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Methyl α-D,L-sorboside

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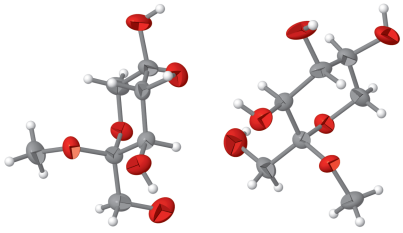
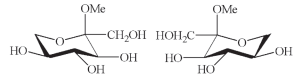
The title compound, $C_7H_{14}O_6$, was prepared from an equimolar mixture of D- and L-sorbose (D:L = 1:1) by Fischer glycosidation in methanol and crystallized from water. The title compound crystallizes in the orthorhombic space group $Pna2_1$. The asymmetric unit contains one molecule each of methyl α-D-sorboside and methyl α-L-sorboside. In the crystal, the molecules are linked by O—H···O hydrogen bonds, forming a two-dimensional network parallel to (001).

3D view



Chemical scheme



Structure description

L-Sorbose is a rare sugar and was the first L-form hexose found in nature (Nordenson *et al.*, 1979). Sorbosides are derivatives of sorbose in which the anomeric hydroxy group at C2 is replaced by an alkoxy group. The crystal structures of racemic α-D,L-sorbose (CSD refcode HELYOP; Taguchi *et al.*, 2018) and methyl α-L-sorboside monohydrate (CSD refcode LAMPAU; Matsumoto *et al.*, 2021) have previously been reported. In the present study, single crystals of anhydrous methyl α-D,L-sorboside were prepared to determine its molecular structure, crystal packing and intermolecular interactions.

The title compound crystallizes in the orthorhombic space group $Pna2_1$. The asymmetric unit contains two crystallographically independent molecules, one molecule each of methyl α-D-sorboside and methyl α-L-sorboside (Fig. 1). The D and L enantiomers adopt mirror-related $^5C_2$ and $^2C_5$ chair conformations, respectively. In both molecules, the methoxy substituent at the anomeric carbon atom (C12 or C22) occupies an axial position. The unit cell therefore contains four molecules of each enantiomer.

The formula weight of methyl α-D,L-sorboside is 194.18, approximately 7.8% greater than that of α-D,L-sorbose (180.16). As both structures have $Z = 8$, their unit-cell volumes can be compared directly. The unit-cell volume of the title compound [1683.06 (13) Å^3] is 232.20 Å^3, or approximately 16.0%, larger than that of α-D,L-sorbose [1450.86 (6) Å^3; Taguchi *et al.*, 2018]. This increase is consistent with the replacement of the anomeric hydroxy group by a methoxy group, although the unit-cell volume also depends on the molecular packing.

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

D—H···A	D—H	H···A	D···A	D—H···A
O11—H11···O13^{i}	0.82	2.00	2.783 (4)	160
O13—H13···O24^{ii}	0.82	1.94	2.748 (4)	167
O23—H23···O14	0.82	2.00	2.805 (4)	169
O24—H24···O26^{iii}	0.82	2.14	2.924 (4)	160
O25—H25···O22^{iv}	0.82	2.27	2.862 (4)	129

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

In the crystal, the molecules are linked by the five intermolecular O—H···O hydrogen bonds listed in Table 1: O23—H23···O14, O24—H24···O26, O25—H25···O22, O11—H11···O13 and O13—H13···O24. The donor···acceptor distances range from 2.748 (4) to 2.924 (4) Å. The methoxy oxygen atom O22 and the ring oxygen atom O26 act as acceptors, while the remaining listed acceptors are hydroxy oxygen atoms. Collectively, these hydrogen bonds generate a two-dimensional network parallel to (001), as shown in Fig. 2.

Synthesis and crystallization

Methyl α-D,L-sorboside was prepared from an equimolar mixture of D- and L-sorbose (D:L = 1:1) by Fischer glycosidation in methanol. The reaction product was purified by ion-exchange chromatography using Dowex 50 W–X2 resin in the Ca^{2+} form, with deionized water as the eluent. Fractions containing the target compound, as identified by HPLC, were combined and concentrated to give a syrup. The product was then dissolved in water, and the solution was allowed to evaporate slowly at room temperature. Colorless block-shaped single crystals suitable for single-crystal X-ray diffraction analysis were obtained.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_7H_{14}O_6$
M_r	194.18
Crystal system, space group	Orthorhombic, $Pna2_1$
Temperature (K)	296
a, b, c (Å)	12.9744 (6), 6.1793 (3), 20.9927 (9)
V (Å^3)	1683.06 (13)
Z	8
Radiation type	Cu $K\alpha$
μ (mm^{-1})	1.17
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}	0.639, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	16861, 3055, 2873
R_{int}	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.602
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.134, 1.06
No. of reflections	3055
No. of parameters	245
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.26
Absolute structure	Flack x determined using 1297 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.29 (7)

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

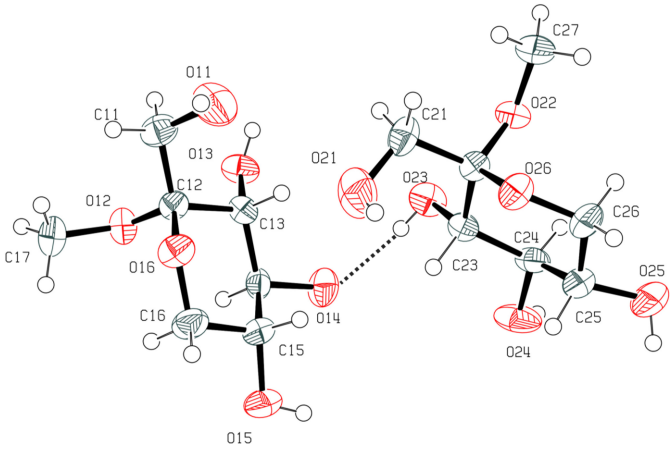


Figure 1
Molecular structure of the two crystallographically independent molecules in the asymmetric unit, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. The O23—H23···O14 hydrogen bond linking the two molecules is shown as a dashed line. H atoms are shown as spheres of arbitrary radius and are not labelled.

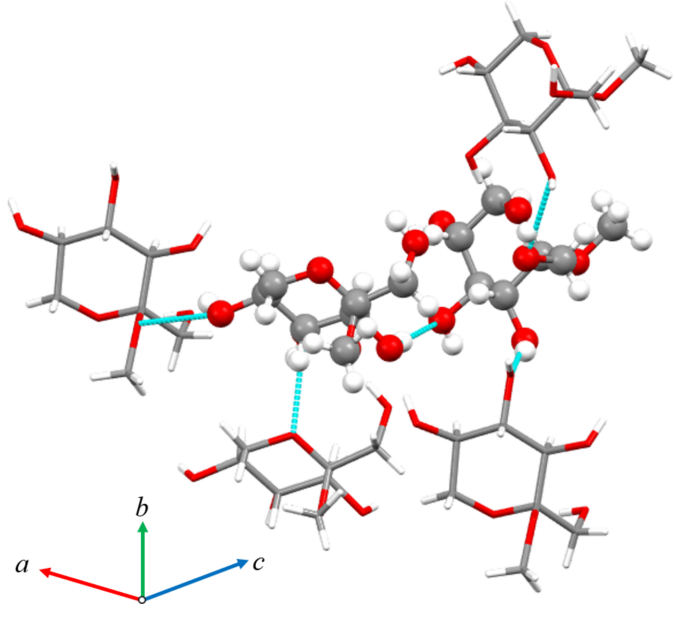


Figure 2
A portion of the crystal packing showing the five O—H···O hydrogen bonds listed in Table 1 as dashed lines. These interactions generate a two-dimensional hydrogen-bonded network parallel to (001). The crystallographic axes are indicated. The molecules highlighted at the centre are shown using a ball-and-stick representation, whereas the surrounding molecules are shown using a capped-stick representation.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The Flack parameter was 0.29 (7), determined using 1297 quotients of the type $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013). Since the crystal contains both enantiomers, this parameter concerns the polarity of the noncentrosymmetric crystal rather than the assignment of the molecular absolute configurations.

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full crystallographic data

IUCrData (2026). **11**, x260858 [https://doi.org/10.1107/S2414314626008588]

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Methyl α-D,L-sorboside

Crystal data

$C_7H_{14}O_6$
M_r = 194.18
Orthorhombic, $Pna2_1$
a = 12.9744 (6) Å
b = 6.1793 (3) Å
c = 20.9927 (9) Å
V = 1683.06 (13) Å^3
Z = 8
$F(000)$ = 832
D_x = 1.533 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54187 Å
Cell parameters from 3106 reflections
θ = 4.4–68.2°
μ = 1.17 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} = 0.639, T_{max} = 1.000
16861 measured reflections
3055 independent reflections
2873 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 68.2°, θ_{min} = 4.2°
h = −14→15
k = −7→7
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.06
3055 reflections
245 parameters
1 restraint
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1016P)^2 + 0.0448P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack x determined using 1297 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.29 (7)

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. The structure was solved using SHELXT (Sheldrick, 2015*a*) and refined against F^2 by full-matrix least-squares methods using SHELXL (Sheldrick, 2015*b*). All non-hydrogen atoms were refined anisotropically. All H atoms were placed in calculated positions and refined using constrained models. C-bound H atoms were refined using riding models, with C—H = 0.96–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl groups. Hydroxy H atoms were treated as rotating groups, with O—H = 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(O)$. The methyl groups at C17 and C27 were refined as rotating groups using AFIX 137. The final refinement gave $R_1 = 0.0481$ for reflections with $I > 2\sigma(I)$ and $wR_2 = 0.1342$ for all data. The maximum and minimum residual electron densities were 0.59 and -0.26 e Å^{-3}, respectively.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O11	−0.4003 (3)	0.3240 (5)	−0.78069 (16)	0.0671 (10)
H11	−0.387471	0.451934	−0.773944	0.101*
O12	−0.4126 (2)	−0.0201 (4)	−0.64021 (12)	0.0396 (6)
O13	−0.4084 (2)	−0.2354 (4)	−0.75361 (13)	0.0410 (6)
H13	−0.436954	−0.186441	−0.785323	0.062*
O14	−0.1999 (2)	−0.3795 (4)	−0.74496 (14)	0.0480 (7)
H14	−0.232748	−0.492633	−0.743066	0.072*
O15	−0.0851 (3)	−0.1770 (7)	−0.64158 (15)	0.0647 (10)
H15	−0.044367	−0.244186	−0.663935	0.097*
O16	−0.2831 (2)	0.2182 (4)	−0.67377 (12)	0.0392 (6)
C11	−0.4427 (3)	0.2310 (6)	−0.72577 (19)	0.0420 (9)
H11A	−0.503304	0.147803	−0.737335	0.050*
H11B	−0.464228	0.344856	−0.696879	0.050*
C12	−0.3666 (3)	0.0849 (5)	−0.69220 (16)	0.0303 (7)
C13	−0.3273 (3)	−0.0967 (5)	−0.73539 (14)	0.0302 (7)
H13A	−0.298012	−0.031393	−0.773888	0.036*
C14	−0.2434 (3)	−0.2254 (5)	−0.70227 (15)	0.0334 (7)
H14A	−0.272427	−0.300395	−0.665259	0.040*
C15	−0.1593 (3)	−0.0737 (6)	−0.68080 (16)	0.0401 (8)
H15A	−0.124857	−0.012794	−0.718270	0.048*
C16	−0.2033 (3)	0.1069 (7)	−0.6415 (2)	0.0461 (9)
H16A	−0.230163	0.048194	−0.601969	0.055*
H16B	−0.148858	0.208235	−0.630911	0.055*
C17	−0.4440 (4)	0.1097 (8)	−0.5876 (2)	0.0565 (11)
H17A	−0.463447	0.250764	−0.602523	0.085*
H17B	−0.387895	0.123021	−0.557999	0.085*
H17C	−0.501660	0.042948	−0.566790	0.085*
O21	−0.1728 (3)	0.2626 (6)	−0.83033 (15)	0.0693 (10)
H21	−0.121087	0.338497	−0.832471	0.104*
O22	−0.16767 (18)	−0.0279 (4)	−0.98010 (10)	0.0352 (5)
O23	−0.1854 (2)	−0.2583 (4)	−0.87343 (12)	0.0432 (6)
H23	−0.184412	−0.307650	−0.837178	0.065*
O24	0.0240 (3)	−0.4150 (5)	−0.86951 (14)	0.0574 (8)
H24	0.021034	−0.534701	−0.886293	0.086*
O25	0.1493 (3)	−0.2152 (8)	−0.97162 (17)	0.0809 (13)
H25	0.197986	−0.259479	−0.950410	0.121*
O26	−0.04060 (18)	0.1940 (4)	−0.93706 (13)	0.0391 (6)

C21	−0.2054 (3)	0.2084 (6)	−0.8919 (2)	0.0443 (9)
H21A	−0.214372	0.339403	−0.916781	0.053*
H21B	−0.271419	0.135103	−0.889677	0.053*
C22	−0.1280 (2)	0.0639 (5)	−0.92409 (15)	0.0295 (7)
C23	−0.0973 (3)	−0.1279 (5)	−0.88316 (15)	0.0313 (7)
H23A	−0.073788	−0.073839	−0.841740	0.038*
C24	−0.0105 (3)	−0.2554 (6)	−0.91335 (17)	0.0373 (8)
H24A	−0.036453	−0.327448	−0.951715	0.045*
C25	0.0787 (3)	−0.1094 (7)	−0.9316 (2)	0.0471 (9)
H25A	0.114018	−0.059367	−0.893078	0.057*
C26	0.0401 (3)	0.0828 (7)	−0.9690 (2)	0.0481 (9)
H26A	0.096793	0.182073	−0.976239	0.058*
H26B	0.015408	0.033996	−1.010144	0.058*
C27	−0.1993 (4)	0.1151 (7)	−1.0295 (2)	0.0519 (10)
H27A	−0.250429	0.045299	−1.055461	0.078*
H27B	−0.140919	0.152506	−1.055372	0.078*
H27C	−0.227987	0.243990	−1.011148	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O11	0.103 (3)	0.0426 (15)	0.0562 (17)	0.0166 (18)	−0.0040 (18)	0.0075 (14)
O12	0.0445 (14)	0.0373 (13)	0.0370 (11)	−0.0016 (11)	0.0099 (10)	−0.0032 (10)
O13	0.0477 (15)	0.0299 (12)	0.0454 (13)	−0.0059 (10)	−0.0151 (11)	−0.0024 (10)
O14	0.0561 (17)	0.0349 (13)	0.0529 (15)	0.0097 (12)	0.0092 (13)	−0.0099 (11)
O15	0.0482 (18)	0.090 (3)	0.0559 (17)	0.0319 (17)	−0.0164 (14)	−0.0109 (17)
O16	0.0336 (13)	0.0310 (11)	0.0529 (14)	−0.0064 (10)	−0.0059 (11)	−0.0074 (10)
C11	0.040 (2)	0.0313 (17)	0.054 (2)	0.0046 (15)	−0.0051 (17)	0.0005 (14)
C12	0.0278 (16)	0.0275 (16)	0.0356 (15)	−0.0033 (12)	−0.0015 (13)	−0.0033 (12)
C13	0.0364 (18)	0.0258 (14)	0.0285 (14)	−0.0027 (13)	−0.0019 (12)	−0.0001 (11)
C14	0.0387 (19)	0.0325 (16)	0.0290 (14)	0.0071 (14)	0.0067 (14)	−0.0001 (12)
C15	0.0277 (18)	0.051 (2)	0.0416 (19)	0.0050 (15)	−0.0044 (13)	−0.0019 (14)
C16	0.032 (2)	0.052 (2)	0.055 (2)	0.0016 (17)	−0.0107 (16)	−0.0136 (16)
C17	0.055 (3)	0.068 (3)	0.047 (2)	0.016 (2)	0.0114 (19)	−0.012 (2)
O21	0.092 (3)	0.0563 (19)	0.0600 (19)	0.0102 (18)	0.0099 (18)	−0.0186 (15)
O22	0.0382 (12)	0.0340 (11)	0.0335 (11)	−0.0021 (10)	−0.0099 (10)	0.0036 (10)
O23	0.0476 (14)	0.0363 (13)	0.0457 (14)	−0.0136 (11)	−0.0039 (12)	0.0085 (11)
O24	0.079 (2)	0.0365 (14)	0.0570 (16)	0.0221 (14)	−0.0342 (15)	−0.0060 (12)
O25	0.051 (2)	0.128 (3)	0.063 (2)	0.050 (2)	−0.0025 (17)	−0.013 (2)
O26	0.0336 (13)	0.0321 (11)	0.0515 (13)	−0.0043 (10)	0.0045 (11)	0.0018 (10)
C21	0.041 (2)	0.038 (2)	0.054 (2)	0.0077 (15)	0.0128 (17)	−0.0017 (15)
C22	0.0285 (16)	0.0250 (14)	0.0351 (15)	−0.0041 (12)	−0.0003 (12)	−0.0006 (12)
C23	0.0353 (18)	0.0281 (16)	0.0306 (15)	−0.0029 (13)	−0.0035 (13)	−0.0007 (12)
C24	0.043 (2)	0.0344 (16)	0.0349 (15)	0.0111 (14)	−0.0144 (15)	−0.0068 (13)
C25	0.0335 (19)	0.066 (3)	0.0417 (17)	0.0126 (17)	−0.0028 (16)	−0.0048 (17)
C26	0.0255 (18)	0.067 (3)	0.052 (2)	0.0012 (16)	0.0050 (16)	0.0044 (18)
C27	0.051 (2)	0.061 (3)	0.044 (2)	0.012 (2)	−0.0096 (17)	0.0136 (18)

Geometric parameters (Å, º)

O11—H11	0.8200	O21—H21	0.8200
O11—C11	1.401 (5)	O21—C21	1.401 (5)
O12—C12	1.403 (4)	O22—C22	1.403 (4)
O12—C17	1.425 (4)	O22—C27	1.424 (4)
O13—H13	0.8200	O23—H23	0.8200
O13—C13	1.410 (4)	O23—C23	1.414 (4)
O14—H14	0.8200	O24—H24	0.8200
O14—C14	1.424 (4)	O24—C24	1.421 (4)
O15—H15	0.8200	O25—H25	0.8200
O15—C15	1.418 (4)	O25—C25	1.404 (5)
O16—C12	1.415 (4)	O26—C22	1.417 (4)
O16—C16	1.416 (5)	O26—C26	1.420 (4)
C11—H11A	0.9700	C21—H21A	0.9700
C11—H11B	0.9700	C21—H21B	0.9700
C11—C12	1.513 (5)	C21—C22	1.504 (5)
C12—C13	1.530 (4)	C22—C23	1.518 (4)
C13—H13A	0.9800	C23—H23A	0.9800
C13—C14	1.517 (4)	C23—C24	1.513 (5)
C14—H14A	0.9800	C24—H24A	0.9800
C14—C15	1.507 (5)	C24—C25	1.516 (6)
C15—H15A	0.9800	C25—H25A	0.9800
C15—C16	1.501 (5)	C25—C26	1.509 (6)
C16—H16A	0.9700	C26—H26A	0.9700
C16—H16B	0.9700	C26—H26B	0.9700
C17—H17A	0.9600	C27—H27A	0.9600
C17—H17B	0.9600	C27—H27B	0.9600
C17—H17C	0.9600	C27—H27C	0.9600
C11—O11—H11	109.5	C21—O21—H21	109.5
C12—O12—C17	117.7 (3)	C22—O22—C27	117.7 (3)
C13—O13—H13	109.5	C23—O23—H23	109.5
C14—O14—H14	109.5	C24—O24—H24	109.5
C15—O15—H15	109.5	C25—O25—H25	109.5
C12—O16—C16	114.0 (3)	C22—O26—C26	114.0 (3)
O11—C11—H11A	109.2	O21—C21—H21A	109.5
O11—C11—H11B	109.2	O21—C21—H21B	109.5
O11—C11—C12	111.8 (3)	O21—C21—C22	110.8 (3)
H11A—C11—H11B	107.9	H21A—C21—H21B	108.1
C12—C11—H11A	109.2	C22—C21—H21A	109.5
C12—C11—H11B	109.2	C22—C21—H21B	109.5
O12—C12—O16	112.5 (3)	O22—C22—O26	111.2 (3)
O12—C12—C11	111.1 (3)	O22—C22—C21	111.8 (3)
O12—C12—C13	105.3 (3)	O22—C22—C23	104.8 (2)
O16—C12—C11	106.2 (3)	O26—C22—C21	106.5 (3)
O16—C12—C13	109.5 (3)	O26—C22—C23	110.0 (3)
C11—C12—C13	112.3 (3)	C21—C22—C23	112.6 (3)

O13—C13—C12	111.0 (3)	O23—C23—C22	108.3 (3)
O13—C13—H13A	108.4	O23—C23—H23A	108.5
O13—C13—C14	109.9 (3)	O23—C23—C24	111.5 (3)
C12—C13—H13A	108.4	C22—C23—H23A	108.5
C14—C13—C12	110.6 (3)	C24—C23—C22	111.4 (3)
C14—C13—H13A	108.4	C24—C23—H23A	108.5
O14—C14—C13	110.3 (3)	O24—C24—C23	108.9 (3)
O14—C14—H14A	109.6	O24—C24—H24A	109.0
O14—C14—C15	108.5 (3)	O24—C24—C25	109.7 (3)
C13—C14—H14A	109.6	C23—C24—H24A	109.0
C15—C14—C13	109.3 (3)	C23—C24—C25	111.4 (3)
C15—C14—H14A	109.6	C25—C24—H24A	109.0
O15—C15—C14	112.6 (3)	O25—C25—C24	111.9 (4)
O15—C15—H15A	109.2	O25—C25—H25A	109.6
O15—C15—C16	105.9 (3)	O25—C25—C26	105.8 (3)
C14—C15—H15A	109.2	C24—C25—H25A	109.6
C16—C15—C14	110.6 (3)	C26—C25—C24	110.3 (3)
C16—C15—H15A	109.2	C26—C25—H25A	109.6
O16—C16—C15	112.1 (3)	O26—C26—C25	112.4 (3)
O16—C16—H16A	109.2	O26—C26—H26A	109.1
O16—C16—H16B	109.2	O26—C26—H26B	109.1
C15—C16—H16A	109.2	C25—C26—H26A	109.1
C15—C16—H16B	109.2	C25—C26—H26B	109.1
H16A—C16—H16B	107.9	H26A—C26—H26B	107.9
O12—C17—H17A	109.5	O22—C27—H27A	109.5
O12—C17—H17B	109.5	O22—C27—H27B	109.5
O12—C17—H17C	109.5	O22—C27—H27C	109.5
H17A—C17—H17B	109.5	H27A—C27—H27B	109.5
H17A—C17—H17C	109.5	H27A—C27—H27C	109.5
H17B—C17—H17C	109.5	H27B—C27—H27C	109.5

O11—C11—C12—O12	−175.4 (3)	O21—C21—C22—O22	167.9 (3)
O11—C11—C12—O16	62.0 (4)	O21—C21—C22—O26	−70.4 (4)
O11—C11—C12—C13	−57.7 (4)	O21—C21—C22—C23	50.2 (4)
O12—C12—C13—O13	57.7 (3)	O22—C22—C23—O23	−58.0 (3)
O12—C12—C13—C14	−64.7 (3)	O22—C22—C23—C24	64.9 (3)
O13—C13—C14—O14	63.0 (4)	O23—C23—C24—O24	−66.3 (4)
O13—C13—C14—C15	−177.8 (3)	O23—C23—C24—C25	172.6 (3)
O14—C14—C15—O15	−68.1 (4)	O24—C24—C25—O25	72.3 (4)
O14—C14—C15—C16	173.7 (3)	O24—C24—C25—C26	−170.3 (3)
O15—C15—C16—O16	−176.9 (3)	O25—C25—C26—O26	173.8 (3)
O16—C12—C13—O13	178.8 (3)	O26—C22—C23—O23	−177.6 (3)
O16—C12—C13—C14	56.5 (4)	O26—C22—C23—C24	−54.7 (3)
C11—C12—C13—O13	−63.4 (3)	C21—C22—C23—O23	63.8 (4)
C11—C12—C13—C14	174.3 (3)	C21—C22—C23—C24	−173.3 (3)
C12—O16—C16—C15	58.2 (4)	C22—O26—C26—C25	−59.0 (4)
C12—C13—C14—O14	−174.0 (3)	C22—C23—C24—O24	172.5 (3)
C12—C13—C14—C15	−54.9 (3)	C22—C23—C24—C25	51.5 (4)

C13—C14—C15—O15	171.6 (3)	C23—C24—C25—O25	−167.1 (3)
C13—C14—C15—C16	53.4 (4)	C23—C24—C25—C26	−49.7 (4)
C14—C15—C16—O16	−54.6 (4)	C24—C25—C26—O26	52.7 (5)
C16—O16—C12—O12	58.4 (4)	C26—O26—C22—O22	−56.7 (4)
C16—O16—C12—C11	−179.8 (3)	C26—O26—C22—C21	−178.8 (3)
C16—O16—C12—C13	−58.3 (4)	C26—O26—C22—C23	58.9 (4)
C17—O12—C12—O16	52.4 (4)	C27—O22—C22—O26	−58.6 (4)
C17—O12—C12—C11	−66.5 (4)	C27—O22—C22—C21	60.3 (4)
C17—O12—C12—C13	171.7 (3)	C27—O22—C22—C23	−177.4 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11···O13^{i}	0.82	2.00	2.783 (4)	160
O13—H13···O24^{ii}	0.82	1.94	2.748 (4)	167
O23—H23···O14	0.82	2.00	2.805 (4)	169
O24—H24···O26^{iii}	0.82	2.14	2.924 (4)	160
O25—H25···O22^{iv}	0.82	2.27	2.862 (4)	129

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) *x*−1/2, −*y*−1/2, *z*; (iii) *x*, *y*−1, *z*; (iv) *x*+1/2, −*y*−1/2, *z*.