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2-[(2-Chloroethoxy)ethyl]-2,3,4,6-tetra-*O*-acetyl-β-D-glucopyranoside

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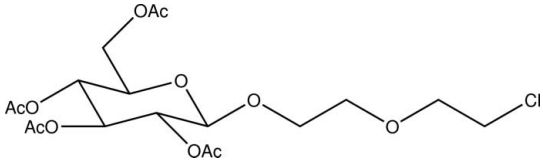
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.048; wR factor = 0.140; data-to-parameter ratio = 14.2.

In the title compound, $C_{18}H_{27}ClO_{11}$, the glucopyranoside ring adopts a chair conformation. All the substituents attached to the six-membered ring are in equatorial positions. In the crystal structure, molecules related by translation along the a axis are linked into chains by weak intermolecular C—H···O hydrogen bonds. The chloroethyl unit is disordered over two sites in a ratio of 0.7:0.3.

Related literature

For the crystal structure of 2,3,4,6-tetra-*O*-acetyl-2-chloroethyl-β-D-glucopyranoside, see: Zhang *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{27}ClO_{11}$
M_r = 454.85
Orthorhombic, $P2_12_12_1$
a = 7.5382 (13) Å
b = 14.195 (3) Å
c = 21.204 (4) Å
V = 2269.0 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
0.50 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.932, T_{max} = 0.956
11900 measured reflections
4018 independent reflections
3116 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.140
S = 1.03
4018 reflections
282 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), with 1705 Friedel pairs
Flack parameter: −0.04 (15)

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15B···O5^{i}	0.97	2.55	3.361 (5)	141
C18—H18B···O9^{i}	0.97	2.48	3.335 (7)	147

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* and *PARST95* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2250).

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Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Zhang, X.-R., Yang, X.-H., Li, X.-M. & Zhang, S.-S. (2006). *Acta Cryst.* E**62**, o3657–o3659.

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supplementary materials

Acta Cryst. (2007). E**63**, o3174 [**doi:10.1107/S1600536807028127**]

2-[(2-Chloroethoxy)ethyl]-2,3,4,6-tetra-*O*-acetyl-*β*-D-glucopyranoside

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Comment

In the title compound, (I) (Fig. 1), all bond lengths and angles are within normal ranges. The galactopyranoside ring adopts a chair conformation. All the substituents attached to the six-membered ring are in equatorial positions, assumed to be the most stable of all possible conformations due to the relatively low energy. There exist five intramolecular hydrogen bonds, forming five closed five-membered rings which contribute to the planarity of the substituents. In the crystal, the molecules are linked into chains along the *a* axis by C15—H15B···O5 and C18—H18B···O9 intermolecular hydrogen bonds.

Experimental

Compound (I) was prepared according to the method of Zhang *et al.* (2006). Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of an ethanol-water (3:1 *v*/*v*) solution over a period of 5 d.

Refinement

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H distances in the range 0.96–0.98 Å, and with U_{iso}(H) = 1.2 U_{eq}(C) and 1.5 U_{eq}(methyl C) H atoms. The chloroethyl fragment (C17—C18—Cl1) was treated as disordered between two positions with occupancy factors 0.70 and 0.30, respectively.

Figures

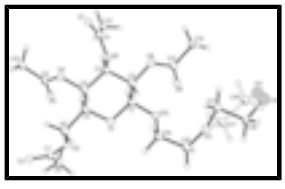


Fig. 1. The molecular structure of (I) showing 50% probability displacement ellipsoids and the atom numbering scheme.

2-[(2-Chloroethoxy)ethyl]-2,3,4,6-tetra-*O*-acetyl-β-*D*-galactopyranoside

Crystal data

$C_{18}H_{27}ClO_{11}$	D_x = 1.332 Mg m^{-3}
M_r = 454.85	Mo *K*α radiation λ = 0.71073 Å
Orthorhombic, $P2_12_12_1$	Cell parameters from 3522 reflections
a = 7.5382 (13) Å	θ = 2.4–21.1°
b = 14.195 (3) Å	μ = 0.22 mm^{-1}
c = 21.204 (4) Å	*T* = 293 (2) K

V = 2269.0 (8) Å^3	Column, colourless
Z = 4	0.50 × 0.22 × 0.16 mm
F_{000} = 960	

Data collection

Bruker SMART CCD area-detector diffractometer	4018 independent reflections
Radiation source: fine-focus sealed tube	3116 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 293(2) K	θ_{max} = 25.1º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→8
T_{min} = 0.932, T_{max} = 0.956	k = −16→8
11900 measured reflections	l = −25→25

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.048	$w = 1/[\sigma^2(F_o^2) + (0.0807P)^2 + 0.2077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.140	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.04	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
4018 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
282 parameters	Extinction correction: none
6 restraints	Absolute structure: Flack (1983), 1705 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.04 (15)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)

C1	0.1755 (4)	0.9731 (2)	0.01052 (13)	0.0561 (7)	
H1A	0.2538	1.0274	0.0167	0.067*	
C2	0.0221 (4)	0.99883 (18)	−0.03236 (13)	0.0533 (6)	
H2A	−0.0508	0.9431	−0.0409	0.064*	
C3	−0.0896 (4)	1.07522 (18)	−0.00178 (13)	0.0510 (6)	
H3A	−0.0239	1.1348	−0.0008	0.061*	
C4	−0.1426 (4)	1.04628 (18)	0.06463 (13)	0.0528 (7)	
H4A	−0.2280	0.9943	0.0626	0.063*	
C5	0.0189 (4)	1.01584 (19)	0.10235 (13)	0.0568 (7)	
H5A	0.1002	1.0693	0.1064	0.068*	
C6	−0.0264 (5)	0.9797 (2)	0.16670 (14)	0.0681 (8)	
H6A	0.0792	0.9560	0.1874	0.082*	
H6B	−0.0755	1.0301	0.1923	0.082*	
C7	−0.2576 (6)	0.8854 (3)	0.20918 (16)	0.0835 (10)	
C8	−0.3918 (7)	0.8146 (3)	0.1925 (2)	0.1123 (16)	
H8A	−0.4642	0.8014	0.2287	0.169*	
H8B	−0.3340	0.7578	0.1790	0.169*	
H8C	−0.4648	0.8383	0.1590	0.169*	
C9	−0.3865 (5)	1.1182 (3)	0.11907 (16)	0.0731 (9)	
C10	−0.4441 (6)	1.2082 (3)	0.14768 (19)	0.0982 (12)	
H10A	−0.5614	1.2011	0.1647	0.147*	
H10B	−0.4447	1.2566	0.1161	0.147*	
H10C	−0.3636	1.2253	0.1808	0.147*	
C11	−0.3081 (4)	1.1719 (2)	−0.05358 (14)	0.0629 (8)	
C12	−0.4690 (5)	1.1648 (3)	−0.09423 (18)	0.0873 (11)	
H12A	−0.5117	1.2269	−0.1038	0.131*	
H12B	−0.5595	1.1303	−0.0724	0.131*	
H12C	−0.4394	1.1328	−0.1327	0.131*	
C13	0.0893 (4)	0.9785 (2)	−0.14137 (14)	0.0649 (8)	
C14	0.1764 (6)	1.0232 (3)	−0.19647 (15)	0.0890 (11)	
H14A	0.1723	0.9810	−0.2318	0.133*	
H14B	0.2977	1.0371	−0.1863	0.133*	
H14C	0.1155	1.0805	−0.2069	0.133*	
C15	0.4186 (5)	0.8690 (3)	0.02034 (18)	0.0858 (11)	
H15A	0.3777	0.8406	0.0593	0.103*	
H15B	0.4904	0.9234	0.0311	0.103*	
C16	0.5271 (5)	0.8010 (3)	−0.0143 (2)	0.0939 (12)	
H16A	0.6003	0.7662	0.0153	0.113*	
H16B	0.4502	0.7564	−0.0356	0.113*	
C17	0.5595 (11)	0.8630 (5)	−0.1191 (2)	0.117 (2)	0.70
H17A	0.5916	0.9248	−0.1349	0.140*	0.70
H17B	0.4313	0.8569	−0.1185	0.140*	0.70
C18	0.6461 (7)	0.7849 (4)	−0.1571 (2)	0.106 (2)	0.70
H18A	0.6190	0.7244	−0.1381	0.127*	0.70
H18B	0.7739	0.7930	−0.1566	0.127*	0.70
Cl1	0.5667 (5)	0.7865 (3)	−0.23801 (13)	0.1242 (10)	0.70
C17'	0.556 (3)	0.8083 (14)	−0.1155 (5)	0.125 (4)*	0.30
H17C	0.4302	0.8229	−0.1149	0.150*	0.30
H17D	0.5673	0.7403	−0.1149	0.150*	0.30

C18'	0.634 (2)	0.8447 (14)	−0.1780 (5)	0.125 (4)*	0.30
H18C	0.7555	0.8237	−0.1822	0.150*	0.30
H18D	0.6327	0.9130	−0.1782	0.150*	0.30
Cl1'	0.5049 (10)	0.8012 (7)	−0.2426 (4)	0.109 (3)*	0.30
O1	0.1055 (3)	0.94203 (13)	0.06919 (9)	0.0574 (5)	
O2	−0.1540 (3)	0.90570 (15)	0.15955 (9)	0.0677 (6)	
O3	−0.2416 (5)	0.9234 (2)	0.25869 (13)	0.1206 (11)	
O4	−0.2231 (3)	1.12583 (13)	0.09468 (9)	0.0610 (5)	
O5	−0.4716 (4)	1.0471 (2)	0.11726 (17)	0.1170 (11)	
O6	−0.2470 (3)	1.08482 (13)	−0.03989 (9)	0.0584 (5)	
O7	−0.2418 (4)	1.24259 (16)	−0.03553 (13)	0.0889 (8)	
O8	0.0921 (3)	1.03612 (13)	−0.09056 (9)	0.0583 (5)	
O9	0.0267 (4)	0.90214 (19)	−0.14093 (12)	0.0970 (9)	
O10	0.2679 (3)	0.89899 (14)	−0.01624 (10)	0.0624 (5)	
O11	0.6350 (4)	0.8454 (3)	−0.05836 (16)	0.1156 (10)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0485 (15)	0.0545 (16)	0.0653 (16)	−0.0021 (14)	0.0042 (13)	−0.0006 (14)
C2	0.0530 (16)	0.0462 (14)	0.0606 (15)	−0.0032 (12)	0.0048 (13)	−0.0032 (12)
C3	0.0485 (15)	0.0427 (13)	0.0618 (15)	−0.0042 (12)	−0.0019 (13)	−0.0019 (12)
C4	0.0554 (16)	0.0424 (13)	0.0608 (15)	−0.0020 (13)	0.0029 (13)	−0.0095 (12)
C5	0.0564 (16)	0.0522 (15)	0.0618 (15)	−0.0027 (14)	−0.0002 (14)	−0.0060 (13)
C6	0.079 (2)	0.0680 (18)	0.0573 (16)	0.0038 (19)	−0.0069 (15)	−0.0057 (15)
C7	0.096 (3)	0.091 (3)	0.063 (2)	0.002 (2)	0.014 (2)	0.0059 (19)
C8	0.129 (4)	0.114 (3)	0.094 (3)	−0.038 (3)	0.021 (3)	0.013 (2)
C9	0.063 (2)	0.078 (2)	0.077 (2)	0.005 (2)	0.0022 (17)	−0.0216 (18)
C10	0.089 (3)	0.103 (3)	0.103 (3)	0.024 (2)	0.005 (2)	−0.039 (2)
C11	0.0656 (19)	0.062 (2)	0.0616 (17)	0.0128 (16)	0.0067 (15)	0.0019 (15)
C12	0.079 (2)	0.092 (2)	0.091 (2)	0.027 (2)	−0.016 (2)	0.001 (2)
C13	0.0557 (17)	0.073 (2)	0.0663 (18)	0.0036 (17)	0.0045 (15)	−0.0106 (16)
C14	0.100 (3)	0.105 (3)	0.0617 (18)	0.009 (3)	0.0110 (19)	0.0005 (19)
C15	0.0603 (19)	0.104 (3)	0.093 (2)	0.024 (2)	−0.0085 (19)	−0.009 (2)
C16	0.060 (2)	0.090 (3)	0.132 (3)	0.012 (2)	0.009 (2)	0.009 (2)
C17	0.114 (5)	0.088 (4)	0.148 (7)	0.032 (4)	0.001 (5)	0.005 (4)
C18	0.065 (3)	0.076 (3)	0.177 (7)	0.002 (3)	0.024 (4)	0.014 (4)
Cl1	0.145 (3)	0.139 (2)	0.0891 (13)	−0.035 (2)	0.0098 (17)	0.0194 (12)
O1	0.0567 (11)	0.0563 (11)	0.0592 (10)	0.0046 (10)	0.0045 (9)	0.0007 (9)
O2	0.0847 (14)	0.0658 (12)	0.0525 (10)	−0.0044 (12)	0.0109 (10)	−0.0010 (9)
O3	0.142 (3)	0.152 (3)	0.0684 (16)	−0.023 (2)	0.0269 (18)	−0.0157 (17)
O4	0.0615 (12)	0.0511 (10)	0.0703 (11)	0.0006 (10)	0.0083 (10)	−0.0140 (10)
O5	0.0772 (16)	0.103 (2)	0.171 (3)	−0.0158 (17)	0.0454 (19)	−0.047 (2)
O6	0.0555 (11)	0.0503 (10)	0.0693 (11)	0.0037 (10)	−0.0078 (10)	−0.0021 (9)
O7	0.0963 (18)	0.0514 (13)	0.1189 (19)	0.0061 (13)	−0.0167 (16)	−0.0007 (13)
O8	0.0637 (12)	0.0525 (10)	0.0588 (10)	−0.0018 (10)	0.0076 (9)	0.0005 (9)
O9	0.113 (2)	0.0815 (16)	0.0962 (17)	−0.0266 (17)	0.0265 (16)	−0.0324 (14)
O10	0.0503 (11)	0.0623 (12)	0.0747 (12)	0.0105 (10)	0.0024 (10)	−0.0038 (10)

O11	0.0740 (17)	0.148 (3)	0.125 (2)	−0.0122 (19)	0.0188 (18)	−0.013 (2)

Geometric parameters (Å, °)

C1—O10	1.383 (3)	C11—O6	1.351 (4)
C1—O1	1.421 (3)	C11—C12	1.492 (5)
C1—C2	1.516 (4)	C12—H12A	0.9600
C1—H1A	0.9800	C12—H12B	0.9600
C2—O8	1.443 (3)	C12—H12C	0.9600
C2—C3	1.518 (4)	C13—O9	1.182 (4)
C2—H2A	0.9800	C13—O8	1.353 (4)
C3—O6	1.442 (3)	C13—C14	1.483 (5)
C3—C4	1.521 (4)	C14—H14A	0.9600
C3—H3A	0.9800	C14—H14B	0.9600
C4—O4	1.432 (3)	C14—H14C	0.9600
C4—C5	1.519 (4)	C15—O10	1.440 (4)
C4—H4A	0.9800	C15—C16	1.462 (5)
C5—O1	1.421 (3)	C15—H15A	0.9700
C5—C6	1.497 (4)	C15—H15B	0.9700
C5—H5A	0.9800	C16—O11	1.390 (5)
C6—O2	1.432 (4)	C16—H16A	0.9700
C6—H6A	0.9700	C16—H16B	0.9700
C6—H6B	0.9700	C17—O11	1.430 (4)
C7—O3	1.186 (4)	C17—C18	1.518 (4)
C7—O2	1.342 (4)	C17—H17A	0.9700
C7—C8	1.469 (6)	C17—H17B	0.9700
C8—H8A	0.9600	C18—Cl1	1.817 (4)
C8—H8B	0.9600	C18—H18A	0.9700
C8—H8C	0.9600	C18—H18B	0.9700
C9—O5	1.197 (4)	C17'—O11	1.450 (5)
C9—O4	1.340 (4)	C17'—C18'	1.536 (5)
C9—C10	1.479 (5)	C17'—H17C	0.9700
C10—H10A	0.9600	C17'—H17D	0.9700
C10—H10B	0.9600	C18'—Cl1'	1.789 (5)
C10—H10C	0.9600	C18'—H18C	0.9700
C11—O7	1.184 (4)	C18'—H18D	0.9700
O10—C1—O1	108.1 (2)	H12A—C12—H12B	109.5
O10—C1—C2	108.7 (2)	C11—C12—H12C	109.5
O1—C1—C2	108.5 (2)	H12A—C12—H12C	109.5
O10—C1—H1A	110.5	H12B—C12—H12C	109.5
O1—C1—H1A	110.5	O9—C13—O8	123.7 (3)
C2—C1—H1A	110.5	O9—C13—C14	125.1 (3)
O8—C2—C1	108.8 (2)	O8—C13—C14	111.2 (3)
O8—C2—C3	107.8 (2)	C13—C14—H14A	109.5
C1—C2—C3	109.8 (2)	C13—C14—H14B	109.5
O8—C2—H2A	110.1	H14A—C14—H14B	109.5
C1—C2—H2A	110.1	C13—C14—H14C	109.5
C3—C2—H2A	110.1	H14A—C14—H14C	109.5
O6—C3—C2	106.5 (2)	H14B—C14—H14C	109.5

O6—C3—C4	109.1 (2)	O10—C15—C16	111.5 (3)
C2—C3—C4	110.4 (2)	O10—C15—H15A	109.3
O6—C3—H3A	110.2	C16—C15—H15A	109.3
C2—C3—H3A	110.2	O10—C15—H15B	109.3
C4—C3—H3A	110.2	C16—C15—H15B	109.3
O4—C4—C5	109.3 (2)	H15A—C15—H15B	108.0
O4—C4—C3	108.1 (2)	O11—C16—C15	111.5 (3)
C5—C4—C3	110.7 (2)	O11—C16—H16A	109.3
O4—C4—H4A	109.6	C15—C16—H16A	109.3
C5—C4—H4A	109.6	O11—C16—H16B	109.3
C3—C4—H4A	109.6	C15—C16—H16B	109.3
O1—C5—C6	107.7 (2)	H16A—C16—H16B	108.0
O1—C5—C4	108.5 (2)	O11—C17—C18	100.3 (4)
C6—C5—C4	113.2 (3)	O11—C17—H17A	111.7
O1—C5—H5A	109.1	C18—C17—H17A	111.7
C6—C5—H5A	109.1	O11—C17—H17B	111.7
C4—C5—H5A	109.1	C18—C17—H17B	111.7
O2—C6—C5	107.9 (2)	H17A—C17—H17B	109.5
O2—C6—H6A	110.1	C17—C18—Cl1	110.5 (4)
C5—C6—H6A	110.1	C17—C18—H18A	109.5
O2—C6—H6B	110.1	Cl1—C18—H18A	109.5
C5—C6—H6B	110.1	C17—C18—H18B	109.5
H6A—C6—H6B	108.4	Cl1—C18—H18B	109.5
O3—C7—O2	122.5 (4)	H18A—C18—H18B	108.1
O3—C7—C8	126.4 (4)	O11—C17'—C18'	116.2 (9)
O2—C7—C8	111.1 (3)	O11—C17'—H17C	108.2
C7—C8—H8A	109.5	C18'—C17'—H17C	108.2
C7—C8—H8B	109.5	O11—C17'—H17D	108.2
H8A—C8—H8B	109.5	C18'—C17'—H17D	108.2
C7—C8—H8C	109.5	H17C—C17'—H17D	107.4
H8A—C8—H8C	109.5	C17'—C18'—Cl1'	109.7 (8)
H8B—C8—H8C	109.5	C17'—C18'—H18C	109.7
O5—C9—O4	123.2 (3)	Cl1'—C18'—H18C	109.7
O5—C9—C10	125.8 (3)	C17'—C18'—H18D	109.7
O4—C9—C10	111.0 (3)	Cl1'—C18'—H18D	109.7
C9—C10—H10A	109.5	H18C—C18'—H18D	108.2
C9—C10—H10B	109.5	C1—O1—C5	112.0 (2)
H10A—C10—H10B	109.5	C7—O2—C6	117.7 (3)
C9—C10—H10C	109.5	C9—O4—C4	119.9 (2)
H10A—C10—H10C	109.5	C11—O6—C3	119.2 (2)
H10B—C10—H10C	109.5	C13—O8—C2	117.0 (2)
O7—C11—O6	124.2 (3)	C1—O10—C15	113.6 (2)
O7—C11—C12	126.0 (3)	C16—O11—C17	116.9 (5)
O6—C11—C12	109.9 (3)	C16—O11—C17'	99.1 (7)
C11—C12—H12A	109.5	C17—O11—C17'	31.4 (8)
C11—C12—H12B	109.5		
O10—C1—C2—O8	−66.3 (3)	O3—C7—O2—C6	−3.4 (6)
O1—C1—C2—O8	176.4 (2)	C8—C7—O2—C6	174.6 (3)
O10—C1—C2—C3	175.9 (2)	C5—C6—O2—C7	−157.5 (3)

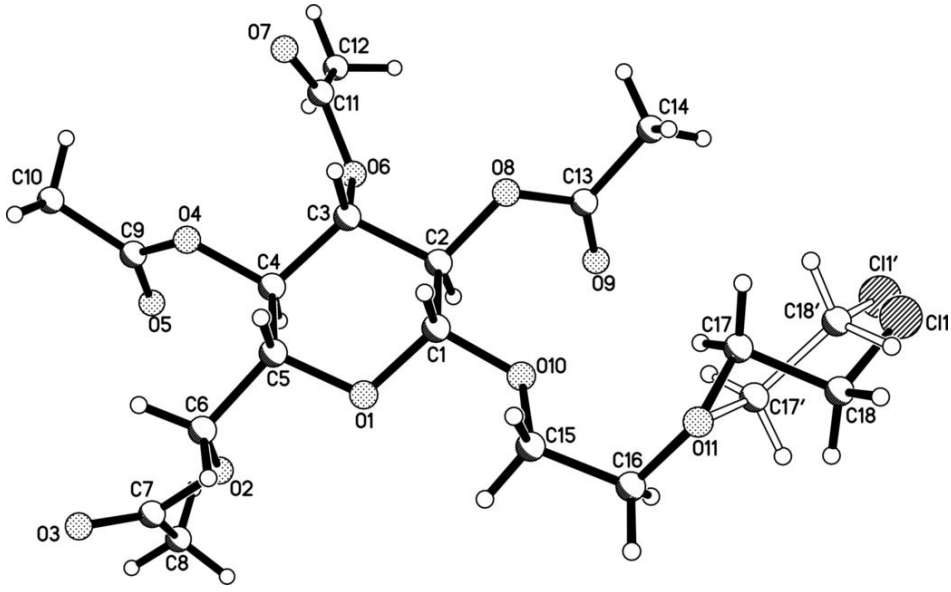
O1—C1—C2—C3	58.6 (3)	O5—C9—O4—C4	0.0 (5)
O8—C2—C3—O6	70.8 (3)	C10—C9—O4—C4	−180.0 (3)
C1—C2—C3—O6	−170.8 (2)	C5—C4—O4—C9	−115.0 (3)
O8—C2—C3—C4	−170.8 (2)	C3—C4—O4—C9	124.5 (3)
C1—C2—C3—C4	−52.4 (3)	O7—C11—O6—C3	−1.0 (4)
O6—C3—C4—O4	−72.1 (3)	C12—C11—O6—C3	178.9 (3)
C2—C3—C4—O4	171.1 (2)	C2—C3—O6—C11	−137.0 (2)
O6—C3—C4—C5	168.3 (2)	C4—C3—O6—C11	103.8 (3)
C2—C3—C4—C5	51.5 (3)	O9—C13—O8—C2	3.3 (5)
O4—C4—C5—O1	−175.2 (2)	C14—C13—O8—C2	−176.0 (3)
C3—C4—C5—O1	−56.3 (3)	C1—C2—O8—C13	103.5 (3)
O4—C4—C5—C6	65.3 (3)	C3—C2—O8—C13	−137.4 (2)
C3—C4—C5—C6	−175.7 (2)	O1—C1—O10—C15	−63.0 (3)
O1—C5—C6—O2	−65.3 (3)	C2—C1—O10—C15	179.4 (3)
C4—C5—C6—O2	54.6 (3)	C16—C15—O10—C1	−171.2 (3)
O10—C15—C16—O11	78.8 (4)	C15—C16—O11—C17	−86.4 (5)
O11—C17—C18—Cl1	177.8 (4)	C15—C16—O11—C17'	−113.8 (11)
O11—C17'—C18'—Cl1'	−173.9 (14)	C18—C17—O11—C16	−103.0 (6)
O10—C1—O1—C5	175.8 (2)	C18—C17—O11—C17'	−42.3 (17)
C2—C1—O1—C5	−66.5 (3)	C18'—C17'—O11—C16	177.2 (19)
C6—C5—O1—C1	−172.1 (2)	C18'—C17'—O11—C17	49.2 (14)
C4—C5—O1—C1	65.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15B···O5^{i}	0.97	2.55	3.361 (5)	141
C18—H18B···O9^{i}	0.97	2.48	3.335 (7)	147

Symmetry codes: (i) *x*+1, *y*, *z*.

Fig. 1


O7
C12
C11
C14
C10
O6
O8
C13
C9
O4
C3
C2
C4
O9
O5
Cl1′
C18′
Cl1
C17
C1
C5
O10
C6
O1
C17′
C18
C15
O11
C16
C7
O2
O3
C8