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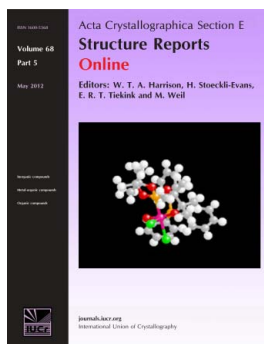
ISSN 1600-5368

{(3a*R*,5*S*,6*R*,6a*R*)-5-[(*R*)-1,2-Dihydroxyethyl]-2,2-dimethyl-tetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl}methyl methanesulfonate

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Acta Cryst. (2014). **E70**, o524–o525

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{(3*aR*,5*S*,6*R*,6*aR*)-5-[(*R*)-1,2-Dihydroxyethyl]-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)methyl methanesulfonate

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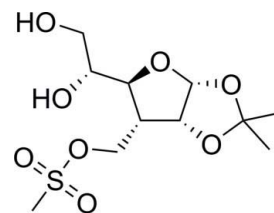
Received 17 February 2014; accepted 2 April 2014

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.027; wR factor = 0.065; data-to-parameter ratio = 17.0.

In the title compound, $\text{C}_{11}\text{H}_{20}\text{O}_8\text{S}$, the furanose ring has a pseudorotation phase angle equal to 31.3° and assumes a 3T_4 conformation, with deviations of 0.297 (4) and -0.152 (4) Å for the corresponding C atoms. The dioxolane ring adopts an envelope conformation. One of the O atoms is at the flap and deviates from the least-squares plane formed by the other four ring atoms by 0.405 (2) Å. The dihedral angle between the planar fragments of the rings is 63.53 (8) $^\circ$. In the crystal, molecules are associated into sheets perpendicular to the b axis by means of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds. A few weak $\text{C}-\text{H}\cdots\text{O}$ interactions are also observed.

Related literature

For the synthesis, properties and applications of the title compound, see: Mikhailopulo *et al.* (1996); Rjabova *et al.* (2012). Its applications in the synthesis of imino sugars and 1'-aza- C -nucleosides are described by Filichev & Pedersen (2001). For a review on the syntheses and biological properties of imino sugars, see: López *et al.* (2012). For reviews on the syntheses and biological properties of aza-nucleosides, see: Romeo *et al.* (2010); Merino (2006).



Experimental

Crystal data

$\text{C}_{11}\text{H}_{20}\text{O}_8\text{S}$	$V = 694.04$ (3) Å ³
$M_r = 312.33$	$Z = 2$
Monoclinic, $P2_1$	Mo $K\alpha$ radiation
$a = 5.5794$ (1) Å	$\mu = 0.27$ mm ⁻¹
$b = 15.6118$ (3) Å	$T = 293$ K
$c = 8.0653$ (2) Å	$0.35 \times 0.30 \times 0.28$ mm
$\beta = 98.913$ (1) $^\circ$	

Data collection

Nonius KappaCCD diffractometer	3005 reflections with $I > 2\sigma(I)$
5266 measured reflections	$R_{\text{int}} = 0.018$
3185 independent reflections	

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.027$	$\Delta\rho_{\text{max}} = 0.16$ e Å ⁻³
$wR(F^2) = 0.065$	$\Delta\rho_{\text{min}} = -0.21$ e Å ⁻³
$S = 1.03$	Absolute structure: Flack (1983),
3185 reflections	1528 Friedel pairs
187 parameters	Absolute structure parameter:
1 restraint	0.00 (5)
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, $^\circ$).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O4}-\text{H41}\cdots\text{O5}^{\text{i}}$	0.82	2.00	2.820 (2)	174
$\text{O5}-\text{H51}\cdots\text{O2}^{\text{ii}}$	0.82	2.24	3.009 (2)	156
$\text{C3}-\text{H3}\cdots\text{O5}^{\text{i}}$	0.98	2.58	3.344 (2)	135
$\text{C8}-\text{H8C}\cdots\text{O6}^{\text{iii}}$	0.96	2.55	3.486 (2)	165
$\text{C9}-\text{H9A}\cdots\text{O4}^{\text{iv}}$	0.96	2.55	3.306 (2)	136
$\text{C11}-\text{H11C}\cdots\text{O8}^{\text{iii}}$	0.96	2.44	3.387 (2)	167

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

Data collection: *COLLECT* (Bruker, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997); 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).

This work was supported by the Latvian Council of Science (grant No 09.1557).

Supporting information for this paper is available from the IUCr electronic archives (Reference: ZP2012).

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supplementary materials

Acta Cryst. (2014). E70, o524–o525 [doi:10.1107/S1600536814007387]

{(3*aR*,5*S*,6*R*,6*aR*)-5-[(*R*)-1,2-Dihydroxyethyl]-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)methyl methanesulfonate

Vitālijs Rjabovs, Anatoly Mishnev, Glebs Kiselovs and Māris Turks

1. Comment

1,2-*O*-isopropylidene-3-deoxy-3-mesyloxymethyl- α -*D*-allofuranose was obtained as the intermediate in the syntheses of 3-*C*-branched 3-*C*-deoxy nucleoside analogs (Mikhailopulo *et al.*, 1996) by an acidic hydrolysis of 5,6-isopropylidene protecting group of the corresponding mesylate. Both the title compound and its precursor can be used for the syntheses of different carbohydrate derivatives such as triazole conjugates of 3-*C*-branched 3-*C*-deoxy allofuranose (Rjabova *et al.*, 2012) and imino sugars and 1'-aza-*C*-nucleosides (Filichev & Pedersen, 2001). For review on syntheses and biological properties of imino sugars, see: López *et al.* (2012). For reviews on syntheses and biological properties of aza-nucleosides, see: Romeo *et al.* (2010) and Merino (2006). Fig. 1 shows a view of the molecular structure of the title compound. The furanose ring has a pseudorotation phase angle equal to 31.3° and assumes ³T₄ conformation with deviations of 0.297 (4) Å and -0.152 (4) Å for corresponding C atoms. The dioxolane ring adopts envelope conformation. One of the O atoms deviates from the least squares plane formed by four other atoms of the dioxolane ring by 0.405 (2) Å. The dihedral angle between plane fragments of the cycles is 63.53 (8)°. In the crystal by means of O—H···O type hydrogen bonds the molecules are associated in sheets perpendicular to crystallographic axis *b* (Fig. 2). A few weak C—H···O hydrogen bond interactions have been also detected in the structure (Table 1).

2. Experimental

Single crystals of ((3*aR*,5*S*,6*R*,6*aR*)-5-((*R*)-1,2-dihydroxyethyl)-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)methyl methanesulfonate were grown from a dichloromethane solution by a slow evaporation at ambient temperature. ¹H-NMR and ¹³C-NMR spectra were recorded at 300 MHz and at 75.5 MHz, respectively. The proton signals for residual non-deuterated solvents (δ 7.26 for CHCl₃) and carbon signals (δ 77.1 for CDCl₃) were used as the internal references for ¹H-NMR and ¹³C-NMR spectra, respectively. Coupling constants are reported in Hz. Analytical thin layer chromatography (TLC) was performed on Kieselgel 60 F254 glass plates precoated with a 0.25 mm thickness of silica gel. 2*M* aqueous solution of H₂SO₄ (1 ml, 2.0 mmol, 0.5 equiv.) was added to a solution of 1,2,5,6-di-*O*-isopropylidene-3-deoxy-3-mesyloxymethyl- α -*D*-allofuranose (1.46 g, 4.1 mmol, 1.0 equiv.) in a mixture of MeOH (11 ml) and DCM (4 ml). The resulting reaction mixture was stirred at 50 °C for 1.5 h (TLC control). The reaction mixture was quenched with saturated aqueous solution of NaHCO₃ (10 ml) and organic solvents were evaporated under reduced pressure. Ethyl acetate (50 ml) was added, the layers were separated, and the organic layer was washed with brine (3 × 10 ml), dried over Na₂SO₄, filtered and evaporated. Crystallization of the crude product from DCM yielded analytically pure mesylate (1.24 g, 96%) as a white solid. *M.p.* 103–104°C (DCM), *R*_f=0.16 (hexanes/EtOAc 1:3), ¹H-NMR (CDCl₃, 300 MHz): 1.34 (s, 3H), 1.52 (s, 3H), 2.36 (b.s., 2H), 2.49 (tt, *J*=9.8 Hz, *J*=4.8 Hz, 1H), 3.05 (s, 3H), 3.69 (m, 2H), 3.83 (m, 2H), 4.42 (t, *J*=10.0 Hz, 1H), 4.67 (dd, *J*=10.0 Hz, *J*=5.0 Hz, 1H), 4.77 (t, *J*=4.0 Hz, 1H), 5.83 (d, *J*=3.6 Hz, 1H), ¹³C-NMR (CDCl₃, 75 MHz): 26.4, 26.7, 37.1, 47.5, 63.7, 66.6, 73.3, 78.8, 80.4, 105.0, 112.4, HRMS: Calculated for C₁₁H₂₀O₈NaS [*M*+Na]⁺: 335.0777.

Found $[M+Na]^+$: 335.0736.

3. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All 20 non-hydrogen atoms were refined anisotropically. All hydrogen atoms were positioned geometrically (O—H = 0.82 Å, C—H = 0.93 to 0.98 Å) and refined as riding on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}, \text{O})$ for methyl and oxy groups and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for others.

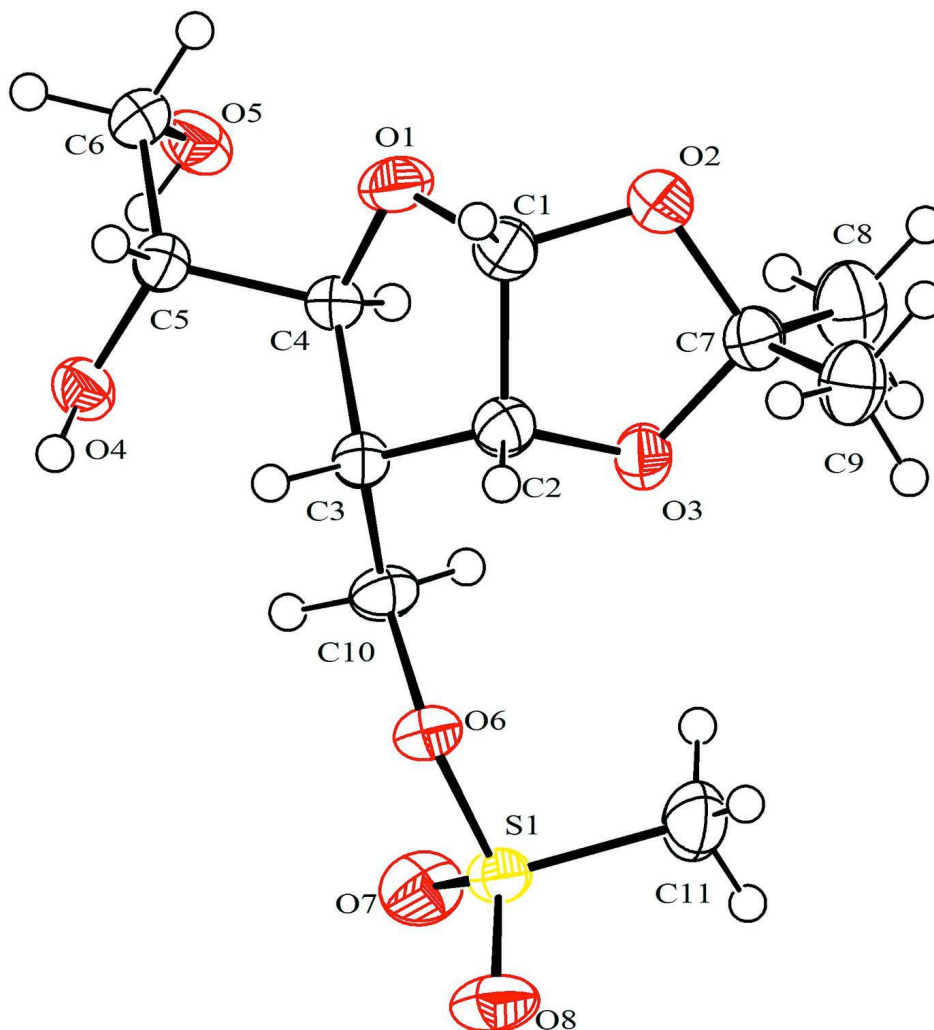
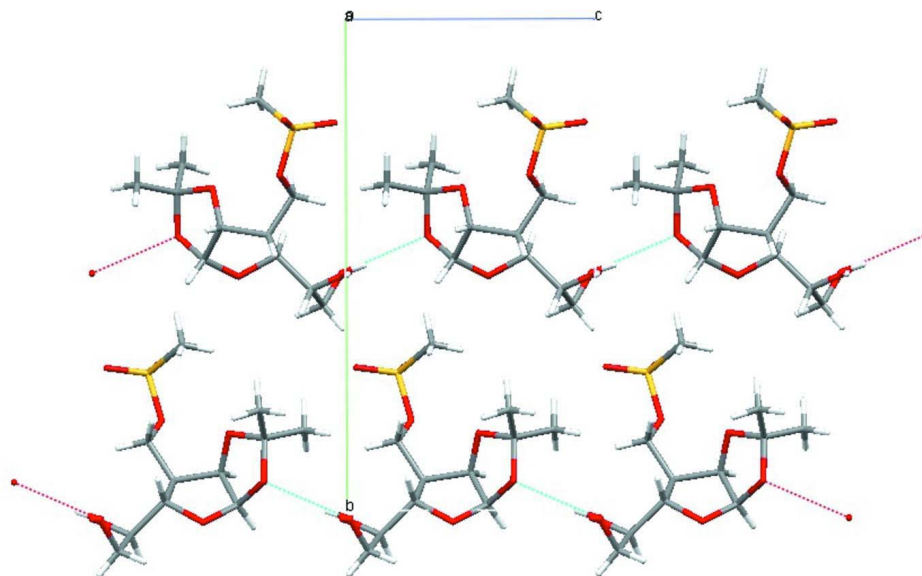


Figure 1

The asymmetric unit of the title compound showing 50% probability displacement ellipsoids and the atom-numbering (hydrogen atoms are shown as small spheres of arbitrary radii)


Figure 2

Packing diagram of the title compound viewed down the *a* axis.

{{(3*aR*,5*S*,6*R*,6*aR*)-5-[(*R*)-1,2-Dihydroxyethyl]-2,2-dimethyltetrahydrofuro[2,3-*d*][1,3]dioxol-6-yl)methyl methanesulfonate

Crystal data

$C_{11}H_{20}O_8S$
 $M_r = 312.33$
 Monoclinic, $P2_1$
 Hall symbol: $P\ 2y_b$
 $a = 5.5794\ (1)\ \text{\AA}$
 $b = 15.6118\ (3)\ \text{\AA}$
 $c = 8.0653\ (2)\ \text{\AA}$
 $\beta = 98.913\ (1)^\circ$
 $V = 694.04\ (3)\ \text{\AA}^3$
 $Z = 2$

$F(000) = 332$
 $D_x = 1.495\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 7583 reflections
 $\theta = 1.0\text{--}27.5^\circ$
 $\mu = 0.27\ \text{mm}^{-1}$
 $T = 293\ \text{K}$
 Prism, colourless
 $0.35 \times 0.30 \times 0.28\ \text{mm}$

Data collection

Nonius KappaCCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 CCD scans
 5266 measured reflections
 3185 independent reflections

3005 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$
 $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.6^\circ$
 $h = -7 \rightarrow 6$
 $k = -20 \rightarrow 20$
 $l = -10 \rightarrow 10$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.065$
 $S = 1.03$
 3185 reflections
 187 parameters

1 restraint
 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
 $w = 1/[\sigma^2(F_o^2) + (0.0319P)^2 + 0.0938P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 0.16 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.064 (4)
 Absolute structure: Flack (1983), 1528 Friedel pairs
 Absolute structure parameter: 0.00 (5)

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 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>	$U_{\text{iso}}^*/U_{\text{eq}}$
C9	0.0490 (4)	0.33494 (13)	-0.8352 (2)	0.0407 (4)
H9A	0.1797	0.3741	-0.8422	0.061*
H9B	-0.0757	0.3429	-0.9302	0.061*
H9C	0.1083	0.2772	-0.8345	0.061*
C7	-0.0536 (3)	0.35157 (11)	-0.6762 (2)	0.0316 (3)
C8	-0.2632 (4)	0.29425 (14)	-0.6553 (2)	0.0470 (5)
H8A	-0.2092	0.2358	-0.6465	0.071*
H8B	-0.3882	0.3003	-0.7507	0.071*
H8C	-0.3262	0.3100	-0.5554	0.071*
S1	0.60651 (6)	0.22002 (2)	-0.20810 (5)	0.02715 (10)
O4	0.22882 (19)	0.51605 (8)	0.01079 (13)	0.0303 (2)
H41	0.3738	0.5199	0.0049	0.046*
O1	-0.0420 (3)	0.52359 (9)	-0.43022 (15)	0.0465 (4)
O6	0.55516 (19)	0.31615 (7)	-0.26299 (14)	0.0278 (2)
O3	0.1263 (2)	0.34259 (7)	-0.53311 (14)	0.0347 (3)
O5	-0.27358 (19)	0.51658 (8)	-0.01728 (15)	0.0364 (3)
H51	-0.1929	0.5014	0.0716	0.055*
O2	-0.1278 (2)	0.44075 (9)	-0.67350 (16)	0.0396 (3)
O8	0.8446 (2)	0.20376 (8)	-0.24301 (17)	0.0427 (3)
O7	0.5551 (2)	0.20875 (9)	-0.04236 (15)	0.0426 (3)
C10	0.3456 (3)	0.35774 (10)	-0.2075 (2)	0.0284 (3)
H10A	0.3819	0.3718	-0.0891	0.034*
H10B	0.2063	0.3198	-0.2244	0.034*
C3	0.2921 (3)	0.43831 (10)	-0.31045 (18)	0.0247 (3)
H3	0.4270	0.4787	-0.2833	0.030*
C1	0.0500 (3)	0.48807 (11)	-0.5677 (2)	0.0329 (4)
H1	0.1185	0.5329	-0.6313	0.039*
C6	-0.1460 (3)	0.58175 (10)	-0.0923 (2)	0.0335 (4)
H6A	-0.1128	0.6293	-0.0147	0.040*
H6B	-0.2477	0.6028	-0.1925	0.040*
C4	0.0556 (3)	0.48076 (10)	-0.2760 (2)	0.0276 (3)

H4	-0.0583	0.4370	-0.2493	0.033*
C2	0.2447 (3)	0.42291 (10)	-0.49929 (19)	0.0277 (3)
H2	0.3917	0.4282	-0.5511	0.033*
C5	0.0908 (3)	0.54919 (10)	-0.13860 (19)	0.0266 (3)
H5	0.1789	0.5976	-0.1777	0.032*
C11	0.3976 (3)	0.16137 (13)	-0.3475 (3)	0.0445 (4)
H11A	0.4188	0.1014	-0.3237	0.067*
H11B	0.4233	0.1724	-0.4605	0.067*
H11C	0.2358	0.1781	-0.3348	0.067*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C9	0.0485 (10)	0.0442 (10)	0.0313 (9)	-0.0040 (8)	0.0124 (8)	-0.0070 (8)
C7	0.0347 (8)	0.0323 (8)	0.0268 (7)	0.0030 (7)	0.0017 (6)	-0.0024 (7)
C8	0.0445 (11)	0.0566 (13)	0.0421 (11)	-0.0097 (9)	0.0132 (8)	-0.0093 (9)
S1	0.02425 (17)	0.02403 (17)	0.03312 (19)	0.00244 (15)	0.00429 (13)	0.00247 (17)
O4	0.0234 (5)	0.0375 (6)	0.0295 (6)	0.0003 (5)	0.0024 (4)	-0.0030 (5)
O1	0.0576 (8)	0.0472 (8)	0.0306 (6)	0.0302 (7)	-0.0062 (5)	-0.0066 (6)
O6	0.0260 (5)	0.0252 (5)	0.0333 (6)	0.0046 (4)	0.0078 (4)	0.0031 (5)
O3	0.0438 (7)	0.0268 (6)	0.0298 (6)	0.0021 (5)	-0.0061 (5)	-0.0033 (5)
O5	0.0227 (5)	0.0496 (7)	0.0359 (6)	0.0025 (5)	0.0013 (4)	-0.0006 (6)
O2	0.0408 (7)	0.0384 (7)	0.0356 (7)	0.0089 (5)	-0.0061 (5)	-0.0052 (5)
O8	0.0284 (6)	0.0370 (7)	0.0640 (8)	0.0093 (5)	0.0112 (5)	0.0074 (6)
O7	0.0536 (7)	0.0392 (7)	0.0362 (6)	0.0050 (6)	0.0101 (5)	0.0113 (6)
C10	0.0281 (7)	0.0300 (8)	0.0287 (8)	0.0076 (6)	0.0093 (6)	0.0022 (6)
C3	0.0228 (7)	0.0248 (7)	0.0262 (7)	0.0009 (6)	0.0032 (5)	-0.0018 (6)
C1	0.0379 (9)	0.0309 (8)	0.0283 (8)	0.0032 (7)	0.0003 (7)	0.0005 (7)
C6	0.0300 (8)	0.0307 (8)	0.0387 (9)	0.0062 (6)	0.0019 (7)	-0.0090 (7)
C4	0.0253 (7)	0.0273 (7)	0.0288 (8)	0.0047 (6)	-0.0003 (6)	-0.0037 (6)
C2	0.0293 (8)	0.0271 (7)	0.0270 (7)	0.0010 (6)	0.0050 (6)	0.0016 (6)
C5	0.0250 (7)	0.0242 (7)	0.0302 (8)	0.0000 (6)	0.0029 (6)	-0.0032 (6)
C11	0.0392 (10)	0.0399 (10)	0.0536 (11)	-0.0059 (8)	0.0051 (8)	-0.0139 (9)

Geometric parameters (\AA , $^\circ$)

C9—C7	1.506 (2)	O5—H51	0.8200
C9—H9A	0.9600	O2—C1	1.413 (2)
C9—H9B	0.9600	C10—C3	1.511 (2)
C9—H9C	0.9600	C10—H10A	0.9700
C7—O3	1.4140 (19)	C10—H10B	0.9700
C7—O2	1.454 (2)	C3—C2	1.524 (2)
C7—C8	1.503 (3)	C3—C4	1.540 (2)
C8—H8A	0.9600	C3—H3	0.9800
C8—H8B	0.9600	C1—C2	1.528 (2)
C8—H8C	0.9600	C1—H1	0.9800
S1—O7	1.4210 (12)	C6—C5	1.515 (2)
S1—O8	1.4226 (12)	C6—H6A	0.9700
S1—O6	1.5782 (11)	C6—H6B	0.9700
S1—C11	1.7480 (18)	C4—C5	1.530 (2)

O4—C5	1.4230 (18)	C4—H4	0.9800
O4—H41	0.8200	C2—H2	0.9800
O1—C1	1.406 (2)	C5—H5	0.9800
O1—C4	1.442 (2)	C11—H11A	0.9600
O6—C10	1.4669 (17)	C11—H11B	0.9600
O3—C2	1.4238 (19)	C11—H11C	0.9600
O5—C6	1.429 (2)		
C7—C9—H9A	109.5	C10—C3—H3	109.5
C7—C9—H9B	109.5	C2—C3—H3	109.5
H9A—C9—H9B	109.5	C4—C3—H3	109.5
C7—C9—H9C	109.5	O1—C1—O2	112.02 (14)
H9A—C9—H9C	109.5	O1—C1—C2	107.70 (13)
H9B—C9—H9C	109.5	O2—C1—C2	105.27 (13)
O3—C7—O2	104.53 (12)	O1—C1—H1	110.6
O3—C7—C8	108.42 (14)	O2—C1—H1	110.6
O2—C7—C8	109.89 (15)	C2—C1—H1	110.6
O3—C7—C9	111.26 (14)	O5—C6—C5	112.10 (13)
O2—C7—C9	108.93 (14)	O5—C6—H6A	109.2
C8—C7—C9	113.43 (15)	C5—C6—H6A	109.2
C7—C8—H8A	109.5	O5—C6—H6B	109.2
C7—C8—H8B	109.5	C5—C6—H6B	109.2
H8A—C8—H8B	109.5	H6A—C6—H6B	107.9
C7—C8—H8C	109.5	O1—C4—C5	106.85 (12)
H8A—C8—H8C	109.5	O1—C4—C3	105.29 (12)
H8B—C8—H8C	109.5	C5—C4—C3	114.43 (12)
O7—S1—O8	119.66 (8)	O1—C4—H4	110.0
O7—S1—O6	109.11 (7)	C5—C4—H4	110.0
O8—S1—O6	104.40 (7)	C3—C4—H4	110.0
O7—S1—C11	109.17 (10)	O3—C2—C3	109.51 (12)
O8—S1—C11	109.23 (9)	O3—C2—C1	103.57 (12)
O6—S1—C11	104.11 (8)	C3—C2—C1	105.03 (12)
C5—O4—H41	109.5	O3—C2—H2	112.7
C1—O1—C4	111.21 (12)	C3—C2—H2	112.7
C10—O6—S1	117.00 (10)	C1—C2—H2	112.7
C7—O3—C2	108.57 (12)	O4—C5—C6	106.96 (12)
C6—O5—H51	109.5	O4—C5—C4	110.57 (12)
C1—O2—C7	109.55 (12)	C6—C5—C4	113.18 (12)
O6—C10—C3	107.43 (11)	O4—C5—H5	108.7
O6—C10—H10A	110.2	C6—C5—H5	108.7
C3—C10—H10A	110.2	C4—C5—H5	108.7
O6—C10—H10B	110.2	S1—C11—H11A	109.5
C3—C10—H10B	110.2	S1—C11—H11B	109.5
H10A—C10—H10B	108.5	H11A—C11—H11B	109.5
C10—C3—C2	114.00 (13)	S1—C11—H11C	109.5
C10—C3—C4	111.15 (12)	H11A—C11—H11C	109.5
C2—C3—C4	103.12 (12)	H11B—C11—H11C	109.5

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>
O4—H41 \cdots O5 ⁱ	0.82	2.00	2.820 (2)	174
O5—H51 \cdots O2 ⁱⁱ	0.82	2.24	3.009 (2)	156
O5—H51 \cdots O4	0.82	2.49	2.777 (2)	102
C3—H3 \cdots O5 ⁱ	0.98	2.58	3.344 (2)	135
C8—H8C \cdots O6 ⁱⁱⁱ	0.96	2.55	3.486 (2)	165
C9—H9A \cdots O4 ^{iv}	0.96	2.55	3.306 (2)	136
C10—H10A \cdots O4	0.97	2.58	3.160 (2)	118
C11—H11C \cdots O8 ⁱⁱⁱ	0.96	2.44	3.387 (2)	167

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