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Methyl 4,6-*O*-benzylidene-*α*-D-glucopyranoside monohydrate

Mari Grobbelaar, Eric Cyriel Hosten and Richard Betz*

Nelson Mandela University, Summerstrand Campus, Department of Chemistry, University Way, Summerstrand, PO Box 77000, Port Elizabeth, 6031, South Africa. *Correspondence e-mail: Richard.Betz@mandela.ac.za

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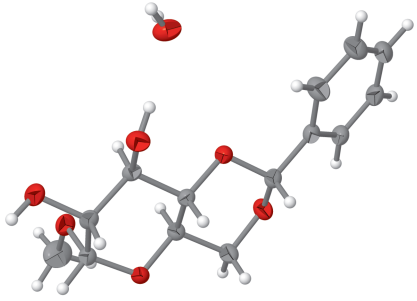
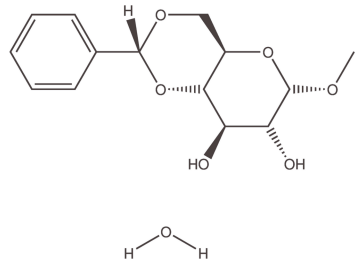
The title compound, $C_{14}H_{18}O_6\cdot H_2O$, is a partially protected derivative of D-glucopyranose. The asymmetric unit contains one sugar molecule and one water molecule of crystallization. Classical hydrogen bonds of the O—H···O type form a cooperative set and are observed next to a C—H···O(water) contact, connecting the entities of the asymmetric unit into a three-dimensional network.

3D view



Chemical scheme



Structure description

Carbohydrates are an important group of biomolecules and form part of the three macronutrients of the human diet. Natural members of this compound class of polyhydroxycarbonyls abound for derivatives with five and six carbon atoms, whose stereochemical diversity is enriched by the ability to form furanoid and pyranoid intramolecular hemiacetal-type addition compounds. As they are the product of natural photosynthesis, they are debated as renewable and carbon-neutral feedstock materials for many industrial processes; however, precisely because of their stereochemical variability, exploiting their synthetic potential often requires a carefully crafted preparative strategy based on protection group chemistry (Lindhorst, 2003).

In connection with the synthesis of coordination compounds, limiting the number of potential donor sites on a polyfunctional carbohydrate is an important measure to ensure the formation of well-defined product species. In connection with a research project around the coordination behaviour of certain hexoses, partially protected derivatives of D-glucose were to be investigated with a specific focus on the *trans*-orientated hydroxyl groups on the six-membered ring. To this end, methyl-4,6-*O*-benzylidene-*α*-D-glucopyranoside was synthesized and characterized in the solid state to allow for the comparison of metrical parameters in the free ligand and in coordination compounds. The structure of the title compound has been reported earlier (Tamaru *et al.*, 2001) but no three-dimensional coordinates were deposited. However, structural information is at

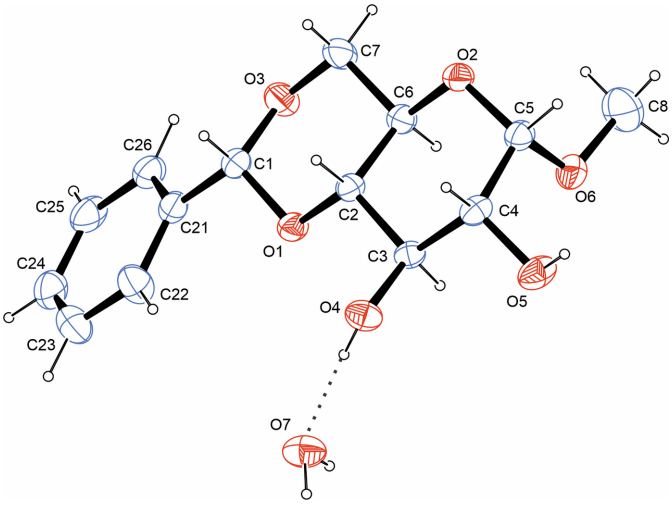


Figure 1
The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at the 50% probability level).

hand for the anhydrous version of the title compound (Luboradzki *et al.*, 2000) as well as the β-anomer of the carbohydrate (Jessen *et al.*, 2001). The stereoisomeric altropyranoside (Bozo & Vasella, 1992), allopyranoside (Muddasani *et al.*, 1994) and idopyranoside (Chu & Jeffrey, 1965; Liu *et al.*, 1993; Orban *et al.*, 2023) equivalents of the title compound have been the focus of diffraction studies on single crystals previously. The present study is a continuation of our interest in structural aspects of coordination compounds of carbohydrate derivatives (Betz & Klüfers, 2007*a*, 2009; Betz *et al.*, 2007*a*) as well as polyheterocyclic compounds (Muller *et al.*, 2021; Betz & Klüfers, 2007*b*,*c*,*d*; Betz & Klüfers, 2008*a*,*b*; Betz *et al.*, 2007*b*) and intends to close the gap of missing three-dimensional coordinates for the title compound.

The title compound (Fig. 1) is a twofold protected derivative of D-glucopyranose with the anomeric hydroxyl group converted into a methoxy group (O6–C8) and the hydroxymethyl and the adjacent ring-bound hydroxyl group capped by a benzylidene protection group. The two *trans*-orientated hydroxyl groups on the pyranose ring remain free. A molecule of water is present in the asymmetric unit. Bond lengths and angles are in good agreement with values reported for comparable compounds whose metrical parameters have been elucidated by means of diffraction studies on single crystals and deposited with the Cambridge Structural Database (Groom *et al.*, 2016). While the methoxy group occupies an axial position, the phenyl group is found in an equatorial position. The two free hydroxyl groups adopt a staggered conformation with a O4—C3—C4—O5 torsion angle of 65.17 (16)°. A conformational analysis of the six-membered rings according to Cremer & Pople (1975) shows the pyranoid ring to adopt a $^{1}C_{4}$ ($^{O2}C_{C3}$) conformation while the six-membered ring established by the condensed benzylidene protection group is present in a $^{4}C_{1}$ ($^{C7}C_{O1}$) conformation (Boeyens, 1978).

In the crystal, classical hydrogen bonds of the O—H···O type are observed next to a C—H···O(water) contact

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

$C_g(1)$ is the centroid of carbon atoms C21–C26.

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4A···O7	0.84	1.86	2.6925 (19)	172
O5—H5A···O5^{i}	0.84	2.48	3.1906 (18)	143
O5—H5A···O6^{i}	0.84	2.12	2.8486 (18)	145
O7—H7C···O4^{ii}	0.84 (1)	2.08 (2)	2.8758 (17)	159 (3)
O7—H7D···O4^{iii}	0.83 (1)	2.02 (1)	2.8444 (19)	175 (3)
C5—H5···O5^{i}	1.00	2.46	3.299 (2)	141
C8—H8C···O7^{iv}	0.98	2.43	3.380 (3)	163
C1—H1···$C_g(1)^{v}$	1.00	2.56	3.516 (2)	161

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

(Table 1) whose range falls by more than 0.1 Å below the sum of van der Waals radii of the atoms participating in them. The hydroxyl group adjacent to the anomeric center establishes a hydrogen bond to the oxygen atom of the methoxy group as acceptor, while the second free hydroxyl group involves the oxygen atom of the free water molecule as acceptor. The water molecule exclusively forms hydrogen bonds to the oxygen atom of the second free hydroxyl group, thus giving rise to a cooperative set of hydrogen bonds. The C—H···O(water) contact is observed between one of the hydrogen atoms of the methoxy group as donor and solvent molecule's oxygen atom as acceptor. A second C—H···O contact between the hydrogen atom of the anomeric center's methine group and the oxygen atom of the hydroxyl group adjacent to the anomeric center is listed for completeness but could be considered an artefact (or consequence) of the hydrogen bonds established by the neighbouring hydroxyl group resulting in distance shortening between the respective C—H and O motifs involved. In terms of graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995), the classical hydrogen bonds require a $DDDC^{1}_{1}(5)$ descriptor on the unary level while the C—H···O contacts require a $DC^{1}_{1}(4)$ descriptor on the same level with the finite pattern reserved for the water-based contact. Furthermore, one C—H···π contact is apparent in between the hydrogen atom of the benzylidene protection

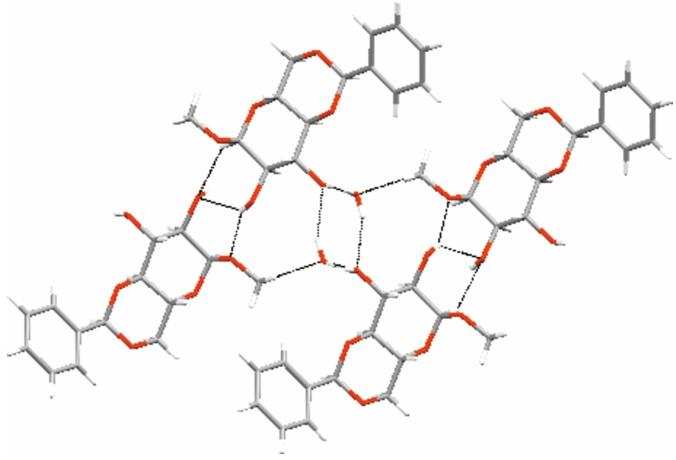


Figure 2
Selected intermolecular contacts, viewed along [010].

group and the aromatic system that connects the molecules to chains along the crystallographic *b* axis. π-Stacking is not a stabilizing factor in the crystal structure of the title compound with the shortest distance in between two centers of gravity measured at 4.8475 (13) Å, which is in agreement with the length of the *b* axis of the unit cell (Fig. 2).

Synthesis and crystallization

The compound was obtained following published standard procedures (Becker *et al.*, 2000; Lindhorst, 2003; Evans, 1972). Crystals suitable for the diffraction study were obtained upon recrystallization from boiling propan-2-ol containing water (alcohol:water approximately 95:5).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{14}H_{18}O_6{\cdot}H_2O$
M_r	300.30
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	200
a, *b*, *c* (Å)	8.9794 (6), 4.8475 (3), 17.3824 (11)
β (°)	103.927 (2)
V (Å^3)	734.37 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.50 × 0.13 × 0.07
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.705, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41341, 3652, 3442
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.081, 1.06
No. of reflections	3652
No. of parameters	204
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.16
Absolute structure	Flack *x* determined using 1467 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.17 (16)

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2020), *SHELXL2019/3* (Sheldrick, 2015) and *PLATON* (Spek, 2020).

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full crystallographic data

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Crystal data

$C_{14}H_{18}O_6 \cdot H_2O$
$M_r = 300.30$
Monoclinic, $P2_1$
$a = 8.9794$ (6) Å
$b = 4.8475$ (3) Å
$c = 17.3824$ (11) Å
$\beta = 103.927$ (2)°
$V = 734.37$ (8) Å^3
$Z = 2$
$F(000) = 320$
$D_x = 1.358$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9923 reflections
$\theta = 2.4$–$28.3°$
$\mu = 0.11$ mm^{-1}
$T = 200$ K
Rod, colourless
0.50 × 0.13 × 0.07 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.705$, $T_{max} = 0.746$
41341 measured reflections
3652 independent reflections
3442 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.3°$
$h = -11 \rightarrow 11$
$k = -6 \rightarrow 6$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.081$
$S = 1.06$
3652 reflections
204 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 0.1456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: SHELXL-2019/2 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.019 (5)
Absolute structure: Flack *x* determined using 1467 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.17 (16)

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 carbon-bound H atoms were placed in calculated positions (C–H 0.98 Å for the methyl group, C–H 0.99 Å for the methylene group and C–H 1.00 Å for the methine groups) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C).
The H atoms of the methyl group were allowed to rotate with a fixed angle around the C–O bond to best fit the experimental electron density (HFIX 137 in the *SHELX* program suite (Sheldrick, 2015), with U(H) set to 1.5U_{eq}(C).
The H atoms of the hydroxyl groups were allowed to rotate with a fixed angle around the C–O bond to best fit the experimental electron density (HFIX 147 in the *SHELX* program suite (Sheldrick, 2015)), with U(H) set to 1.5U_{eq}(O).
The hydrogen atoms of the water molecule were located on a difference Fourier map and refined freely with the O—H bonds restrained to 0.84 (1) Å and the H···H distance restrained to 1.34 (2) Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.46554 (13)	0.5554 (2)	0.74863 (6)	0.0238 (3)
O2	0.12794 (13)	0.9982 (3)	0.71868 (7)	0.0254 (3)
O3	0.40114 (14)	0.6184 (3)	0.87039 (7)	0.0314 (3)
O4	0.42598 (14)	0.7276 (3)	0.58470 (7)	0.0276 (3)
H4A	0.471173	0.574777	0.588148	0.044 (7)*
O5	0.11857 (16)	0.8527 (3)	0.50945 (7)	0.0326 (3)
H5A	0.073092	0.989590	0.484881	0.043 (7)*
O6	−0.02371 (13)	0.7058 (3)	0.62439 (7)	0.0297 (3)
O7	0.57272 (16)	0.2455 (3)	0.58050 (8)	0.0348 (3)
C1	0.52160 (18)	0.6135 (4)	0.83089 (9)	0.0244 (3)
H1	0.574134	0.796858	0.837146	0.029*
C2	0.36312 (17)	0.7704 (3)	0.71266 (9)	0.0206 (3)
H2	0.418578	0.950973	0.720224	0.025*
C3	0.30499 (17)	0.7132 (3)	0.62492 (9)	0.0206 (3)
H3	0.257645	0.525372	0.617432	0.025*
C4	0.18457 (19)	0.9274 (3)	0.58932 (9)	0.0233 (3)
H4	0.236211	1.110364	0.589884	0.028*
C5	0.06150 (19)	0.9515 (3)	0.63686 (10)	0.0244 (3)
H5	−0.007931	1.109256	0.615502	0.029*
C6	0.23033 (18)	0.7808 (3)	0.75229 (9)	0.0233 (3)
H6	0.174321	0.600724	0.744613	0.028*
C7	0.2933 (2)	0.8339 (4)	0.84008 (10)	0.0312 (4)
H7A	0.344631	1.015908	0.848362	0.037*
H7B	0.208970	0.832990	0.867783	0.037*
C8	−0.1524 (2)	0.7112 (6)	0.65891 (16)	0.0531 (6)
H8A	−0.213356	0.877348	0.641402	0.080*
H8B	−0.116555	0.712809	0.716801	0.080*
H8C	−0.215818	0.547268	0.642267	0.080*
C21	0.63591 (19)	0.3933 (4)	0.86650 (10)	0.0259 (3)
C22	0.7440 (2)	0.3128 (5)	0.82542 (12)	0.0357 (4)
H22	0.740831	0.389879	0.774803	0.043*

C23	0.8563 (2)	0.1213 (5)	0.85770 (13)	0.0411 (5)
H23	0.931025	0.071158	0.829763	0.049*
C24	0.8597 (2)	0.0029 (5)	0.93049 (12)	0.0392 (5)
H24	0.936355	−0.128995	0.952543	0.047*
C25	0.7510 (2)	0.0775 (4)	0.97097 (11)	0.0357 (4)
H25	0.751721	−0.006604	1.020429	0.043*
C26	0.6400 (2)	0.2755 (4)	0.93970 (10)	0.0300 (4)
H26	0.567370	0.329480	0.968532	0.036*
H7C	0.599 (3)	0.242 (7)	0.5371 (11)	0.063 (8)*
H7D	0.527 (3)	0.099 (4)	0.5837 (15)	0.049 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0261 (5)	0.0249 (6)	0.0194 (5)	0.0041 (5)	0.0033 (4)	−0.0010 (4)
O2	0.0268 (6)	0.0252 (6)	0.0228 (5)	0.0056 (5)	0.0032 (4)	−0.0036 (5)
O3	0.0303 (6)	0.0431 (8)	0.0214 (5)	0.0104 (6)	0.0075 (5)	0.0041 (5)
O4	0.0324 (6)	0.0276 (6)	0.0260 (6)	0.0030 (5)	0.0134 (5)	0.0026 (5)
O5	0.0455 (7)	0.0300 (7)	0.0183 (5)	0.0057 (6)	−0.0001 (5)	0.0007 (5)
O6	0.0252 (5)	0.0319 (7)	0.0309 (6)	−0.0053 (5)	0.0050 (4)	−0.0046 (5)
O7	0.0444 (7)	0.0294 (7)	0.0362 (7)	−0.0025 (6)	0.0207 (6)	−0.0032 (6)
C1	0.0241 (7)	0.0283 (8)	0.0195 (7)	0.0012 (7)	0.0030 (6)	−0.0016 (6)
C2	0.0228 (7)	0.0189 (7)	0.0196 (6)	0.0001 (6)	0.0039 (5)	−0.0010 (6)
C3	0.0248 (7)	0.0172 (7)	0.0207 (6)	−0.0014 (6)	0.0070 (5)	−0.0008 (6)
C4	0.0304 (8)	0.0176 (8)	0.0204 (7)	−0.0005 (6)	0.0033 (6)	0.0006 (6)
C5	0.0258 (8)	0.0226 (8)	0.0229 (7)	0.0023 (6)	0.0019 (6)	−0.0015 (6)
C6	0.0235 (7)	0.0245 (8)	0.0216 (7)	0.0021 (6)	0.0047 (6)	−0.0005 (6)
C7	0.0301 (8)	0.0410 (10)	0.0224 (7)	0.0110 (8)	0.0064 (6)	−0.0006 (7)
C8	0.0343 (10)	0.0628 (16)	0.0679 (15)	−0.0120 (11)	0.0235 (10)	−0.0125 (13)
C21	0.0246 (7)	0.0265 (8)	0.0242 (7)	−0.0005 (7)	0.0008 (6)	−0.0034 (6)
C22	0.0310 (9)	0.0427 (12)	0.0342 (9)	0.0064 (8)	0.0096 (7)	0.0068 (8)
C23	0.0303 (9)	0.0487 (12)	0.0438 (10)	0.0108 (9)	0.0080 (8)	−0.0016 (10)
C24	0.0350 (9)	0.0380 (11)	0.0372 (10)	0.0098 (9)	−0.0060 (8)	−0.0039 (9)
C25	0.0442 (10)	0.0344 (10)	0.0227 (8)	0.0058 (8)	−0.0034 (7)	−0.0005 (7)
C26	0.0322 (8)	0.0331 (10)	0.0219 (7)	0.0037 (7)	0.0011 (6)	−0.0023 (7)

Geometric parameters (Å, º)

O1—C1	1.4250 (18)	C4—C5	1.535 (2)
O1—C2	1.4305 (18)	C4—H4	1.0000
O2—C5	1.4218 (19)	C5—H5	1.0000
O2—C6	1.4280 (19)	C6—C7	1.516 (2)
O3—C1	1.4141 (19)	C6—H6	1.0000
O3—C7	1.436 (2)	C7—H7A	0.9900
O4—C3	1.4281 (17)	C7—H7B	0.9900
O4—H4A	0.8400	C8—H8A	0.9800
O5—C4	1.4191 (19)	C8—H8B	0.9800
O5—H5A	0.8400	C8—H8C	0.9800

O6—C5	1.404 (2)	C21—C26	1.387 (2)
O6—C8	1.425 (2)	C21—C22	1.392 (2)
O7—H7C	0.841 (12)	C22—C23	1.386 (3)
O7—H7D	0.832 (13)	C22—H22	0.9500
C1—C21	1.507 (2)	C23—C24	1.383 (3)
C1—H1	1.0000	C23—H23	0.9500
C2—C3	1.5140 (19)	C24—C25	1.382 (3)
C2—C6	1.515 (2)	C24—H24	0.9500
C2—H2	1.0000	C25—C26	1.396 (3)
C3—C4	1.519 (2)	C25—H25	0.9500
C3—H3	1.0000	C26—H26	0.9500

C1—O1—C2	109.23 (11)	O2—C6—C2	109.77 (12)
C5—O2—C6	111.43 (12)	O2—C6—C7	109.48 (13)
C1—O3—C7	111.18 (13)	C2—C6—C7	108.66 (12)
C3—O4—H4A	109.5	O2—C6—H6	109.6
C4—O5—H5A	109.5	C2—C6—H6	109.6
C5—O6—C8	112.74 (16)	C7—C6—H6	109.6
H7C—O7—H7D	107 (2)	O3—C7—C6	107.50 (14)
O3—C1—O1	111.33 (12)	O3—C7—H7A	110.2
O3—C1—C21	109.72 (13)	C6—C7—H7A	110.2
O1—C1—C21	108.27 (13)	O3—C7—H7B	110.2
O3—C1—H1	109.2	C6—C7—H7B	110.2
O1—C1—H1	109.2	H7A—C7—H7B	108.5
C21—C1—H1	109.2	O6—C8—H8A	109.5
O1—C2—C3	109.66 (12)	O6—C8—H8B	109.5
O1—C2—C6	108.61 (12)	H8A—C8—H8B	109.5
C3—C2—C6	110.24 (12)	O6—C8—H8C	109.5
O1—C2—H2	109.4	H8A—C8—H8C	109.5
C3—C2—H2	109.4	H8B—C8—H8C	109.5
C6—C2—H2	109.4	C26—C21—C22	119.16 (17)
O4—C3—C2	111.45 (12)	C26—C21—C1	122.25 (15)
O4—C3—C4	108.54 (12)	C22—C21—C1	118.55 (15)
C2—C3—C4	108.92 (12)	C23—C22—C21	120.60 (18)
O4—C3—H3	109.3	C23—C22—H22	119.7
C2—C3—H3	109.3	C21—C22—H22	119.7
C4—C3—H3	109.3	C24—C23—C22	120.16 (19)
O5—C4—C3	108.23 (13)	C24—C23—H23	119.9
O5—C4—C5	111.15 (13)	C22—C23—H23	119.9
C3—C4—C5	111.52 (12)	C25—C24—C23	119.63 (18)
O5—C4—H4	108.6	C25—C24—H24	120.2
C3—C4—H4	108.6	C23—C24—H24	120.2
C5—C4—H4	108.6	C24—C25—C26	120.48 (18)
O6—C5—O2	111.81 (13)	C24—C25—H25	119.8
O6—C5—C4	106.76 (13)	C26—C25—H25	119.8
O2—C5—C4	111.56 (13)	C21—C26—C25	119.94 (17)
O6—C5—H5	108.9	C21—C26—H26	120.0
O2—C5—H5	108.9	C25—C26—H26	120.0

C4—C5—H5	108.9		
C7—O3—C1—O1	−62.57 (18)	C5—O2—C6—C2	63.05 (16)
C7—O3—C1—C21	177.59 (14)	C5—O2—C6—C7	−177.76 (14)
C2—O1—C1—O3	62.49 (17)	O1—C2—C6—O2	178.67 (12)
C2—O1—C1—C21	−176.82 (13)	C3—C2—C6—O2	−61.17 (16)
C1—O1—C2—C3	179.03 (12)	O1—C2—C6—C7	58.97 (17)
C1—O1—C2—C6	−60.45 (15)	C3—C2—C6—C7	179.13 (14)
O1—C2—C3—O4	−65.88 (16)	C1—O3—C7—C6	59.08 (18)
C6—C2—C3—O4	174.60 (13)	O2—C6—C7—O3	−177.12 (13)
O1—C2—C3—C4	174.40 (12)	C2—C6—C7—O3	−57.25 (18)
C6—C2—C3—C4	54.88 (16)	O3—C1—C21—C26	−16.3 (2)
O4—C3—C4—O5	65.17 (16)	O1—C1—C21—C26	−138.00 (16)
C2—C3—C4—O5	−173.32 (13)	O3—C1—C21—C22	165.85 (16)
O4—C3—C4—C5	−172.26 (12)	O1—C1—C21—C22	44.2 (2)
C2—C3—C4—C5	−50.76 (16)	C26—C21—C22—C23	−1.2 (3)
C8—O6—C5—O2	63.6 (2)	C1—C21—C22—C23	176.72 (19)
C8—O6—C5—C4	−174.09 (16)	C21—C22—C23—C24	1.6 (3)
C6—O2—C5—O6	60.50 (16)	C22—C23—C24—C25	−0.3 (3)
C6—O2—C5—C4	−58.97 (17)	C23—C24—C25—C26	−1.4 (3)
O5—C4—C5—O6	51.55 (16)	C22—C21—C26—C25	−0.4 (3)
C3—C4—C5—O6	−69.32 (16)	C1—C21—C26—C25	−178.28 (17)
O5—C4—C5—O2	173.98 (13)	C24—C25—C26—C21	1.7 (3)
C3—C4—C5—O2	53.10 (17)		

Hydrogen-bond geometry (Å, º)

C_g(1) is the centroid of carbon atoms C21–C26.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O7	0.84	1.86	2.6925 (19)	172
O5—H5*A*···O5^{i}	0.84	2.48	3.1906 (18)	143
O5—H5*A*···O6^{i}	0.84	2.12	2.8486 (18)	145
O7—H7*C*···O4^{ii}	0.84 (1)	2.08 (2)	2.8758 (17)	159 (3)
O7—H7*D*···O4^{iii}	0.83 (1)	2.02 (1)	2.8444 (19)	175 (3)
C5—H5···O5^{i}	1.00	2.46	3.299 (2)	141
C8—H8*C*···O7^{iv}	0.98	2.43	3.380 (3)	163
C1—H1···C_g(1)^{v}	1.00	2.56	3.516 (2)	161

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