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2-(2,6-Dimethoxyphenyl)-5-hydroxy-7-methoxy-4*H*-1-benzopyran-4-oneR. Ravi Kumar,^a M. Krishnaiah,^a N. Jagadesh Kumar,^a
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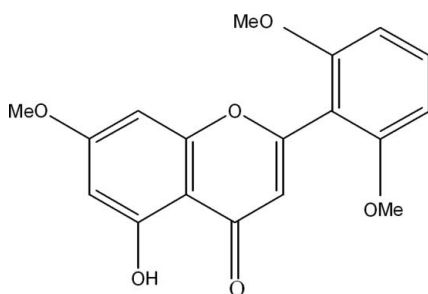
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.037; wR factor = 0.096; data-to-parameter ratio = 12.1.

In the title compound, $\text{C}_{18}\text{H}_{16}\text{O}_6$, the dimethoxyphenyl ring is rotated by 61.8 (1°) from the plane of the benzopyran system. The molecule is stabilized by an intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bond.

Related literature

The title compound, along with a terpinoid and six other flavonoids, was isolated from the roots and the aerial parts of *Andrographis peniculata* Nees (Reddy *et al.*, 2003), a herb widely distributed in the plains of India and Sri Lanka (Gamble, 1956). In traditional Indian medicine, the whole plant of *A. peniculata* is extensively used in the treatment of dyspepsia, dysentery, malaria, respiratory infections and as an antidote for snake bites, see: Kirtikar & Basu (1975); Chopra *et al.* (1980).



Experimental

Crystal data

 $\text{C}_{18}\text{H}_{16}\text{O}_6$ $M_r = 328.31$ Monoclinic, $P2_1/n$
 $a = 11.003$ (7) Å
 $b = 11.015$ (7) Å
 $c = 13.734$ (9) Å
 $\beta = 113.159$ (10°)
 $V = 1530.4$ (17) Å³ $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.11$ mm⁻¹
 $T = 295$ K
 $0.69 \times 0.37 \times 0.36$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.929$, $T_{\max} = 0.969$ 7431 measured reflections
2675 independent reflections
2300 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.096$
 $S = 1.04$
2675 reflections221 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.17$ e Å⁻³
 $\Delta\rho_{\min} = -0.18$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O}6-\text{H}6\cdots\text{O}4$	0.82	1.82	2.560 (2)	149

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 for Windows (Farrugia, 1999); software used to prepare material for publication: enCIFer (Allen *et al.*, 2004) and PARST (Nardelli, 1995).

MK thanks the University Grants Commission, New Delhi, for financial support as a major project.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2533).

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supporting information

Acta Cryst. (2009). E65, o2262 [doi:10.1107/S1600536809032383]

2-(2,6-Dimethoxyphenyl)-5-hydroxy-7-methoxy-4H-1-benzopyran-4-one

R. Ravi Kumar, M. Krishnaiah, N. Jagadesh Kumar, D. Gunasekhar Reddy and V. G. Puranik

S1. Comment

The title compound along with a terpinoid and six other flavonoids were isolated from the roots and the aerial parts of *Andrographis paniculata* Nees (Reddy *et al.*, 2003), an erect herb widely distributed in the plains throughout India and Srilanka (Gamble, 1956). In traditional Indian medicine the whole plant of *A. paniculata* is extensively used in the treatment of dyspepsia, dysentery, malaria, respiratory infections and as an antidote for snake bites (Kirtikar & Basu, 1975; Chopra *et al.*, 1980). As a part of our ongoing investigation on medicinal plants, we report the structure of the title compound (I) (Fig.1).

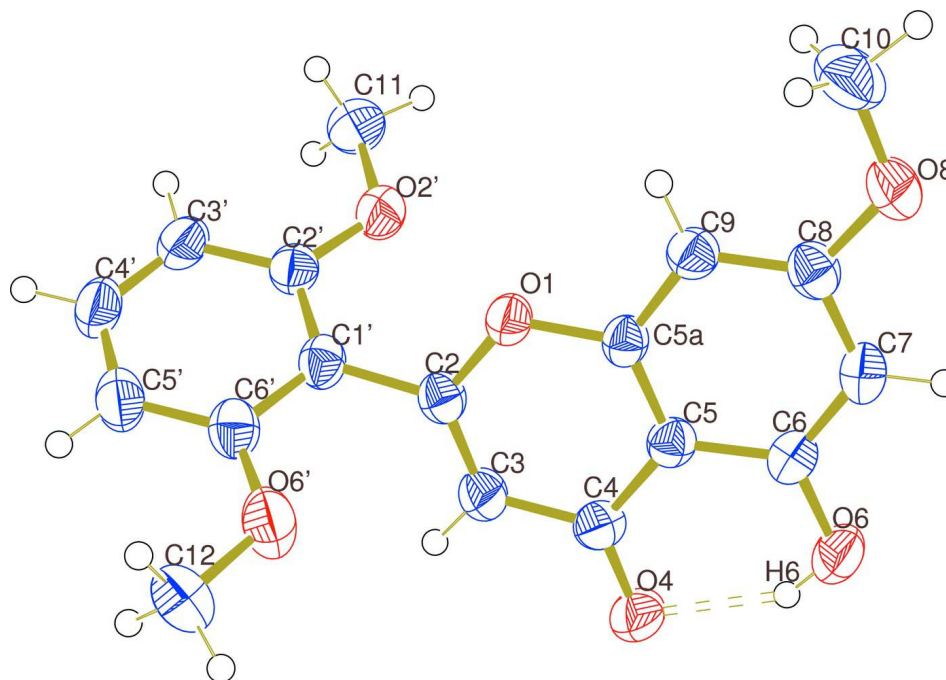
The benzopyran ring is slightly planar with a maximum deviation from the plane of 0.034 (1) Å. The dihedral angle between the least-squares planes of the phenyl ring and the benzopyran moiety is 61.8 (1)°. The non planarity of the phenolic ring is due to the presence of the steric hindrance caused by 2',6' dioxygenation resulting the decrease in the conjugation of the phenyl ring with the carbonyl group. The absence of conjugation means that there will be more delocalization of π -electrons in C2, C3, C4, and O4 unit. The C2–C1' bond length (1.475 (2)Å) is within the 3σ of the average $4sp^2$ – $4sp^3$ bond distance of 1.48 Å.

S2. Experimental

The shade dried and powdered roots of whole plant of *A. paniculata* Nees (3 kg) was successively extracted with n-hexane, Me₂CO and MeOH. The acetone extract on purification over a silica gel column using n-hexane EtoAc step gradients yielded 18 mg of the title compound with a m.p. of 196–198°C and recrystallized by slow evaporation from a hexane solution.

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93Å (aromatic H) or 0.96Å (methyl H) or 0.82Å (oxygen H) and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}$ (C-aromatic) or $U_{iso}(H) = 1.5U_{eq}$ for methyl and oxygen atoms.

**Figure 1**

View of the molecule showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary radius.

2-(2,6-Dimethoxyphenyl)-5-hydroxy-7-methoxy-4H-1-benzopyran-4-one

Crystal data

$C_{18}H_{16}O_6$
 $M_r = 328.31$
 Monoclinic, $P2_1/n$
 Hall symbol: $-P 2_1n$
 $a = 11.003 (7) \text{ \AA}$
 $b = 11.015 (7) \text{ \AA}$
 $c = 13.734 (9) \text{ \AA}$
 $\beta = 113.159 (10)^\circ$
 $V = 1530.4 (17) \text{ \AA}^3$
 $Z = 4$
 $F(000) = 688$

$D_x = 1.425 \text{ Mg m}^{-3}$
 $D_m = 1.42 \text{ Mg m}^{-3}$
 D_m measured by none
 Melting point: 469 K
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 2-25^\circ$
 $\mu = 0.11 \text{ mm}^{-1}$
 $T = 295 \text{ K}$
 Needle, colourless
 $0.69 \times 0.37 \times 0.36 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 Detector resolution: 0 pixels mm^{-1}
 ω scans
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2001)
 $T_{\min} = 0.929$, $T_{\max} = 0.969$

7431 measured reflections
 2675 independent reflections
 2300 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.5^\circ$
 $h = -7 \rightarrow 13$
 $k = -13 \rightarrow 13$
 $l = -16 \rightarrow 16$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.096$
 $S = 1.04$
 2675 reflections
 221 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-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.3516P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$

Special details

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 ?t 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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.95634 (9)	0.63933 (8)	0.16154 (8)	0.0376 (3)
C2	0.97394 (14)	0.75775 (13)	0.14376 (12)	0.0361 (3)
C3	1.06401 (15)	0.79404 (13)	0.10773 (12)	0.0412 (4)
H3	1.0720	0.8764	0.0967	0.049*
C4	1.14884 (15)	0.71009 (13)	0.08555 (12)	0.0391 (3)
O4	1.23188 (12)	0.74190 (10)	0.04933 (10)	0.0526 (3)
C5	1.13251 (14)	0.58600 (13)	0.10870 (11)	0.0350 (3)
C6	1.21312 (15)	0.49245 (14)	0.09621 (12)	0.0393 (3)
O6	1.30566 (12)	0.52024 (11)	0.05872 (11)	0.0560 (3)
H6	1.3026	0.5931	0.0458	0.084*
C7	1.19766 (16)	0.37579 (14)	0.12164 (12)	0.0436 (4)
H7	1.2524	0.3151	0.1146	0.052*
C8	1.09978 (15)	0.34760 (13)	0.15815 (12)	0.0403 (3)
O8	1.09338 (12)	0.22951 (9)	0.18118 (10)	0.0537 (3)
C9	1.01709 (14)	0.43571 (13)	0.16945 (11)	0.0375 (3)
H9	0.9506	0.4162	0.1926	0.045*
C5A	1.03645 (13)	0.55351 (13)	0.14532 (11)	0.0333 (3)
C10	0.9930 (2)	0.19296 (17)	0.21541 (17)	0.0638 (5)
H10A	1.0044	0.2346	0.2798	0.096*
H10B	0.9987	0.1070	0.2278	0.096*
H10C	0.9080	0.2125	0.1618	0.096*
C1'	0.88314 (14)	0.83990 (13)	0.16728 (12)	0.0376 (3)
C2'	0.88837 (14)	0.85308 (13)	0.26936 (12)	0.0396 (4)
O2'	0.97735 (11)	0.78129 (10)	0.34356 (8)	0.0467 (3)
C3'	0.80767 (16)	0.93686 (15)	0.28990 (14)	0.0479 (4)

H3'	0.8119	0.9467	0.3584	0.057*
C4'	0.72169 (17)	1.00504 (15)	0.20869 (15)	0.0521 (4)
H4'	0.6680	1.0613	0.2231	0.063*
C5'	0.71262 (16)	0.99273 (14)	0.10730 (14)	0.0493 (4)
H5'	0.6523	1.0388	0.0530	0.059*
C6'	0.79435 (15)	0.91074 (14)	0.08648 (13)	0.0426 (4)
O6'	0.79624 (13)	0.89242 (11)	-0.00985 (9)	0.0594 (3)
C12	0.70572 (18)	0.95611 (16)	-0.09779 (14)	0.0551 (4)
H12A	0.6172	0.9317	-0.1097	0.083*
H12B	0.7232	0.9381	-0.1595	0.083*
H12C	0.7152	1.0418	-0.0840	0.083*
C11	0.99169 (19)	0.79582 (17)	0.44992 (13)	0.0557 (5)
H11A	1.0145	0.8785	0.4713	0.084*
H11B	1.0603	0.7430	0.4947	0.084*
H11C	0.9100	0.7757	0.4558	0.084*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0400 (6)	0.0327 (5)	0.0456 (6)	0.0029 (4)	0.0227 (5)	-0.0012 (4)
C2	0.0384 (8)	0.0313 (7)	0.0373 (8)	0.0008 (6)	0.0135 (6)	-0.0020 (6)
C3	0.0455 (9)	0.0317 (8)	0.0498 (9)	0.0011 (6)	0.0223 (7)	0.0006 (7)
C4	0.0404 (8)	0.0408 (8)	0.0390 (8)	-0.0015 (7)	0.0187 (7)	-0.0003 (7)
O4	0.0583 (7)	0.0444 (6)	0.0717 (8)	-0.0006 (5)	0.0435 (7)	0.0037 (6)
C5	0.0362 (7)	0.0364 (8)	0.0322 (7)	0.0005 (6)	0.0132 (6)	-0.0025 (6)
C6	0.0388 (8)	0.0418 (8)	0.0404 (8)	0.0018 (6)	0.0188 (7)	-0.0038 (7)
O6	0.0579 (7)	0.0495 (7)	0.0795 (8)	0.0053 (6)	0.0474 (7)	0.0004 (6)
C7	0.0447 (9)	0.0378 (8)	0.0496 (9)	0.0081 (7)	0.0200 (7)	-0.0040 (7)
C8	0.0442 (8)	0.0336 (8)	0.0394 (8)	0.0001 (7)	0.0127 (7)	-0.0025 (7)
O8	0.0639 (8)	0.0317 (6)	0.0708 (8)	0.0032 (5)	0.0323 (7)	0.0043 (5)
C9	0.0387 (8)	0.0360 (8)	0.0395 (8)	-0.0017 (6)	0.0172 (7)	-0.0011 (6)
C5A	0.0340 (7)	0.0334 (7)	0.0317 (7)	0.0024 (6)	0.0120 (6)	-0.0037 (6)
C10	0.0678 (12)	0.0427 (10)	0.0818 (13)	-0.0062 (9)	0.0305 (11)	0.0124 (10)
C1'	0.0361 (8)	0.0315 (7)	0.0463 (8)	-0.0001 (6)	0.0176 (7)	-0.0041 (7)
C2'	0.0389 (8)	0.0347 (8)	0.0493 (9)	-0.0009 (6)	0.0217 (7)	0.0001 (7)
O2'	0.0522 (6)	0.0483 (7)	0.0443 (6)	0.0107 (5)	0.0242 (5)	0.0017 (5)
C3'	0.0542 (10)	0.0445 (9)	0.0574 (10)	0.0042 (8)	0.0353 (9)	-0.0015 (8)
C4'	0.0529 (10)	0.0408 (9)	0.0753 (12)	0.0102 (8)	0.0388 (10)	0.0004 (9)
C5'	0.0445 (9)	0.0408 (9)	0.0623 (11)	0.0094 (7)	0.0207 (8)	0.0033 (8)
C6'	0.0418 (8)	0.0356 (8)	0.0487 (9)	0.0010 (7)	0.0162 (7)	-0.0045 (7)
O6'	0.0695 (8)	0.0590 (8)	0.0417 (6)	0.0255 (6)	0.0131 (6)	-0.0009 (6)
C12	0.0575 (10)	0.0465 (10)	0.0509 (10)	0.0044 (8)	0.0101 (8)	0.0066 (8)
C11	0.0676 (11)	0.0585 (11)	0.0481 (10)	0.0069 (9)	0.0301 (9)	0.0014 (8)

Geometric parameters (Å, °)

O1—C2	1.3549 (19)	C10—H10B	0.9600
O1—C5A	1.3692 (17)	C10—H10C	0.9600

C2—C3	1.331 (2)	C1'—C2'	1.388 (2)
C2—C1'	1.475 (2)	C1'—C6'	1.394 (2)
C3—C4	1.429 (2)	C2'—O2'	1.3555 (19)
C3—H3	0.9300	C2'—C3'	1.384 (2)
C4—O4	1.2500 (18)	O2'—C11	1.415 (2)
C4—C5	1.431 (2)	C3'—C4'	1.369 (2)
C5—C5A	1.384 (2)	C3'—H3'	0.9300
C5—C6	1.413 (2)	C4'—C5'	1.363 (3)
C6—O6	1.3445 (18)	C4'—H4'	0.9300
C6—C7	1.360 (2)	C5'—C6'	1.381 (2)
O6—H6	0.8200	C5'—H5'	0.9300
C7—C8	1.390 (2)	C6'—O6'	1.346 (2)
C7—H7	0.9300	O6'—C12	1.413 (2)
C8—O8	1.347 (2)	C12—H12A	0.9600
C8—C9	1.380 (2)	C12—H12B	0.9600
O8—C10	1.418 (2)	C12—H12C	0.9600
C9—C5A	1.376 (2)	C11—H11A	0.9600
C9—H9	0.9300	C11—H11B	0.9600
C10—H10A	0.9600	C11—H11C	0.9600
C2—O1—C5A	119.25 (11)	H10A—C10—H10C	109.5
C3—C2—O1	122.42 (13)	H10B—C10—H10C	109.5
C3—C2—C1'	124.37 (14)	C2'—C1'—C6'	118.90 (13)
O1—C2—C1'	113.21 (12)	C2'—C1'—C2	121.52 (13)
C2—C3—C4	121.93 (14)	C6'—C1'—C2	119.49 (13)
C2—C3—H3	119.0	O2'—C2'—C3'	124.56 (14)
C4—C3—H3	119.0	O2'—C2'—C1'	115.41 (13)
O4—C4—C3	122.98 (14)	C3'—C2'—C1'	120.03 (14)
O4—C4—C5	122.11 (13)	C2'—O2'—C11	117.66 (12)
C3—C4—C5	114.91 (13)	C4'—C3'—C2'	119.54 (15)
C5A—C5—C6	117.44 (13)	C4'—C3'—H3'	120.2
C5A—C5—C4	120.55 (13)	C2'—C3'—H3'	120.2
C6—C5—C4	122.00 (13)	C5'—C4'—C3'	121.82 (15)
O6—C6—C7	120.24 (13)	C5'—C4'—H4'	119.1
O6—C6—C5	119.10 (14)	C3'—C4'—H4'	119.1
C7—C6—C5	120.66 (14)	C4'—C5'—C6'	118.98 (16)
C6—O6—H6	109.5	C4'—C5'—H5'	120.5
C6—C7—C8	119.78 (14)	C6'—C5'—H5'	120.5
C6—C7—H7	120.1	O6'—C6'—C5'	124.35 (15)
C8—C7—H7	120.1	O6'—C6'—C1'	114.93 (13)
O8—C8—C9	123.71 (14)	C5'—C6'—C1'	120.72 (15)
O8—C8—C7	114.82 (13)	C6'—O6'—C12	119.16 (13)
C9—C8—C7	121.46 (14)	O6'—C12—H12A	109.5
C8—O8—C10	118.13 (13)	O6'—C12—H12B	109.5
C5A—C9—C8	117.69 (14)	H12A—C12—H12B	109.5
C5A—C9—H9	121.2	O6'—C12—H12C	109.5
C8—C9—H9	121.2	H12A—C12—H12C	109.5
O1—C5A—C9	116.19 (13)	H12B—C12—H12C	109.5

O1—C5A—C5	120.86 (13)	O2'—C11—H11A	109.5
C9—C5A—C5	122.94 (13)	O2'—C11—H11B	109.5
O8—C10—H10A	109.5	H11A—C11—H11B	109.5
O8—C10—H10B	109.5	O2'—C11—H11C	109.5
H10A—C10—H10B	109.5	H11A—C11—H11C	109.5
O8—C10—H10C	109.5	H11B—C11—H11C	109.5
C5A—O1—C2—C3	2.1 (2)	C6—C5—C5A—O1	178.64 (12)
C5A—O1—C2—C1'	-178.43 (12)	C4—C5—C5A—O1	-0.9 (2)
O1—C2—C3—C4	-0.2 (2)	C6—C5—C5A—C9	0.0 (2)
C1'—C2—C3—C4	-179.53 (14)	C4—C5—C5A—C9	-179.56 (14)
C2—C3—C4—O4	178.26 (15)	C3—C2—C1'—C2'	-115.93 (18)
C2—C3—C4—C5	-2.2 (2)	O1—C2—C1'—C2'	64.66 (18)
O4—C4—C5—C5A	-177.77 (14)	C3—C2—C1'—C6'	60.8 (2)
C3—C4—C5—C5A	2.7 (2)	O1—C2—C1'—C6'	-118.64 (15)
O4—C4—C5—C6	2.7 (2)	C6'—C1'—C2'—O2'	-179.85 (13)
C3—C4—C5—C6	-176.84 (14)	C2—C1'—C2'—O2'	-3.1 (2)
C5A—C5—C6—O6	178.63 (13)	C6'—C1'—C2'—C3'	-1.0 (2)
C4—C5—C6—O6	-1.8 (2)	C2—C1'—C2'—C3'	175.73 (14)
C5A—C5—C6—C7	-1.4 (2)	C3'—C2'—O2'—C11	-2.1 (2)
C4—C5—C6—C7	178.17 (15)	C1'—C2'—O2'—C11	176.67 (14)
O6—C6—C7—C8	-178.61 (14)	O2'—C2'—C3'—C4'	179.69 (15)
C5—C6—C7—C8	1.4 (2)	C1'—C2'—C3'—C4'	0.9 (2)
C6—C7—C8—O8	-179.87 (14)	C2'—C3'—C4'—C5'	0.2 (3)
C6—C7—C8—C9	0.0 (2)	C3'—C4'—C5'—C6'	-1.2 (3)
C9—C8—O8—C10	2.3 (2)	C4'—C5'—C6'—O6'	-178.63 (15)
C7—C8—O8—C10	-177.86 (15)	C4'—C5'—C6'—C1'	1.2 (2)
O8—C8—C9—C5A	178.53 (14)	C2'—C1'—C6'—O6'	179.76 (13)
C7—C8—C9—C5A	-1.3 (2)	C2—C1'—C6'—O6'	3.0 (2)
C2—O1—C5A—C9	177.17 (13)	C2'—C1'—C6'—C5'	-0.1 (2)
C2—O1—C5A—C5	-1.57 (19)	C2—C1'—C6'—C5'	-176.86 (14)
C8—C9—C5A—O1	-177.40 (12)	C5'—C6'—O6'—C12	-2.9 (2)
C8—C9—C5A—C5	1.3 (2)	C1'—C6'—O6'—C12	177.24 (14)

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>
O6—H6...O4	0.82	1.82	2.560 (2)	149