Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(6*S**)-6-[(1*S**,2*R**)-1,2-Dihydroxypentyl]-4-methoxy-5,6-dihydro-2*H*-pyran-2-one

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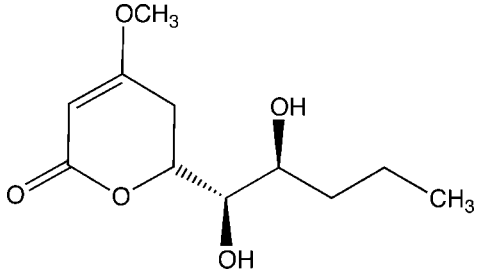
Received 11 September 2013; accepted 1 October 2013

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.052; wR factor = 0.121; data-to-parameter ratio = 8.6.

The title compound, $C_{11}H_{18}O_5$, was isolated from a liquid culture of *Pestalotiopsis sp*. In the molecule, the pyran-2-one ring assumes a half-chair conformation. The two terminal C atoms of the pentyl group were refined as disordered over two sets of sites, with refined occupancies of 0.881 (10) and 0.119 (10). In the crystal, molecules are linked *via* O—H···O hydrogen bonds forming a three-dimensional network.

Related literature

For the first isolation of the title compound, see: McGahren *et al.* (1973). For the natural and unnatural stereospecific synthesis, see: Kirihata *et al.* (1990, 1992*a*,*b*); Masaki *et al.* (1994). For closely related products from other fungi, see: Kimura *et al.* (1986); Kirihata *et al.* (1996); Lee *et al.* (1995); Davies-Coleman & Rivett (1989). For biological activity, see: Venkatasubbaiah & Van Dyke (1991). For crystal structures of related compounds, see: Yoshino & Nowacki (1972); Engel & Nowacki (1972*a*,*b*).



Experimental

Crystal data

$C_{11}H_{18}O_5$
M_r = 230.25
Orthorhombic, $P2_12_12_1$
a = 5.0375 (3) Å
b = 11.4515 (13) Å
c = 20.802 (2) Å
V = 1200.02 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 200 K
0.28 × 0.18 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
T_{min} = 0.973, T_{max} = 0.992
2711 measured reflections
1616 independent reflections
1153 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.121
S = 1.06
1616 reflections
188 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1′—H1′*O*···O2^{i}	0.85 (3)	1.93 (3)	2.778 (3)	177 (3)
O2′—H2′*O*···O2′^{ii}	0.80 (4)	2.05 (4)	2.8178 (18)	163 (4)

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *WinGX* (Farrugia, 2012), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5653).

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supporting information

Acta Cryst. (2013). E**69**, o1657–o1658 [doi:10.1107/S1600536813027025]

(6*S**)-6-[(1*S**,2*R**)-1,2-Dihydroxypentyl]-4-methoxy-5,6-dihydro-2*H*-pyran-2-one

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S1. Comment

The title compound was first isolated from an unidentified *Penicillium sp*. (McGahren *et al.*, 1973). Multiple routes have been reported for the total synthesis (Kirihata *et al.*, 1990; Kirihata *et al.*, 1992*a*; Masaki *et al.*, 1994) including syntheses creating unnatral stereoisomers (Kirihata *et al.*, 1992*b*). Closely related products have been reported from other fungi (Kirihata *et al.*, 1996; Lee *et al.*, 1995). The 6-substituted 5,6-dihydropyran-2-one moiety present in the title compound is also found in natural products from several species of plants and fungi (Davies-Coleman & Rivett, 1989). Although many structures with this moiety exhibit bioactivity, it appears that the title compound displays none of the reported activities. Notably, the gibberellin synergistic activity of the very closely related compound pestalotin is not found (Kimura *et al.*, 1986; Venkatasubbaiah & Van Dyke, 1991). In our lab we observed moderate antifungal activity. Crystal structures for the related natural products, kavain, dihydrokavain and methysticin have been reported (Yoshino & Nowacki, 1972; Engel & Nowacki, 1972*a*; Engel & Nowacki, 1972*b*). In the title compound, the atoms of the pyran-2-one assume a half-chair conformation. The conformations of the methoxy and dihydroxypentyl groups are shown in Fig. 1. Carbons 4′ and 5′ are disordered over two sites with occupancies of 0.881 (10):0.119 (10). In the crystal, molecules are linked via O—H···O hydrogen bonds forming a three-dimensional network (see Table 1 and Fig. 2).

S2. Experimental

The title compound was obtained by liquid-liquid extraction (CH_2Cl_2/H_2O) of a culture of an endophytic *Pestalotiopsis sp*. The CH_2Cl_2 fraction was evaporated under reduced pressure then purified by chromatography on a silica column with $CHCl_3$/CH_3OH (8/2) as eluent. After pooling common fractions, a crystal was grown by slow evaporation of a MeOH solution.

S3. Refinement

The molecule exhibits orientational disorder at atoms C4 and C5. Hydrogen atoms were located and refined isotropically except those on C4 and C5 which were placed in calculated positions of C—H = 0.98 and 0.99Å and assigned isotropic displacement parameters of $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C_{methyl})$, and their coordinates were allowed to ride on their respective carbons using *SHELXL97* (Sheldrick, 2008). In the absence of anomalous dispersion effects the Friedel pairs were merged. The absolute configuration is not known.

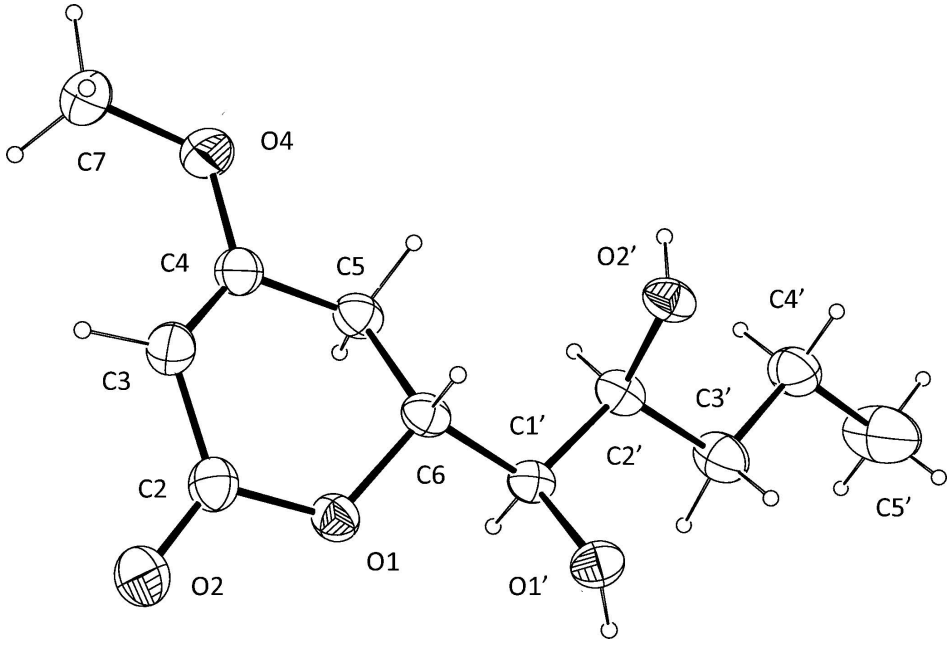

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are shown at the 50% probability level on non-hydrogen atoms. The disorder is not shown.

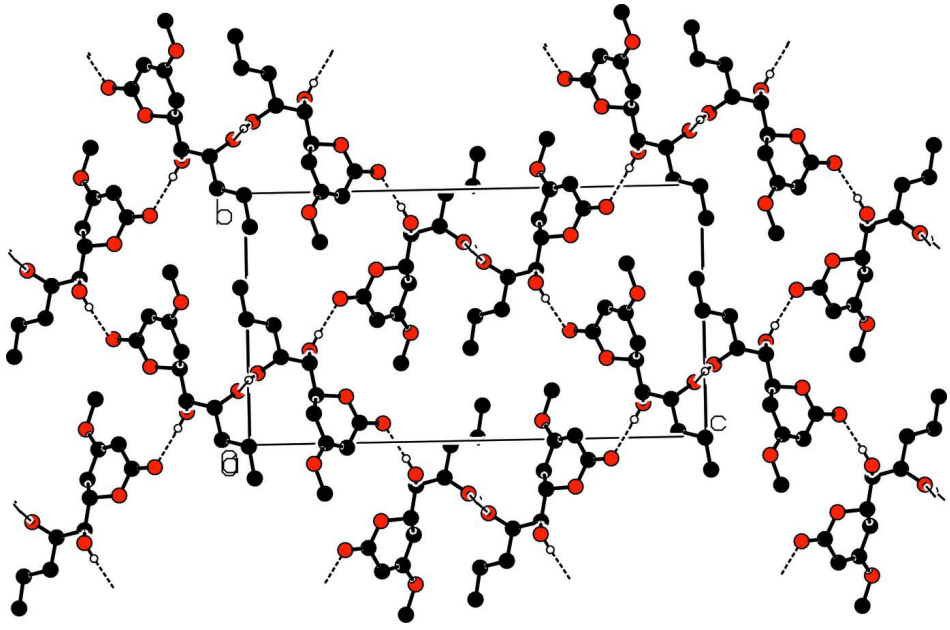

Figure 2

A portion of the crystal structure viewed along the *a* axis. The dashed lines indicate O—H···O hydrogen bonds. The disorder is not shown.

(6*S)-6-[(1*S**,2*R**)-1,2-Dihydroxypentyl]-4-methoxy-5,6-dihydro-2*H*-pyran-2-one**

Crystal data

$C_{11}H_{18}O_5$
$M_r = 230.25$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.0375$ (3) Å
$b = 11.4515$ (13) Å
$c = 20.802$ (2) Å
$V = 1200.02$ (19) Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.274$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 17230 reflections
$\theta = 1.0$–$27.5°$
$\mu = 0.10$ mm^{-1}
$T = 200$ K
Plate, colorless
0.28 × 0.18 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ plus ω scans
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
$T_{min} = 0.973$, $T_{max} = 0.992$
2711 measured reflections
1616 independent reflections
1153 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.4°$
$h = -6 \rightarrow 6$
$k = -14 \rightarrow 14$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.121$
$S = 1.06$
1616 reflections
188 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.1236P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.033 (6)

Special details

Experimental. The program DENZO-SMN (Otwinowski & Minor, 1997) uses a scaling algorithm that effectively corrects for absorption effects. High redundancy data were used in the scaling program thus the 'multi-scan′ code word was used. No transmission coefficients are available from the program (only scale factors for each frame). The scale factors in the experimental table are calculated from the 'size′ command in the SHELXL97<i/> input file.

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.4082 (4)	0.31378 (17)	0.78556 (9)	0.0429 (5)	
O2	0.5372 (5)	0.4250 (2)	0.70604 (12)	0.0678 (7)	
O4	−0.0742 (6)	0.5734 (2)	0.85714 (11)	0.0685 (8)	
O1′	0.5361 (4)	0.1294 (2)	0.86362 (10)	0.0451 (6)	
H1′O	0.516 (7)	0.066 (3)	0.8434 (15)	0.050 (10)*	
O2′	0.2491 (5)	0.21272 (19)	0.97762 (9)	0.0443 (5)	
H2′O	0.125 (8)	0.238 (3)	0.9970 (17)	0.051 (10)*	
C2	0.4146 (7)	0.4194 (3)	0.75666 (15)	0.0481 (8)	
C3	0.2702 (8)	0.5156 (3)	0.78511 (15)	0.0541 (8)	
H3	0.302 (8)	0.590 (3)	0.7637 (17)	0.070 (11)*	
C4	0.0890 (7)	0.4946 (3)	0.83017 (13)	0.0520 (8)	
C5	0.0460 (6)	0.3748 (3)	0.85552 (15)	0.0454 (7)	
H5A	−0.004 (7)	0.381 (2)	0.9013 (15)	0.048 (8)*	
H5B	−0.094 (8)	0.335 (3)	0.8314 (15)	0.056 (9)*	
C6	0.3007 (6)	0.3053 (3)	0.85045 (13)	0.0395 (7)	
H6	0.433 (6)	0.340 (2)	0.8789 (12)	0.028 (6)*	
C1′	0.2742 (5)	0.1766 (3)	0.86336 (14)	0.0376 (6)	
H1′	0.168 (5)	0.146 (2)	0.8299 (12)	0.026 (7)*	
C2′	0.1275 (6)	0.1490 (3)	0.92562 (14)	0.0421 (7)	
H2′	−0.057 (6)	0.174 (3)	0.9211 (14)	0.044 (8)*	
C3′A	0.1175 (9)	0.0209 (3)	0.94034 (14)	0.0598 (9)	0.881 (10)
H3′A	0.3000	−0.0079	0.9481	0.072*	0.881 (10)
H3′B	0.0454	−0.0213	0.9027	0.072*	0.881 (10)
C4′A	−0.0549 (13)	−0.0058 (5)	0.99940 (18)	0.0624 (14)	0.881 (10)
H4′A	0.0249	0.0315	1.0377	0.075*	0.881 (10)
H4′B	−0.2335	0.0283	0.9930	0.075*	0.881 (10)
C5′A	−0.0814 (18)	−0.1325 (4)	1.0111 (3)	0.118 (3)	0.881 (10)
H5′A	−0.1905	−0.1454	1.0495	0.177*	0.881 (10)
H5′B	0.0949	−0.1666	1.0178	0.177*	0.881 (10)
H5′C	−0.1660	−0.1695	0.9739	0.177*	0.881 (10)
C3′B	0.1175 (9)	0.0209 (3)	0.94034 (14)	0.0598 (9)	0.119 (10)
H3′C	0.2915	−0.0094	0.9258	0.072*	0.119 (10)
H3′D	−0.0147	−0.0109	0.9098	0.072*	0.119 (10)
C4′B	0.064 (7)	−0.043 (3)	1.0025 (13)	0.036 (7)*	0.119 (10)
H4′C	0.1133	0.0035	1.0409	0.043*	0.119 (10)
H4′D	0.1484	−0.1207	1.0041	0.043*	0.119 (10)
C5′B	−0.244 (5)	−0.049 (2)	0.9920 (11)	0.038 (8)*	0.119 (10)
H5′D	−0.3267	−0.0887	1.0287	0.057*	0.119 (10)
H5′E	−0.2819	−0.0932	0.9526	0.057*	0.119 (10)
H5′F	−0.3161	0.0299	0.9881	0.057*	0.119 (10)
C7	−0.0519 (12)	0.6930 (3)	0.83475 (18)	0.0924 (17)	
H7A	−0.1803	0.7420	0.8577	0.139*	
H7B	−0.0884	0.6960	0.7885	0.139*	
H7C	0.1282	0.7218	0.8430	0.139*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0439 (11)	0.0449 (12)	0.0398 (10)	−0.0023 (9)	0.0045 (9)	0.0010 (9)
O2	0.0802 (18)	0.0588 (15)	0.0645 (14)	0.0010 (13)	0.0250 (14)	0.0148 (12)
O4	0.0831 (18)	0.0673 (15)	0.0549 (13)	0.0342 (14)	−0.0025 (13)	−0.0027 (11)
O1′	0.0373 (11)	0.0457 (13)	0.0525 (12)	0.0014 (9)	0.0025 (9)	−0.0052 (11)
O2′	0.0365 (11)	0.0575 (13)	0.0388 (10)	−0.0012 (11)	−0.0009 (9)	−0.0102 (9)
C2	0.0505 (18)	0.0443 (17)	0.0497 (17)	−0.0040 (15)	−0.0004 (15)	0.0035 (15)
C3	0.071 (2)	0.0453 (19)	0.0460 (17)	0.0060 (18)	−0.0063 (16)	0.0010 (16)
C4	0.057 (2)	0.058 (2)	0.0406 (15)	0.0203 (18)	−0.0105 (15)	−0.0035 (15)
C5	0.0386 (16)	0.0567 (19)	0.0408 (16)	0.0048 (14)	0.0013 (13)	−0.0036 (14)
C6	0.0356 (14)	0.0472 (17)	0.0356 (14)	−0.0013 (12)	−0.0022 (11)	−0.0066 (12)
C1′	0.0315 (13)	0.0438 (16)	0.0375 (14)	−0.0017 (12)	−0.0029 (12)	−0.0064 (13)
C2′	0.0328 (15)	0.0548 (19)	0.0388 (15)	−0.0060 (13)	−0.0019 (12)	−0.0054 (14)
C3′A	0.078 (2)	0.053 (2)	0.0477 (17)	−0.0177 (19)	0.0093 (16)	−0.0044 (16)
C4′A	0.077 (4)	0.058 (3)	0.053 (2)	−0.004 (3)	0.016 (2)	0.002 (2)
C5′A	0.197 (8)	0.061 (3)	0.097 (4)	−0.029 (4)	0.070 (5)	0.002 (3)
C7	0.152 (5)	0.067 (3)	0.059 (2)	0.053 (3)	−0.006 (3)	0.0042 (19)

Geometric parameters (Å, º)

O1—C2	1.351 (3)	C2′—C3′A	1.499 (5)
O1—C6	1.458 (3)	C2′—H2′	0.98 (3)
O2—C2	1.222 (4)	C3′A—C4′A	1.536 (5)
O4—C4	1.343 (4)	C3′A—H3′A	0.9900
O4—C7	1.451 (4)	C3′A—H3′B	0.9900
O1′—C1′	1.426 (3)	C4′A—C5′A	1.477 (7)
O1′—H1′O	0.85 (3)	C4′A—H4′A	0.9900
O2′—C2′	1.442 (3)	C4′A—H4′B	0.9900
O2′—H2′O	0.80 (4)	C5′A—H5′A	0.9800
C2—C3	1.447 (5)	C5′A—H5′B	0.9800
C3—C4	1.330 (5)	C5′A—H5′C	0.9800
C3—H3	0.98 (4)	C4′B—C5′B	1.57 (4)
C4—C5	1.486 (5)	C4′B—H4′C	0.9900
C5—C6	1.513 (4)	C4′B—H4′D	0.9900
C5—H5A	0.99 (3)	C5′B—H5′D	0.9800
C5—H5B	0.97 (4)	C5′B—H5′E	0.9800
C6—C1′	1.504 (4)	C5′B—H5′F	0.9800
C6—H6	0.98 (3)	C7—H7A	0.9800
C1′—C2′	1.524 (4)	C7—H7B	0.9800
C1′—H1′	0.94 (3)	C7—H7C	0.9800
C2—O1—C6	118.7 (2)	C3′A—C2′—H2′	105.9 (18)
C4—O4—C7	116.9 (3)	C1′—C2′—H2′	108.6 (17)
C1′—O1′—H1′O	102 (3)	C2′—C3′A—C4′A	112.2 (3)
C2′—O2′—H2′O	103 (3)	C2′—C3′A—H3′A	109.2
O2—C2—O1	116.3 (3)	C4′A—C3′A—H3′A	109.2

O2—C2—C3	124.5 (3)	C2′—C3′A—H3′B	109.2
O1—C2—C3	119.2 (3)	C4′A—C3′A—H3′B	109.2
C4—C3—C2	119.7 (3)	H3′A—C3′A—H3′B	107.9
C4—C3—H3	126 (2)	C5′A—C4′A—C3′A	112.3 (4)
C2—C3—H3	113 (2)	C5′A—C4′A—H4′A	109.1
C3—C4—O4	126.4 (3)	C3′A—C4′A—H4′A	109.1
C3—C4—C5	121.1 (3)	C5′A—C4′A—H4′B	109.1
O4—C4—C5	112.5 (3)	C3′A—C4′A—H4′B	109.1
C4—C5—C6	109.7 (3)	H4′A—C4′A—H4′B	107.9
C4—C5—H5A	108.2 (17)	C4′A—C5′A—H5′A	109.5
C6—C5—H5A	108.9 (19)	C4′A—C5′A—H5′B	109.5
C4—C5—H5B	110.5 (19)	H5′A—C5′A—H5′B	109.5
C6—C5—H5B	109 (2)	C4′A—C5′A—H5′C	109.5
H5A—C5—H5B	110 (3)	H5′A—C5′A—H5′C	109.5
O1—C6—C1′	105.3 (2)	H5′B—C5′A—H5′C	109.5
O1—C6—C5	110.2 (2)	C5′B—C4′B—H4′C	112.8
C1′—C6—C5	115.3 (2)	C5′B—C4′B—H4′D	112.8
O1—C6—H6	106.3 (15)	H4′C—C4′B—H4′D	110.3
C1′—C6—H6	110.7 (15)	C4′B—C5′B—H5′D	109.5
C5—C6—H6	108.7 (15)	C4′B—C5′B—H5′E	109.5
O1′—C1′—C6	106.9 (2)	H5′D—C5′B—H5′E	109.5
O1′—C1′—C2′	111.5 (2)	C4′B—C5′B—H5′F	109.5
C6—C1′—C2′	113.4 (2)	H5′D—C5′B—H5′F	109.5
O1′—C1′—H1′	112.6 (16)	H5′E—C5′B—H5′F	109.5
C6—C1′—H1′	106.5 (15)	O4—C7—H7A	109.5
C2′—C1′—H1′	106.0 (16)	O4—C7—H7B	109.5
O2′—C2′—C3′A	110.9 (3)	H7A—C7—H7B	109.5
O2′—C2′—C1′	109.1 (2)	O4—C7—H7C	109.5
C3′A—C2′—C1′	113.1 (3)	H7A—C7—H7C	109.5
O2′—C2′—H2′	109.1 (18)	H7B—C7—H7C	109.5

C6—O1—C2—O2	170.8 (3)	C4—C5—C6—C1′	−169.6 (2)
C6—O1—C2—C3	−11.9 (4)	O1—C6—C1′—O1′	64.9 (3)
O2—C2—C3—C4	162.4 (3)	C5—C6—C1′—O1′	−173.5 (2)
O1—C2—C3—C4	−14.7 (5)	O1—C6—C1′—C2′	−171.8 (2)
C2—C3—C4—O4	−174.4 (3)	C5—C6—C1′—C2′	−50.2 (3)
C2—C3—C4—C5	4.7 (5)	O1′—C1′—C2′—O2′	68.4 (3)
C7—O4—C4—C3	0.3 (5)	C6—C1′—C2′—O2′	−52.4 (3)
C7—O4—C4—C5	−178.8 (3)	O1′—C1′—C2′—C3′A	−55.5 (3)
C3—C4—C5—C6	28.2 (4)	C6—C1′—C2′—C3′A	−176.2 (3)
O4—C4—C5—C6	−152.6 (3)	O2′—C2′—C3′A—C4′A	63.0 (4)
C2—O1—C6—C1′	169.7 (2)	C1′—C2′—C3′A—C4′A	−174.2 (3)
C2—O1—C6—C5	44.8 (3)	C2′—C3′A—C4′A—C5′A	175.7 (5)
C4—C5—C6—O1	−50.7 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1′—H1′*O*···O2^{i}	0.85 (3)	1.93 (3)	2.778 (3)	177 (3)
O2′—H2′*O*···O2′^{ii}	0.80 (4)	2.05 (4)	2.8178 (18)	163 (4)

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) *x*−1/2, −*y*+1/2, −*z*+2.