

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

 Methyl 6-deoxy-6-iodo-2,3-O-isopropylidene- α -D-mannopyranoside

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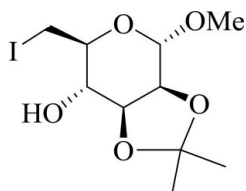
Received 1 August 2013; accepted 12 August 2013

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.016; wR factor = 0.043; data-to-parameter ratio = 25.0.

In the title compound, $\text{C}_{10}\text{H}_{17}\text{IO}_5$, the six-membered tetrahydropyran ring and the five-membered 1,3-dioxolane ring adopt sofa and envelope conformations, respectively. In the crystal, $\text{O}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into layers nearly parallel to the bc plane.

Related literature

For carbohydrates which are important for the preparation of unsaturated aldehydes, see: Kleban *et al.* (2000); Dransfield *et al.* (1999); Greul *et al.* (2001). For conversions of unsaturated aldehydes to oximes, nitrones and nitrile oxides, see: Dransfield *et al.* (1999); Bernet & Vasella (1979); Greul *et al.* (2001); Gallos *et al.* (1999); Kleban *et al.* (2001). For the methods reported in the literature for the preparation of the title compound, see: Garegg & Samuelsson (1980); Bundle *et al.* (1988); Ichikawa *et al.* (2004). For the synthesis of methyl 2,3-*O*-isopropylidene- α -D-mannopyranoside, see: Evans & Parrish (1977); Isobe *et al.* (1981). For ring-puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$\text{C}_{10}\text{H}_{17}\text{IO}_5$
 $M_r = 344.14$
 Monoclinic, $P2_1$
 $a = 8.3121$ (8) Å
 $b = 10.3911$ (10) Å
 $c = 8.3128$ (8) Å
 $\beta = 118.639$ (3)°

$V = 630.15$ (11) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.55$ mm⁻¹
 $T = 100$ K
 $0.99 \times 0.58 \times 0.44$ mm

Data collection

Bruker Kappa APEXII DUO
 diffractometer
 Absorption correction: numerical
 (Blessing, 1995)
 $T_{\min} = 0.187$, $T_{\max} = 0.401$

13656 measured reflections
 3827 independent reflections
 3803 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.043$
 $S = 1.24$
 3827 reflections
 153 parameters
 3 restraints

$\Delta\rho_{\max} = 0.86$ e Å⁻³
 $\Delta\rho_{\min} = -0.82$ e Å⁻³
 Absolute structure: Flack (1983),
 1811 Friedel pairs
 Absolute structure parameter: 0.003
 (12)

H atoms treated by a mixture of independent and constrained refinement

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O2}-\text{H2A}\cdots\text{O3}^i$	0.82 (3)	2.03 (3)	2.807 (2)	157 (3)
$\text{C10}-\text{H10C}\cdots\text{O2}^{ii}$	0.98	2.51	3.390 (3)	149

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); 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, 2012); software used to prepare material for publication: WinGX (Farrugia, 2012) and PLATON (Spek, 2009).

The authors are indebted to the Research Fund of Çankırı Karatekin University (grant No. BAP:2011/06) for financial support, and thank Professor V. Jäger of Stuttgart University, Germany, for helpful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5727).

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supporting information

Acta Cryst. (2013). E69, o1449–o1450 [doi:10.1107/S1600536813022629]

Methyl 6-deoxy-6-iodo-2,3-*O*-isopropylidene- α -D-mannopyranoside

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S1. Comment

Various carbohydrates have been considerably important for the preparation of unsaturated aldehydes (Kleban *et al.*, 2000; Dransfield *et al.*, 1999; Greul *et al.*, 2001). Conversions of unsaturated aldehydes to oximes (Dransfield *et al.*, 1999), nitrones (Bernet & Vasella, 1979; Greul *et al.*, 2001), nitrile oxides (Gallos *et al.*, 1999; Kleban *et al.*, 2001) and their intramolecular cycloadditions have been reported. These cycloadducts are useful intermediates for the syntheses of polyhydroxylated aminocyclopentane derivatives (Greul *et al.*, 2001; Kleban *et al.*, 2001).

In the title compound (Fig. 1), the ring A (C1–C5/O1) is not planar, but adopts a sofa conformation with puckering parameters (Cremer & Pople, 1975) $Q_T = 0.551(2) \text{ \AA}$, $\varphi = -113.1(5)^\circ$ and $\theta = 158.5(2)^\circ$. The conformation of ring B (O4/O5/C3/C4/C8) is an envelope, with atom C4 at the flap position, $-0.573(2) \text{ \AA}$ from the mean plane through the other four atoms. Rings A and B have local pseudo-mirror planes running through C1 and C4 (for ring A), and running through C4 and the midpoint of the O4–C8 bond (for ring B).

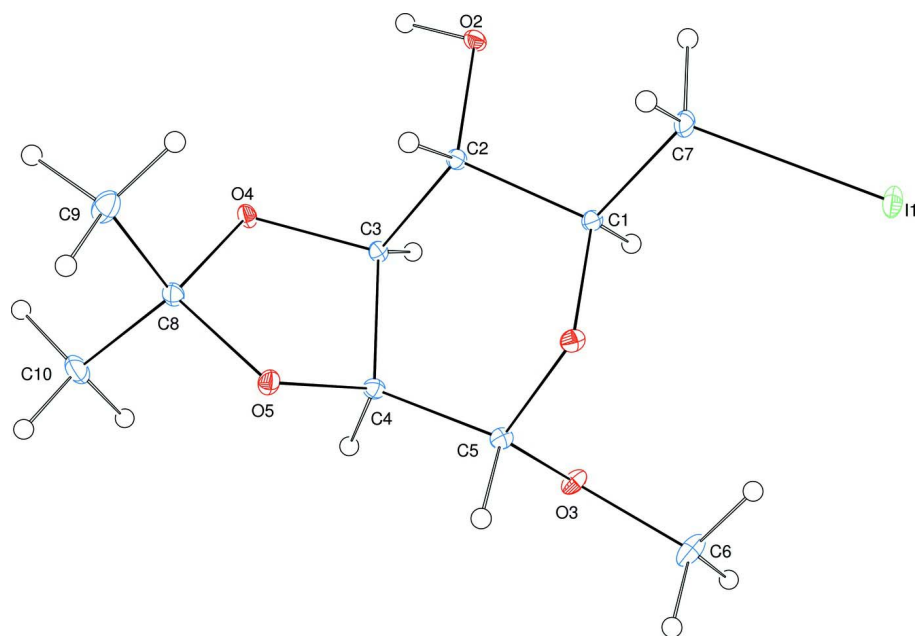
In the crystal structure, intermolecular O—H \cdots O and C—H \cdots O hydrogen bonds (Table 1) link the molecules into layers nearly parallel to the *bc* plane (Fig. 2).

S2. Experimental

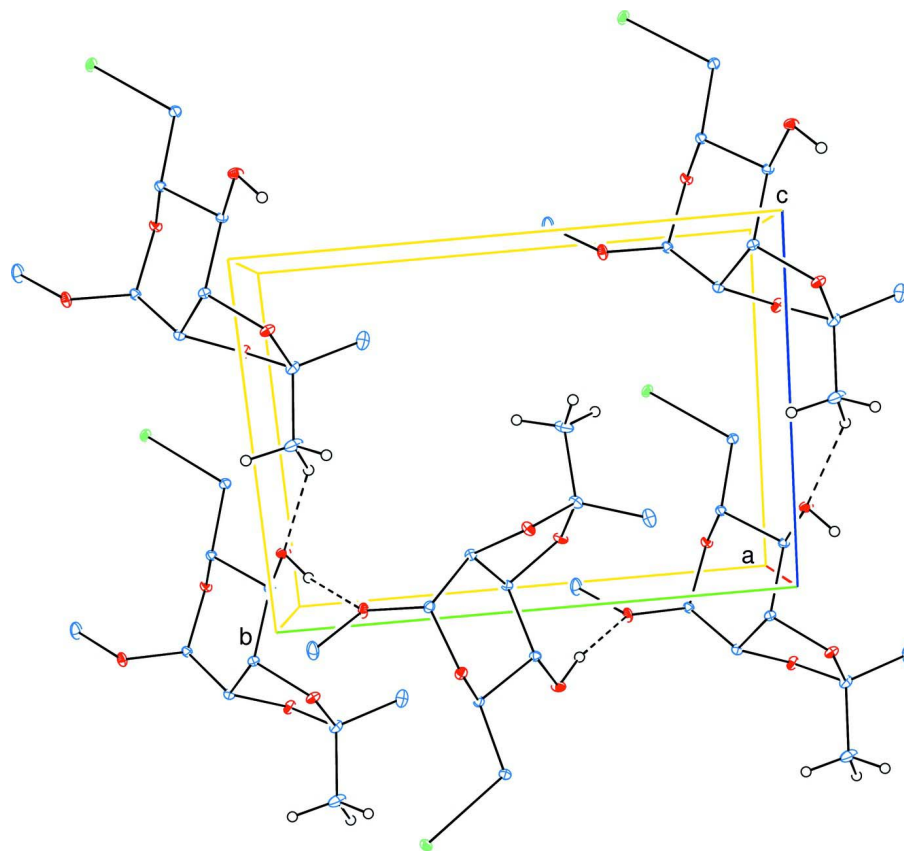
The title compound was synthesized in two steps starting from α -D-mannopyranoside by the literature methods (Garegg & Samuelsson, 1980; Bundle *et al.*, 1988; Ichikawa *et al.*, 2004). To a solution of methyl 2,3-*O*-isopropylidene- α -D-mannopyranoside (Evans & Parrish, 1977; Isobe *et al.*, 1981) (2.50 g, 10.66 mmol) in dry toluene (70 ml, dissolved at 353 K) were added PPh₃ (4.30 g, 15.90 mmol), imidazole (2.17 g, 31.98 mmol) and iodine (3.80 g, 14.90 mmol) sequentially. The reaction mixture was refluxed for 3 h. 20 ml water was added, and then the mixture was extracted with EtOAc (4 \times 20 ml). The combined organic phase was washed with brine (300 ml) and then dried over MgSO₄. The filtrate was concentrated under reduced pressure, and the residue was purified by chromatography (PE:EE 70:30) to afford the iodo compound as a colourless crystalline solid (yield: 90%), m.p. 383–384 K.

S3. Refinement

Atom H2A (for OH) was located in a difference Fourier map and refined freely. The C-bound H atoms were positioned geometrically, with C—H = 1.00, 0.99 and 0.98 \AA for methine, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = kU_{\text{eq}}(\text{C})$, where $k = 1.2$ for methine and methylene and $k = 1.5$ for methyl H atoms.

**Figure 1**

The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

A partial packing diagram. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity.

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Crystal data

$C_{10}H_{17}IO_5$
 $M_r = 344.14$
 Monoclinic, $P2_1$
 Hall symbol: P 2yb
 $a = 8.3121$ (8) Å
 $b = 10.3911$ (10) Å
 $c = 8.3128$ (8) Å
 $\beta = 118.639$ (3)°
 $V = 630.15$ (11) Å³
 $Z = 2$

$F(000) = 340$
 $D_x = 1.814$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 3798 reflections
 $\theta = 2.8$ – 30.5 °
 $\mu = 2.55$ mm⁻¹
 $T = 100$ K
 Prism, colourless
 $0.99 \times 0.58 \times 0.44$ mm

Data collection

Bruker Kappa APEXII DUO
 diffractometer
 Radiation source: fine-focus sealed tube
 Triumph monochromator
 φ and ω scans
 Absorption correction: numerical
 (Blessing, 1995)
 $T_{\min} = 0.187$, $T_{\max} = 0.401$

13656 measured reflections
 3827 independent reflections
 3803 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\max} = 30.5$ °, $\theta_{\min} = 2.8$ °
 $h = -11 \rightarrow 11$
 $k = -14 \rightarrow 14$
 $l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.043$

$S = 1.24$

3827 reflections

153 parameters

3 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

$w = 1/[\sigma^2(F_o^2) + (0.0159P)^2 + 0.0596P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.82 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0949 (17)

Absolute structure: Flack (1983), 1811 Friedel
pairs

Absolute structure parameter: 0.003 (12)

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. 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 $F^2 > 2\sigma(F^2)$ 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
I1	0.388710 (12)	0.741920 (17)	0.435425 (11)	0.01675 (5)
O1	0.59121 (17)	0.64971 (12)	0.87699 (17)	0.0126 (2)
O2	0.91193 (19)	0.47140 (13)	0.78471 (18)	0.0150 (2)
H2A	0.998 (4)	0.426 (3)	0.855 (4)	0.045 (10)*
O3	0.76827 (18)	0.82125 (12)	1.0565 (2)	0.0143 (2)
O4	1.04540 (17)	0.44287 (13)	1.19016 (17)	0.0130 (2)
O5	0.80476 (18)	0.50343 (12)	1.23592 (19)	0.0143 (2)
C1	0.6958 (2)	0.62356 (15)	0.7844 (2)	0.0113 (3)
H1	0.7689	0.7009	0.7875	0.014*
C2	0.8224 (2)	0.51098 (16)	0.8849 (2)	0.0111 (3)
H2	0.7473	0.4379	0.8912	0.013*
C3	0.9584 (2)	0.55251 (16)	1.0784 (2)	0.0105 (3)
H3	1.0518	0.6125	1.0768	0.013*
C4	0.8628 (2)	0.61411 (15)	1.1762 (2)	0.0119 (3)
H4	0.9530	0.6646	1.2845	0.014*
C5	0.6980 (3)	0.69768 (17)	1.0559 (2)	0.0118 (3)
H5	0.6183	0.7038	1.1152	0.014*
C6	0.6277 (3)	0.91625 (18)	0.9709 (3)	0.0226 (4)
H6A	0.5518	0.8950	0.8409	0.034*
H6B	0.6839	1.0010	0.9823	0.034*
H6C	0.5510	0.9178	1.0309	0.034*
C7	0.5644 (3)	0.58663 (17)	0.5897 (3)	0.0158 (3)

H7A	0.4882	0.5136	0.5903	0.019*
H7B	0.6351	0.5574	0.5287	0.019*
C8	0.9482 (3)	0.40997 (16)	1.2897 (2)	0.0143 (3)
C9	0.8614 (3)	0.27863 (19)	1.2334 (3)	0.0220 (4)
H9A	0.7752	0.2655	1.2809	0.033*
H9B	0.9570	0.2124	1.2832	0.033*
H9C	0.7957	0.2727	1.0993	0.033*
C10	1.0810 (3)	0.4196 (2)	1.4915 (3)	0.0231 (4)
H10A	1.1313	0.5070	1.5203	0.035*
H10B	1.1809	0.3579	1.5237	0.035*
H10C	1.0172	0.4004	1.5618	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.01472 (6)	0.01220 (5)	0.01494 (6)	0.00098 (5)	0.00036 (4)	0.00353 (5)
O1	0.0087 (5)	0.0137 (5)	0.0134 (6)	0.0003 (4)	0.0036 (5)	-0.0021 (4)
O2	0.0145 (6)	0.0201 (6)	0.0104 (6)	0.0058 (5)	0.0060 (5)	0.0004 (5)
O3	0.0097 (6)	0.0093 (5)	0.0215 (7)	-0.0009 (4)	0.0055 (5)	-0.0018 (4)
O4	0.0107 (6)	0.0189 (6)	0.0111 (6)	0.0046 (5)	0.0065 (5)	0.0047 (5)
C1	0.0102 (7)	0.0112 (6)	0.0108 (7)	0.0007 (5)	0.0037 (6)	-0.0009 (5)
C2	0.0096 (7)	0.0130 (6)	0.0099 (7)	0.0014 (6)	0.0042 (6)	0.0002 (5)
C3	0.0078 (7)	0.0132 (6)	0.0101 (7)	0.0008 (5)	0.0039 (6)	0.0009 (5)
C4	0.0113 (7)	0.0131 (7)	0.0118 (7)	0.0001 (6)	0.0061 (6)	-0.0006 (6)
C5	0.0102 (7)	0.0116 (6)	0.0125 (8)	-0.0010 (5)	0.0046 (7)	-0.0018 (5)
O5	0.0138 (6)	0.0148 (5)	0.0175 (6)	0.0041 (4)	0.0102 (5)	0.0048 (5)
C6	0.0155 (9)	0.0131 (8)	0.0329 (11)	0.0036 (6)	0.0065 (8)	0.0002 (7)
C7	0.0150 (8)	0.0134 (7)	0.0118 (8)	0.0023 (6)	0.0005 (7)	0.0008 (6)
C8	0.0146 (8)	0.0173 (7)	0.0147 (8)	0.0044 (6)	0.0100 (7)	0.0039 (6)
C9	0.0234 (10)	0.0161 (7)	0.0313 (11)	0.0018 (6)	0.0171 (9)	0.0045 (6)
C10	0.0239 (10)	0.0326 (10)	0.0132 (9)	0.0095 (8)	0.0093 (8)	0.0069 (7)

Geometric parameters (Å, °)

I1—C7	2.1414 (18)	C4—O5	1.425 (2)
O1—C1	1.4362 (19)	C4—C5	1.522 (3)
O1—C5	1.408 (2)	C4—H4	1.0000
O2—C2	1.4182 (18)	C5—H5	1.0000
O2—H2A	0.823 (16)	C6—H6A	0.9800
O3—C5	1.409 (2)	C6—H6B	0.9800
O3—C6	1.432 (2)	C6—H6C	0.9800
O4—C8	1.4480 (19)	C7—H7A	0.9900
O5—C8	1.433 (2)	C7—H7B	0.9900
C1—C2	1.527 (2)	C8—C9	1.509 (3)
C1—C7	1.505 (2)	C8—C10	1.506 (3)
C1—H1	1.0000	C9—H9A	0.9800
C2—C3	1.519 (2)	C9—H9B	0.9800
C2—H2	1.0000	C9—H9C	0.9800

C3—O4	1.428 (2)	C10—H10A	0.9800
C3—C4	1.524 (2)	C10—H10B	0.9800
C3—H3	1.0000	C10—H10C	0.9800
C5—O1—C1	113.31 (13)	O3—C5—H5	108.2
C2—O2—H2A	106 (3)	C4—C5—H5	108.2
C5—O3—C6	112.85 (13)	O3—C6—H6A	109.5
C3—O4—C8	108.25 (12)	O3—C6—H6B	109.5
C4—O5—C8	106.61 (12)	O3—C6—H6C	109.5
O1—C1—C2	106.69 (13)	H6A—C6—H6B	109.5
O1—C1—C7	108.12 (14)	H6A—C6—H6C	109.5
O1—C1—H1	110.5	H6B—C6—H6C	109.5
C2—C1—H1	110.5	I1—C7—H7A	109.0
C7—C1—C2	110.34 (13)	I1—C7—H7B	109.0
C7—C1—H1	110.5	C1—C7—I1	112.76 (11)
O2—C2—C1	108.61 (13)	C1—C7—H7A	109.0
O2—C2—C3	111.71 (13)	C1—C7—H7B	109.0
O2—C2—H2	109.1	H7A—C7—H7B	107.8
C1—C2—H2	109.1	O4—C8—C9	110.52 (14)
C3—C2—C1	109.25 (13)	O4—C8—C10	107.99 (15)
C3—C2—H2	109.1	O5—C8—O4	105.68 (13)
O4—C3—C2	110.49 (14)	O5—C8—C9	108.28 (16)
O4—C3—C4	102.62 (12)	O5—C8—C10	111.02 (14)
O4—C3—H3	110.6	C10—C8—C9	113.10 (16)
C2—C3—C4	111.72 (14)	C8—C9—H9A	109.5
C2—C3—H3	110.6	C8—C9—H9B	109.5
C4—C3—H3	110.6	C8—C9—H9C	109.5
O5—C4—C3	101.37 (12)	H9A—C9—H9B	109.5
O5—C4—C5	109.94 (14)	H9A—C9—H9C	109.5
O5—C4—H4	110.0	H9B—C9—H9C	109.5
C3—C4—H4	110.0	C8—C10—H10A	109.5
C5—C4—C3	115.09 (14)	C8—C10—H10B	109.5
C5—C4—H4	110.0	C8—C10—H10C	109.5
O1—C5—O3	112.13 (14)	H10A—C10—H10B	109.5
O1—C5—C4	113.92 (14)	H10A—C10—H10C	109.5
O1—C5—H5	108.2	H10B—C10—H10C	109.5
O3—C5—C4	106.06 (14)		
C5—O1—C1—C2	67.22 (16)	C2—C1—C7—I1	-177.65 (10)
C5—O1—C1—C7	-174.10 (14)	O2—C2—C3—O4	-75.14 (16)
C1—O1—C5—O3	67.12 (17)	O2—C2—C3—C4	171.29 (13)
C1—O1—C5—C4	-53.35 (18)	C1—C2—C3—O4	164.67 (12)
C6—O3—C5—O1	63.69 (19)	C1—C2—C3—C4	51.10 (17)
C6—O3—C5—C4	-171.39 (15)	C2—C3—O4—C8	-95.94 (15)
C3—O4—C8—O5	-0.79 (18)	C4—C3—O4—C8	23.30 (17)
C3—O4—C8—C9	116.14 (17)	O4—C3—C4—O5	-37.10 (16)
C3—O4—C8—C10	-119.67 (15)	O4—C3—C4—C5	-155.67 (14)
C4—O5—C8—O4	-24.18 (18)	C2—C3—C4—O5	81.28 (16)

C4—O5—C8—C9	-142.61 (15)	C2—C3—C4—C5	-37.29 (19)
C4—O5—C8—C10	92.67 (16)	C3—C4—O5—C8	37.73 (17)
O1—C1—C2—O2	172.83 (13)	C5—C4—O5—C8	159.94 (14)
O1—C1—C2—C3	-65.09 (16)	O5—C4—C5—O1	-76.30 (17)
C7—C1—C2—O2	55.61 (18)	O5—C4—C5—O3	159.88 (12)
C7—C1—C2—C3	177.69 (13)	C3—C4—C5—O1	37.36 (19)
O1—C1—C7—I1	66.01 (15)	C3—C4—C5—O3	-86.45 (16)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O2—H2A \cdots O3 ⁱ	0.82 (3)	2.03 (3)	2.807 (2)	157 (3)
C10—H10C \cdots O2 ⁱⁱ	0.98	2.51	3.390 (3)	149

Symmetry codes: (i) $-x+2, y-1/2, -z+2$; (ii) $x, y, z+1$.