlandCorrespondence e-mail:  
catherine.housecroft@unibas.ch**Key indicators**Single-crystal X-ray study  
 $T = 173\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.029  
 $wR$  factor = 0.033  
Data-to-parameter ratio = 14.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**2,3,5-Tri-*O*-acetyl-1-(2-chloroethyl)- $\beta$ -D-ribofuranose**In the crystal structure of the title compound,  $\text{C}_{13}\text{H}_{19}\text{ClO}_8$ , extensive intermolecular hydrogen bonding leads to a three-dimensional network, but the Cl substituent is not involved in these interactions.Received 26 June 2006  
Accepted 27 June 2006**Comment**We have recently prepared a series of 1-(2-haloethyl)-2,3,5-tri-*O*-acetyl- $\beta$ -D-ribofuranose derivatives for use in the synthesis of ribose-functionalized 2,2'-bipyridine (Constable *et al.*, 2004) and 2,2':6',2''-terpyridine ligands. Crystals of 1-(2-chloroethyl)-2,3,5-tri-*O*-acetyl- $\beta$ -D-ribofuranose, (I), were grown by freeze-thawing the colourless oil that was obtained after chromatographic purification of the compound.Fig. 1 shows the molecular structure of (I). Bond distances and angles are unexceptional. The conformation of (I) is very similar to that found in polymorph *B* of 1,2,3,5-tetra-*O*-acetyl- $\beta$ -D-ribofuranose (Bombicz *et al.*, 2003; James & Stevens, 1973; Poppleton, 1976), and the conformations of the two molecules**Figure 1**  
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.



**Figure 2**  
The conformation of compound (I).

are compared in Figs. 2 and 3. Both compounds crystallize in the non-centrosymmetric space group  $P2_12_12_1$ , with cell dimensions that are similar, suggesting similar packing. Two polymorphs of 1,2,3,5-tetra-*O*-acetyl- $\beta$ -D-ribofuranose exist (Bombicz *et al.*, 2003; Czugler *et al.*, 1981; James & Stevens, 1973; Patterson & Groshens, 1954; Poppleton, 1976) and the relative instability of polymorph *A* has been attributed to extremely short H $\cdots$ H contacts (Bombicz *et al.*, 2003).

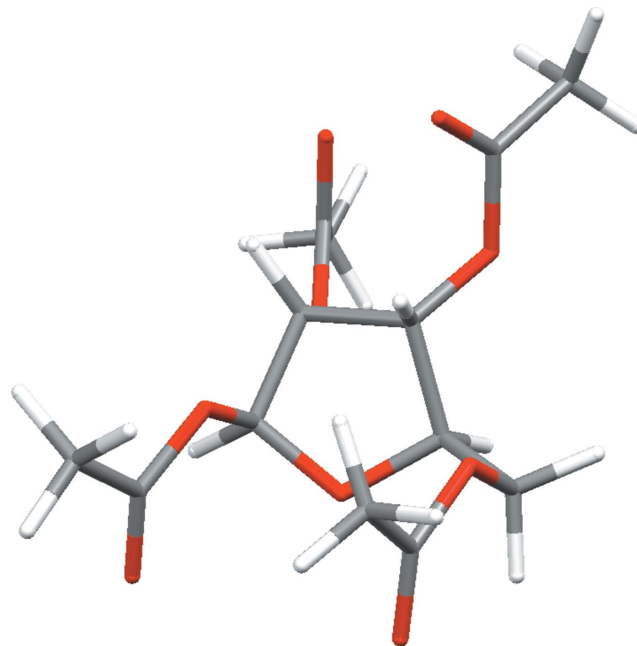
The molecule of (I) exhibits two short intramolecular C—H $\cdots$ O contacts [C2—H21 $\cdots$ O8 = 2.25 Å and C2 $\cdots$ O8 = 2.679 (2) Å, and C5—H51 $\cdots$ O4 = 2.26 Å and C5 $\cdots$ O4 = 2.671 (2) Å]. These are, however, non-directional (C2—H21 $\cdots$ O8 = 106° and C5—H51 $\cdots$ O4 = 105°) (Desiraju & Steiner, 1999). Similar short contacts are observed in 1,2,3,5-tetra-*O*-acetyl- $\beta$ -D-ribofuranose. Intermolecular interactions involve C—H $\cdots$ O contacts (Table 2) and lead to the formation of an extensive network of interconnected molecules. The Cl substituent is not involved in any intermolecular interactions.

## Experimental

The title compound was prepared as a colourless oil from 1,2,3,5-tri-*O*-acetyl- $\beta$ -D-ribofuranose and 2-chloroethanol in the presence of SnCl<sub>4</sub> by a method previously described for the analogous reaction starting from arabinofuranose (Pathak *et al.*, 2001). Crystals were grown by repeatedly dipping a sample of the compound contained in a tube under high vacuum into liquid nitrogen.

### Crystal data

C <sub>13</sub> H <sub>19</sub> ClO <sub>8</sub>	Z = 4
M <sub>r</sub> = 338.74	D <sub>x</sub> = 1.465 Mg m <sup>-3</sup>
Orthorhombic, $P2_12_12_1$	Mo K $\alpha$ radiation
a = 7.3407 (5) Å	$\mu$ = 0.29 mm <sup>-1</sup>
b = 13.5532 (14) Å	T = 173 K
c = 15.4384 (9) Å	Block, colourless
V = 1536.0 (2) Å <sup>3</sup>	0.28 × 0.26 × 0.22 mm



**Figure 3**  
The conformation of polymorph *B* of 1,2,3,5-tetra-*O*-acetyl- $\beta$ -D-ribofuranose.

### Data collection

Nonius KappaCCD area-detector diffractometer	46023 measured reflections
$\varphi$ and $\omega$ scans	3896 independent reflections
Absorption correction: multi-scan (DENZO/SCALEPACK; Otwinowski & Minor, 1997)	2801 reflections with $I > 3\sigma(I)$
$T_{\min} = 0.93$ , $T_{\max} = 0.94$	$R_{\text{int}} = 0.075$
	$\theta_{\text{max}} = 28.5^\circ$

### Refinement

Refinement on $F$	+ 0.288 $T_4(x)$ ,
$R[F > 2\sigma(F)] = 0.029$	where $T_i$ are the Chebyshev
$wR(F) = 0.033$	polynomials and $x = F_c/F_{\text{max}}$
$S = 1.07$	(Prince, 1982; Watkin, 1994)
2801 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
200 parameters	$\Delta\rho_{\text{max}} = 0.20 \text{ e \AA}^{-3}$
H-atom parameters constrained	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
$w = [1 - (F_o - F_c)^2/36\sigma^2(F)]^2 / [2.46T_o(x) - 0.945T_1(x) + 1.98T_2(x) - 0.132T_3(x)]$	Absolute structure: Flack (1983),
	with 1663 Friedel pairs
	Flack parameter: -0.01 (6)

**Table 1**

Selected geometric parameters (Å, °).

C11—C7	1.7847 (19)	C3—C4	1.516 (2)
C1—C2	1.513 (2)	C3—O5	1.428 (2)
C1—O1	1.397 (2)	C4—C5	1.506 (2)
C1—O2	1.421 (2)	C4—O2	1.428 (2)
C2—C3	1.515 (2)	C5—O3	1.436 (2)
C2—O7	1.435 (2)		
C2—C1—O1	106.34 (13)	C2—C3—O5	114.33 (13)
C2—C1—O2	105.66 (14)	C4—C3—O5	108.65 (13)
O1—C1—O2	111.71 (13)	C3—C4—C5	115.53 (14)
C1—C2—C3	100.45 (14)	C3—C4—O2	104.72 (13)
C1—C2—O7	106.62 (13)	C5—C4—O2	110.94 (13)
C3—C2—O7	109.57 (13)	C4—O2—C1	110.50 (12)
C2—C3—C4	102.56 (13)		

**Table 2**  
Intermolecular C—H...O interactions (Å, °) in (I).

	H...O	C...O	H—C...O
C1—H11...O4 <sup>i</sup>	2.56	3.453 (2)	157
C9—H92...O6 <sup>ii</sup>	2.55	3.447 (3)	156
C11—H113...O5 <sup>iii</sup>	2.48	3.428 (2)	168
C7—H72...O4 <sup>iv</sup>	2.61	3.391 (3)	139
C6—H61...O2 <sup>i</sup>	2.71	3.249 (2)	117

Symmetry codes: (i)  $-\frac{1}{2} + x, \frac{3}{2} - y, 2 - z$ ; (ii)  $-x, \frac{1}{2} + y, \frac{3}{2} - z$ ; (iii)  $-\frac{1}{2} + x, \frac{1}{2} - y, 2 - z$ ; (iv)  $x - 1, y, z$ .

All H atoms were treated as riding atoms, with C—H = 0.96 Å and  $U_{\text{iso}}(\text{H})$  between  $1.0U_{\text{eq}}(\text{C})$  and  $1.2U_{\text{eq}}(\text{C})$ .

Data collection: *COLLECT* (Nonius, 2001); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CRYSTALS*.

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