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1,3,4,5,6-Penta-*O*-acetyl-L-sorbose

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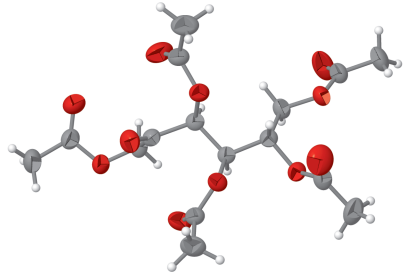
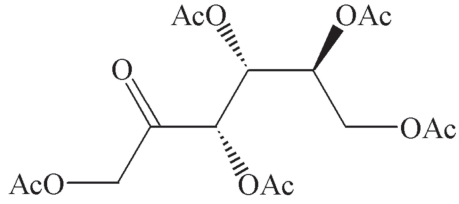
The crystal structure of the title compound, $C_{16}H_{22}O_{11}$, was determined. The compound crystallizes in the monoclinic space group $P2_1$, with one molecule in the asymmetric unit. Unlike unmodified L-sorbose, which adopts an α-L-sorbopyranose form and forms an extensive three-dimensional O—H···O hydrogen-bonding network in the crystal, the title compound adopts an acyclic keto form. Acetylation of all five hydroxy groups removes the O—H hydrogen-bond donors; consequently, no conventional intermolecular O—H···O hydrogen bonds are present. The crystal packing features intermolecular C—H···O contacts involving the acetyl groups.

3D view



Chemical scheme



Structure description

The title compound, $C_{16}H_{22}O_{11}$, was obtained by acetylation of L-sorbose. The molecular structure is shown in Fig. 1. The compound crystallizes in the monoclinic space group $P2_1$, with one molecule in the asymmetric unit. Unmodified L-sorbose crystallizes as α-L-sorbopyranose (CSD refcode SORBOL01; Nordenson *et al.*, 1979), whereas the title compound adopts an acyclic keto form, as indicated by the C2═O2 bond length of 1.194 (4) Å. In the crystal structure of unmodified L-sorbose, the five hydroxy groups act as hydrogen-bond donors and acceptors, linking the molecules through an extended three-dimensional O—H···O hydrogen-bond network. Unmodified L-sorbose crystallizes in the orthorhombic space group $P2_12_12_1$, with a reported unit-cell volume of approximately 745 Å^3 for Z = 4 (CSD refcode SORBOL01; Nordenson *et al.*, 1979). In the title compound, all five hydroxy groups of L-sorbose are converted into acetate ester groups. Consequently, the molecule has no O—H hydrogen-bond donors, and no conventional O—H···O hydrogen bonds are present in the crystal. Selected C—H···O contacts are listed in Table 1 and shown as black dashed lines in Fig. 2. The absolute configuration is consistent with that of the L-sorbose starting material and is supported by a Flack parameter of 0.02 (10), determined using 1441 quotients.

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O10^{i}	0.98	2.48	3.285 (4)	139
C6—H6A···O10^{i}	0.97	2.58	3.394 (4)	141
C8—H8C···O8^{ii}	0.96	2.58	3.536 (5)	172
C12—H12A···O11^{iii}	0.96	2.60	3.531 (6)	164
C12—H12C···O1^{iv}	0.96	2.51	3.393 (5)	154

Symmetry codes: (i) $x+1, y, z$; (ii) $x, y, z-1$; (iii) $x-1, y, z-1$; (iv) $x-1, y, z$.

Synthesis and crystallization

L-Sorbose (20.0 g) was suspended in dichloromethane (100 ml) and stirred at room temperature. Acetic anhydride (80 ml) and 4-dimethylaminopyridine (DMAP) were added, and the reaction mixture was stirred for 24 h. The reaction was quenched by the addition of methanol, and the solvents were removed under reduced pressure. The residue was dissolved in ethyl acetate and washed with hydrochloric acid and water to remove DMAP, followed successively by saturated aqueous sodium hydrogen carbonate solution and water. The organic layer was concentrated under reduced pressure to afford the crude product as a syrup.

The crude product was purified by silica-gel column chromatography. The fractions containing the major product were collected and concentrated. Crystallization from an ethyl acetate/hexane solvent system, followed by recrystallization from the same solvent system, afforded colorless block-shaped crystals of the title compound (6.5 g, 15.0% yield based on L-sorbose), suitable for single-crystal X-ray diffraction.

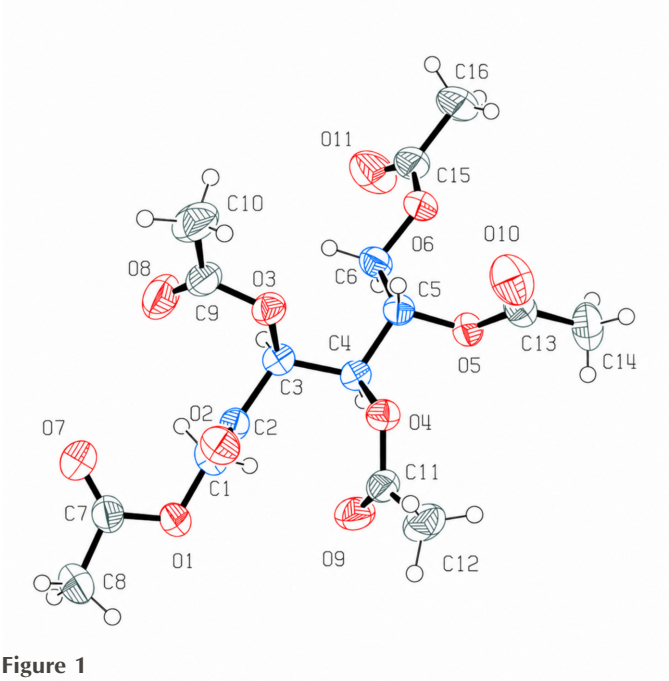

Figure 1
Molecular structure of the title compound showing the atom-labelling scheme. The carbon atoms of the original L-sorbose skeleton are shown in blue, and the carbon atoms of the acetyl groups in grey. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as small spheres of arbitrary radii.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{22}O_{11}$
M_r	390.33
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	296
a, b, c (Å)	6.1780 (7), 20.434 (2), 7.9015 (8)
β (°)	105.199 (7)
V (Å^3)	962.58 (18)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.00
Crystal size (mm)	0.10 × 0.10 × 0.10
Data collection	
Diffractometer	Rigaku R-AXIS RAPID
Absorption correction	Multi-scan (*ABSCOR*; Rigaku, 1995)
T_{min}, T_{max}	0.522, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10458, 3422, 3273
R_{int}	0.054
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.046, 0.113, 1.10
No. of reflections	3422
No. of parameters	249
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.32
Absolute structure	Flack x determined using 1441 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.02 (10)

Computer programs: *RAPID-AUTO* (Rigaku, 2009), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

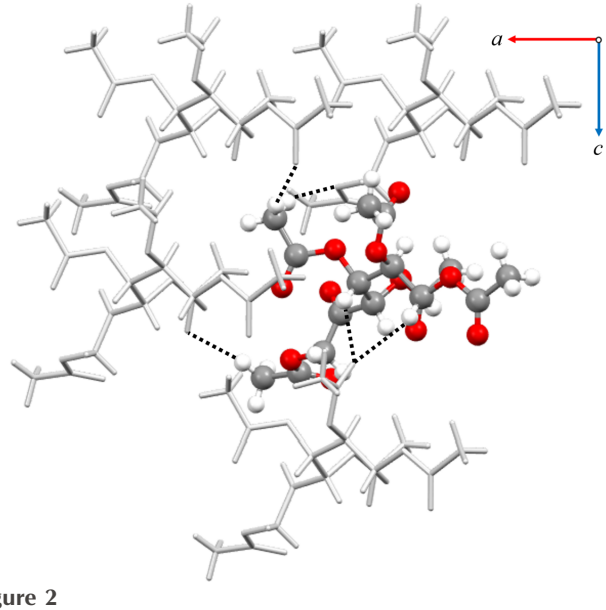

Figure 2
Crystal-packing diagram of the title compound, viewed along the b axis. Selected intermolecular C—H···O contacts are shown as black dashed lines (details in Table 1).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{16}H_{22}O_{11}$
M_r = 390.33
Monoclinic, $P2_1$
a = 6.1780 (7) Å
b = 20.434 (2) Å
c = 7.9015 (8) Å
β = 105.199 (7)°
V = 962.58 (18) Å^3
Z = 2
$F(000)$ = 412
D_x = 1.347 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.5418 Å
Cell parameters from 10151 reflections
θ = 4.3–68.3°
μ = 1.00 mm^{-1}
T = 296 K
Block, clear light colourless
0.1 × 0.1 × 0.1 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (ABSCOR; Rigaku, 1995)
T_{min} = 0.522, T_{max} = 1.000
10458 measured reflections
3422 independent reflections
3273 reflections with $I > 2\sigma(I)$
R_{int} = 0.054
θ_{max} = 68.2°, θ_{min} = 4.3°
h = −7→7
k = −24→24
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.113
S = 1.10
3422 reflections
249 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0693P)^2 + 0.0505P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Absolute structure: Flack x determined using 1441 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.02 (10)

Special details

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

Refinement. All H atoms were placed in geometrically calculated positions and refined using a riding model, with C—H distances of 0.96–0.98 Å. Their isotropic displacement parameters were set at U_{iso}(H) = 1.2U_{eq}(C) for methine and methylene H atoms and 1.5U_{eq}(C) for methyl H atoms. Methyl groups were allowed to rotate about their C—C bonds. The absolute structure was determined using 1441 quotients of the form [(I+) - (I–)]/[(I+) + (I–)], giving a Flack parameter of 0.02 (10) (Parsons *et al.*, 2013).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	1.1314 (4)	0.61300 (11)	0.3088 (3)	0.0492 (5)
O2	0.7378 (4)	0.62487 (11)	0.4003 (3)	0.0503 (5)
O3	0.6634 (4)	0.56616 (10)	0.6939 (3)	0.0426 (5)
O4	0.4932 (3)	0.48793 (11)	0.3710 (2)	0.0390 (4)
O5	0.5064 (3)	0.37254 (9)	0.5541 (3)	0.0404 (5)
O6	0.6531 (4)	0.37666 (11)	0.9092 (3)	0.0475 (5)
O7	1.2431 (5)	0.69183 (14)	0.5087 (3)	0.0678 (7)
O8	0.9614 (5)	0.62743 (16)	0.8212 (4)	0.0728 (8)
O9	0.7110 (4)	0.48931 (15)	0.1837 (3)	0.0577 (6)
O10	0.1614 (4)	0.39293 (17)	0.5829 (4)	0.0745 (8)
O11	0.9864 (6)	0.3561 (2)	1.0954 (4)	0.0857 (10)
C1	1.0909 (5)	0.57142 (16)	0.4421 (4)	0.0463 (7)
H1A	1.204134	0.579410	0.550999	0.056*
H1B	1.103443	0.526106	0.409333	0.056*
C2	0.8636 (5)	0.58266 (14)	0.4701 (4)	0.0382 (6)
C3	0.8045 (5)	0.53460 (14)	0.6011 (4)	0.0369 (6)
H3	0.943816	0.521460	0.686033	0.044*
C4	0.6851 (5)	0.47292 (13)	0.5143 (3)	0.0344 (6)
H4	0.790640	0.446029	0.471078	0.041*
C5	0.5902 (5)	0.43266 (14)	0.6410 (4)	0.0369 (6)
H5	0.468004	0.456706	0.670845	0.044*
C6	0.7665 (6)	0.41474 (17)	0.8062 (4)	0.0449 (7)
H6A	0.885523	0.389430	0.778394	0.054*
H6B	0.831168	0.453810	0.869289	0.054*
C7	1.2058 (6)	0.67348 (16)	0.3604 (5)	0.0502 (8)
C8	1.2355 (9)	0.7120 (2)	0.2084 (6)	0.0781 (14)
H8A	1.391260	0.712445	0.209468	0.117*
H8B	1.184981	0.756077	0.216245	0.117*
H8C	1.149530	0.692442	0.101426	0.117*
C9	0.7682 (6)	0.61372 (17)	0.8059 (4)	0.0496 (7)
C10	0.6165 (9)	0.6434 (2)	0.9033 (6)	0.0716 (11)
H10A	0.465041	0.642506	0.831137	0.107*
H10B	0.660841	0.687839	0.932870	0.107*
H10C	0.625932	0.618896	1.008680	0.107*
C11	0.5274 (5)	0.49127 (16)	0.2087 (4)	0.0440 (7)
C12	0.3111 (6)	0.4964 (2)	0.0716 (4)	0.0609 (9)
H12A	0.235497	0.454908	0.059101	0.091*
H12B	0.339506	0.508457	−0.038020	0.091*
H12C	0.218697	0.529035	0.105211	0.091*

C13	0.2902 (5)	0.35653 (17)	0.5416 (4)	0.0475 (7)
C14	0.2420 (7)	0.2890 (2)	0.4686 (6)	0.0687 (11)
H14A	0.284440	0.285803	0.360406	0.103*
H14B	0.084588	0.280055	0.447516	0.103*
H14C	0.325876	0.257838	0.550988	0.103*
C15	0.7878 (7)	0.35047 (17)	1.0555 (5)	0.0545 (8)
C16	0.6523 (10)	0.3151 (2)	1.1598 (6)	0.0775 (13)
H16A	0.654682	0.339533	1.263955	0.116*
H16B	0.715418	0.272468	1.191641	0.116*
H16C	0.500265	0.310598	1.090212	0.116*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0562 (13)	0.0454 (12)	0.0503 (11)	−0.0113 (10)	0.0216 (10)	−0.0018 (9)
O2	0.0520 (13)	0.0427 (12)	0.0554 (12)	0.0105 (10)	0.0128 (10)	0.0109 (9)
O3	0.0444 (11)	0.0434 (11)	0.0418 (11)	0.0004 (9)	0.0148 (9)	−0.0057 (8)
O4	0.0354 (10)	0.0443 (11)	0.0364 (9)	0.0025 (8)	0.0079 (8)	0.0021 (8)
O5	0.0373 (10)	0.0383 (11)	0.0460 (10)	−0.0019 (8)	0.0120 (8)	−0.0012 (8)
O6	0.0561 (13)	0.0481 (12)	0.0402 (10)	−0.0062 (10)	0.0156 (9)	0.0068 (9)
O7	0.086 (2)	0.0589 (16)	0.0601 (16)	−0.0127 (14)	0.0210 (14)	−0.0134 (12)
O8	0.0650 (18)	0.080 (2)	0.0706 (17)	−0.0182 (15)	0.0129 (14)	−0.0279 (15)
O9	0.0595 (14)	0.0738 (16)	0.0443 (11)	−0.0043 (13)	0.0213 (10)	−0.0069 (12)
O10	0.0398 (14)	0.084 (2)	0.103 (2)	0.0011 (14)	0.0248 (14)	0.0035 (17)
O11	0.071 (2)	0.104 (2)	0.0721 (18)	−0.0015 (18)	0.0026 (15)	0.0419 (17)
C1	0.0419 (16)	0.0419 (16)	0.0564 (18)	−0.0011 (13)	0.0150 (14)	0.0063 (13)
C2	0.0397 (15)	0.0349 (14)	0.0384 (14)	−0.0012 (11)	0.0070 (11)	−0.0021 (11)
C3	0.0343 (13)	0.0377 (14)	0.0374 (14)	0.0053 (11)	0.0072 (11)	0.0006 (11)
C4	0.0317 (13)	0.0356 (14)	0.0344 (13)	0.0040 (10)	0.0062 (10)	0.0013 (10)
C5	0.0359 (14)	0.0371 (14)	0.0384 (13)	0.0016 (11)	0.0111 (11)	−0.0010 (10)
C6	0.0440 (17)	0.0497 (17)	0.0406 (15)	−0.0046 (13)	0.0103 (12)	0.0082 (12)
C7	0.0500 (18)	0.0451 (17)	0.0561 (19)	−0.0076 (14)	0.0152 (15)	−0.0022 (14)
C8	0.102 (4)	0.065 (3)	0.065 (2)	−0.033 (2)	0.017 (2)	0.009 (2)
C9	0.061 (2)	0.0471 (17)	0.0392 (15)	−0.0004 (15)	0.0101 (13)	−0.0054 (12)
C10	0.096 (3)	0.066 (2)	0.058 (2)	0.010 (2)	0.027 (2)	−0.0168 (18)
C11	0.0535 (18)	0.0396 (15)	0.0381 (14)	−0.0017 (14)	0.0107 (12)	−0.0037 (12)
C12	0.061 (2)	0.072 (2)	0.0401 (16)	0.0010 (19)	−0.0038 (14)	0.0003 (16)
C13	0.0368 (15)	0.0527 (18)	0.0481 (16)	−0.0043 (14)	0.0026 (12)	0.0132 (14)
C14	0.060 (2)	0.053 (2)	0.080 (3)	−0.0185 (18)	−0.003 (2)	0.0095 (19)
C15	0.073 (2)	0.0473 (19)	0.0441 (16)	−0.0028 (17)	0.0160 (16)	0.0079 (14)
C16	0.113 (4)	0.069 (3)	0.057 (2)	−0.015 (3)	0.033 (2)	0.019 (2)

Geometric parameters (Å, º)

O1—C1	1.426 (4)	C5—H5	0.9800
O1—C7	1.344 (4)	C5—C6	1.510 (4)
O2—C2	1.194 (4)	C6—H6A	0.9700
O3—C3	1.432 (3)	C6—H6B	0.9700

O3—C9	1.359 (4)	C7—C8	1.487 (5)
O4—C4	1.441 (3)	C8—H8A	0.9600
O4—C11	1.355 (3)	C8—H8B	0.9600
O5—C5	1.436 (3)	C8—H8C	0.9600
O5—C13	1.353 (4)	C9—C10	1.488 (5)
O6—C6	1.435 (4)	C10—H10A	0.9600
O6—C15	1.345 (4)	C10—H10B	0.9600
O7—C7	1.194 (4)	C10—H10C	0.9600
O8—C9	1.201 (5)	C11—C12	1.487 (5)
O9—C11	1.202 (4)	C12—H12A	0.9600
O10—C13	1.195 (5)	C12—H12B	0.9600
O11—C15	1.189 (5)	C12—H12C	0.9600
C1—H1A	0.9700	C13—C14	1.495 (5)
C1—H1B	0.9700	C14—H14A	0.9600
C1—C2	1.496 (4)	C14—H14B	0.9600
C2—C3	1.538 (4)	C14—H14C	0.9600
C3—H3	0.9800	C15—C16	1.505 (5)
C3—C4	1.529 (4)	C16—H16A	0.9600
C4—H4	0.9800	C16—H16B	0.9600
C4—C5	1.527 (4)	C16—H16C	0.9600

C7—O1—C1	115.8 (3)	C7—C8—H8B	109.5
C9—O3—C3	114.0 (2)	C7—C8—H8C	109.5
C11—O4—C4	117.0 (2)	H8A—C8—H8B	109.5
C13—O5—C5	117.8 (2)	H8A—C8—H8C	109.5
C15—O6—C6	114.8 (3)	H8B—C8—H8C	109.5
O1—C1—H1A	109.3	O3—C9—C10	111.8 (3)
O1—C1—H1B	109.3	O8—C9—O3	121.6 (3)
O1—C1—C2	111.8 (3)	O8—C9—C10	126.6 (3)
H1A—C1—H1B	107.9	C9—C10—H10A	109.5
C2—C1—H1A	109.3	C9—C10—H10B	109.5
C2—C1—H1B	109.3	C9—C10—H10C	109.5
O2—C2—C1	124.4 (3)	H10A—C10—H10B	109.5
O2—C2—C3	122.1 (3)	H10A—C10—H10C	109.5
C1—C2—C3	113.5 (2)	H10B—C10—H10C	109.5
O3—C3—C2	109.9 (2)	O4—C11—C12	111.1 (3)
O3—C3—H3	108.4	O9—C11—O4	122.8 (3)
O3—C3—C4	108.3 (2)	O9—C11—C12	126.1 (3)
C2—C3—H3	108.4	C11—C12—H12A	109.5
C4—C3—C2	113.3 (2)	C11—C12—H12B	109.5
C4—C3—H3	108.4	C11—C12—H12C	109.5
O4—C4—C3	112.2 (2)	H12A—C12—H12B	109.5
O4—C4—H4	109.3	H12A—C12—H12C	109.5
O4—C4—C5	104.6 (2)	H12B—C12—H12C	109.5
C3—C4—H4	109.3	O5—C13—C14	110.1 (3)
C5—C4—C3	111.9 (2)	O10—C13—O5	123.0 (3)
C5—C4—H4	109.3	O10—C13—C14	126.9 (3)
O5—C5—C4	107.4 (2)	C13—C14—H14A	109.5

O5—C5—H5	109.9	C13—C14—H14B	109.5
O5—C5—C6	107.1 (2)	C13—C14—H14C	109.5
C4—C5—H5	109.9	H14A—C14—H14B	109.5
C6—C5—C4	112.6 (2)	H14A—C14—H14C	109.5
C6—C5—H5	109.9	H14B—C14—H14C	109.5
O6—C6—C5	105.9 (2)	O6—C15—C16	110.7 (4)
O6—C6—H6A	110.6	O11—C15—O6	123.5 (3)
O6—C6—H6B	110.6	O11—C15—C16	125.8 (4)
C5—C6—H6A	110.6	C15—C16—H16A	109.5
C5—C6—H6B	110.6	C15—C16—H16B	109.5
H6A—C6—H6B	108.7	C15—C16—H16C	109.5
O1—C7—C8	110.3 (3)	H16A—C16—H16B	109.5
O7—C7—O1	123.3 (3)	H16A—C16—H16C	109.5
O7—C7—C8	126.4 (3)	H16B—C16—H16C	109.5
C7—C8—H8A	109.5		

O1—C1—C2—O2	−5.8 (4)	C3—C4—C5—O5	−173.2 (2)
O1—C1—C2—C3	174.8 (3)	C3—C4—C5—C6	−55.5 (3)
O2—C2—C3—O3	−31.4 (4)	C4—O4—C11—O9	−8.2 (5)
O2—C2—C3—C4	89.9 (3)	C4—O4—C11—C12	170.9 (3)
O3—C3—C4—O4	70.2 (3)	C4—C5—C6—O6	−179.2 (2)
O3—C3—C4—C5	−47.0 (3)	C5—O5—C13—O10	7.9 (4)
O4—C4—C5—O5	65.1 (3)	C5—O5—C13—C14	−172.7 (3)
O4—C4—C5—C6	−177.2 (2)	C6—O6—C15—O11	−2.4 (5)
O5—C5—C6—O6	−61.3 (3)	C6—O6—C15—C16	176.5 (3)
C1—O1—C7—O7	2.1 (5)	C7—O1—C1—C2	83.9 (3)
C1—O1—C7—C8	−178.6 (3)	C9—O3—C3—C2	−68.6 (3)
C1—C2—C3—O3	147.9 (2)	C9—O3—C3—C4	167.1 (2)
C1—C2—C3—C4	−90.7 (3)	C11—O4—C4—C3	92.4 (3)
C2—C3—C4—O4	−52.1 (3)	C11—O4—C4—C5	−146.1 (2)
C2—C3—C4—C5	−169.3 (2)	C13—O5—C5—C4	−125.0 (2)
C3—O3—C9—O8	0.8 (4)	C13—O5—C5—C6	113.9 (3)
C3—O3—C9—C10	−178.1 (3)	C15—O6—C6—C5	173.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O10^{i}	0.98	2.48	3.285 (4)	139
C6—H6*A*···O10^{i}	0.97	2.58	3.394 (4)	141
C8—H8*C*···O8^{ii}	0.96	2.58	3.536 (5)	172
C12—H12*A*···O11^{iii}	0.96	2.60	3.531 (6)	164
C12—H12*C*···O1^{iv}	0.96	2.51	3.393 (5)	154

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, *y*, *z*−1; (iii) *x*−1, *y*, *z*−1; (iv) *x*−1, *y*, *z*.