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

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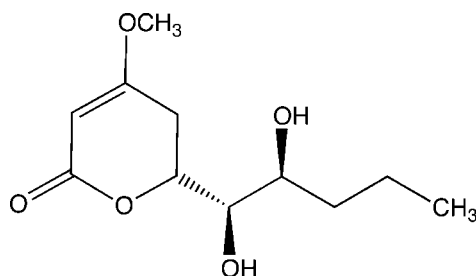
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Key indicators: single-crystal X-ray study; $T = 200$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; disorder in main residue; R factor = 0.052; wR factor = 0.121; data-to-parameter ratio = 8.6.

The title compound, $\text{C}_{11}\text{H}_{18}\text{O}_5$, 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

$\text{C}_{11}\text{H}_{18}\text{O}_5$
 $M_r = 230.25$
 Orthorhombic, $P2_12_12_1$
 $a = 5.0375$ (3) Å
 $b = 11.4515$ (13) Å
 $c = 20.802$ (2) Å
 $V = 1200.02$ (19) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 200$ K
 $0.28 \times 0.18 \times 0.08$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$

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, °).

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|--|----------|-------------|-------------|---------------|
| $\text{O1}'-\text{H1}'\text{O}\cdots\text{O2}^{\text{i}}$ | 0.85 (3) | 1.93 (3) | 2.778 (3) | 177 (3) |
| $\text{O2}'-\text{H2}'\text{O}\cdots\text{O2}^{\text{ii}}$ | 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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supplementary materials

Acta Cryst. (2013). E69, 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

Domenic J. Valenti, Atta M. Arif, Gary A. Strobel and James K. Harper

1. 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 unnatural 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).

2. Experimental

The title compound was obtained by liquid-liquid extraction (CH₂Cl₂/H₂O) of a culture of an endophytic *Pestalotiopsis* sp. The CH₂Cl₂ fraction was evaporated under reduced pressure then purified by chromatography on a silica column with CHCl₃/CH₃OH (8/2) as eluent. After pooling common fractions, a crystal was grown by slow evaporation of a MeOH solution.

3. 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 0.99 Å and assigned isotropic displacement parameters of $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$, 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.

Computing details

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); 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 (Sheldrick, 2008).

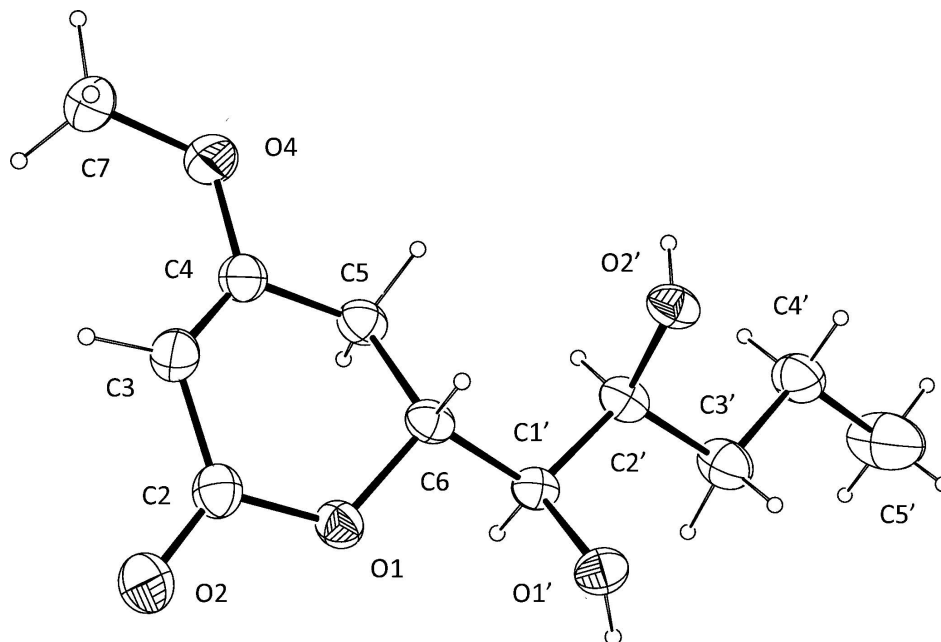


Figure 1

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

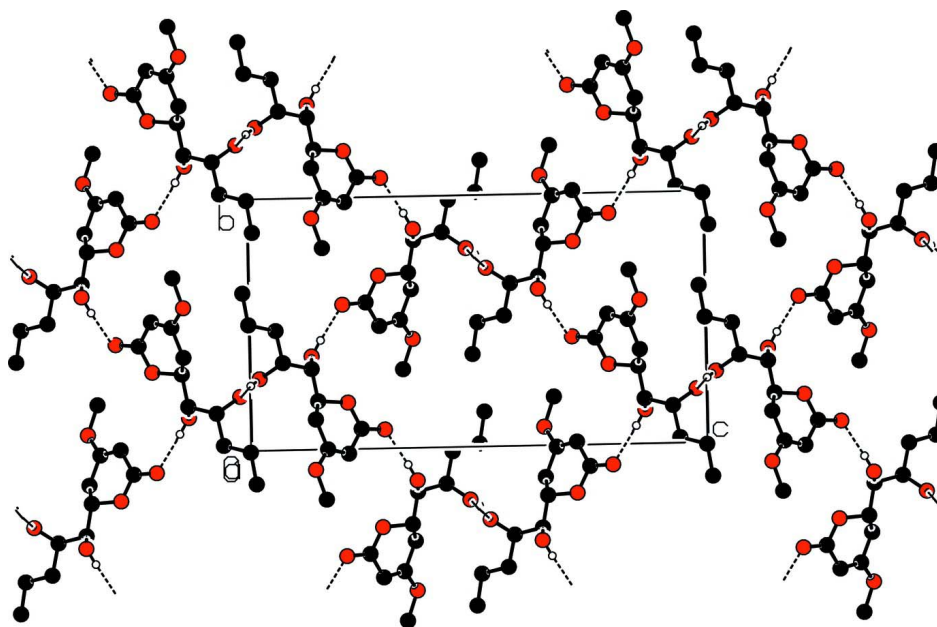


Figure 2

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.

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

Crystal data

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

Data collection

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

Refinement

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

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>/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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | 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 (\AA^2)

| | 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 (\AA , $^\circ$)

| | | | |
|--------------|-----------|----------------|------------|
| 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, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|-----------------------------|-------------|---------------|-----------------------|-------------------------|
| 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) $x-1/2, -y+1/2, -z+2$.