Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

8-Formyl-4-methyl-2-oxo-2*H*-chromen-7-yl 4-methylbenzenesulfonate

H. Yuvaraj,[a]* D. Gayathri,[b] Rajesh G. Kalkhambkar,[c] Geeta M. Kulkarni[c] and Rajendra M. Bapset[d]

[a]School of Display and Chemical Engineering, Yeungnam University, Gyeongsan, Gyeoungbuk 712-749, Republic of Korea, [b]Department of Physics, Dr. M.G.R. Educational and Research Institute University, Periyar E.V.R. High Road, Maduravoyal, Chennai 600 095, India, [c]Department of Chemistry, Karnatak University's Karnatak Science College, Dharwad 580 001, Karnataka, India, and [d]Department of Chemistry, B.K. College, Belgaum 590 001, Karnataka, India
Correspondence e-mail: yuvraj_pd@yahoo.co.in

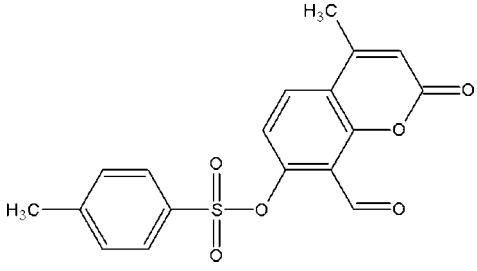
Received 18 April 2011; accepted 18 May 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.043; wR factor = 0.135; data-to-parameter ratio = 17.8.

In the title compound, $C_{18}H_{14}O_6S$, the coumarin ring system is nearly planar, with a maximum out-of-plane deviation of 0.032 (2) Å. The dihedral angle between the benzene ring and the coumarin ring system is 32.41 (8)°. The crystal packing is stabilized by intermolecular C—H···O interactions, generating $C(8)$, $C(10)$ and $C(11)$ chains and an $R_2^2(10)$ ring. The formyl group is disordered over two sets of sites, with occupancies of 0.548 (5) and 0.452 (5).

Related literature

For the biological activity of coumarins, see: Carlton *et al.* (1996); El-Agrody *et al.* (2001); Emmanuel-Giota *et al.* (2001); Kulkarni *et al.* (2006); Kalkhambkar *et al.* (2008); Shaker (1996); Yang *et al.* (2005); Zhou *et al.* (2000). For a related structure, see: Yuvaraj *et al.* (2011).



Experimental

Crystal data

$C_{18}H_{14}O_6S$ M_r = 358.35
Orthorhombic, *Pbca*
a = 17.6174 (7) Å
b = 7.2025 (3) Å
c = 25.7706 (10) Å
V = 3270.0 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 293 K
0.14 × 0.13 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
48911 measured reflections
4234 independent reflections
3095 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.135
S = 1.02
4234 reflections
238 parameters
14 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O6^{i}	0.93	2.56	3.326 (2)	140
C13—H13···O6^{ii}	0.93	2.52	3.343 (2)	148
C16—H16···O2^{iii}	0.93	2.51	3.433 (2)	175

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

HY acknowledges Yeungnam University for the opportunity to work as a Full-Time Foreign Instructor.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2704).

References

Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Carlton, B. D., Aubrun, J. C. & Simon, G. S. (1996). *Fundam. Appl. Toxicol.* **30**, 145–151.
El-Agrody, A. M., Abd El-Latif, M. S., El-Hady, N. A., Fakery, A. H. & Bedair, A. H. (2001). *Molecules*, **6**, 519–527.
Emmanuel-Giota, A. A., Fylaktakidou, K. C., Hadjipavlou-Litina, D. J., Litinas, K. E. & Nicolaides, D. N. (2001). *J. Heterocycl. Chem.* **38**, 717–722.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Kalkhambkar, R.G., Kulkarni, G.M., Kamanavalli, Premkumar, N. Asdaq, S.M.B. & Sun, C.M. (2008). *Eur. J. Med. Chem.* **43**, 2178–2188.
Kulkarni, M. V., Kulkarni, G. M., Lin, C. H. & Sun, C. M. (2006). *Curr. Med. Chem.* **13**, 2795–2818.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Shaker, R. M. (1996). *Pharmazie*, **51**, 148–148.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yang, H., Protiva, P., Gil, R. R., Jiang, B., Baggett, S., Basile, M. J., Reynertson, K. A., Weinstein, I. B. & Kennelly, E. J. (2005). *Planta Med.* **71**, 852–60.
Yuvaraj, H., Gayathri, D., Kalkhambkar, R. G., Kulkarni, G. M. & Bapset, R. M. (2011). *Acta Cryst.* E**67**, o323.
Zhou, P., Takaishi, Y. & Duan, H. (2000). *Phytochemistry*, **53**, 689–697.

supporting information

Acta Cryst. (2011). E**67**, o1513 [doi:10.1107/S1600536811018927]

8-Formyl-4-methyl-2-oxo-2*H*-chromen-7-yl 4-methylbenzenesulfonate

H. Yuvaraj, D. Gayathri, Rajesh G. Kalkhambkar, Geeta M. Kulkarni and Rajendra M. Bapset

S1. Comment

Coumarins are the class of lactones with extensive occurrence in plants possessing wide range of biological activities (Kulkarni *et al.*, 2006). Many synthetic and naturally occurring coumarins are well documented for their wide range of biological activities such as antibacterial (El-Agrody *et al.*, 2001), antifungal (Shaker, 1996), antioxidant (Yang *et al.*, 2005), analgesic (Kalkhambkar *et al.*, 2008) and anti-inflammatory (Emmanuel-Giota *et al.*, 2001) properties. A large number of natural and semisynthetic coumarin and bicoumarin derivatives have been reported to demonstrate chemopreventive (Carlton *et al.*, 1996) and anti-HIV (Zhou *et al.*, 2000) activities. In view of various biological properties associated with coumarins, we have synthesized the title compound and report here its structure.

The molecular structure of the title compound is shown in Fig.1. Bond lengths and bond angles are comparable with the similar structure (Yuvaraj *et al.*, 2011). Positional disorder has been observed for formyl oxygen atom with C14—O4A and C14—O4B bond lengths being 1.137 (3) and 1.109 (4) Å, respectively. The coumarin ring system is nearly planar with a maximum out-of-plane deviation of 0.032 (2) Å (r.m.s. deviation = 0.021 Å). Dihedral angle between the C2–C7 benzene ring and the C8–C13 benzene ring of the coumarin moeity is 33.3 (1)°. Atoms O6 and C18 lie -0.017 (3) and 0.073 (3) Å, respectively, from the least-squares plane of the atoms (C10/C11/C17/C16/C15/O5, r.m.s. deviation = 0.012 Å). Atom C1 lies 0.030 (4) Å from the least-squares plane of the phenyl ring (r.m.s. deviation = 0.007 Å).

The crystal packing is stabilized by C—H···O intermolecular interactions. C4—H4···O6^{i} interaction generates a helical C(11) chain along the [010] direction. Interactions C13—H13···O6^{ii} and C16—H16···O2^{iii} generate C(8) and C(10) chains, respectively, running along [100]. In addition, the interactions C13—H13···O6^{ii} and C16—H16···O2^{iii} generate an $R_2^2(10)$ ring.

S2. Experimental

A mixture of 8-formyl-7-hydroxy-4-methyl coumarin (6 mmol), *p*-toluenesulfonylchloride (6 mmol) and powdered anhydrous K_2CO_3 (6 mmol) in 20 ml of super dry acetone was stirred in room temperature for 12 h. After the completion of the reaction, the solvent was removed under reduced pressure and separated the solids by filtration. It was then washed with 50 ml of dilute hydrochloric acid, excess of cold water, dried and crystallized from ethanol and dioxan mixture. Yield 80%; Light green crystalline solid (ethanol + dioxan); m.p. 180–182 °C; R_f 0.43 (benzene); IR (KBr) cm^{-1} 1734, 1708, 1303; ^{1}H NMR ($CDCl_3$) δ 2.47 (3*H*, s), 2.51 (3*H*, s), 6.35 (1*H*, s), 7.32 (6*H*, m), 10.34 (1*H*, s); Anal. Calcd. for $C_{18}H_{14}O_6S$: C 60.33, H 3.94; Found: C 60.13, H 3.70.

S3. Refinement

All H-atoms were refined using a riding model, with d(C—H) = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for the aromatic CH, and with d(C—H) = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for the CH_3 group. The formyl group is disordered over two sites with occupancies of 0.548 (5) and 0.452 (5). Atoms O4A and O4B were restrained to be approximately isotropic by an *ISOR*

0.01 command. The distances of C14—O4A and C14—O4B have been restrained to 1.20 (1) Å.

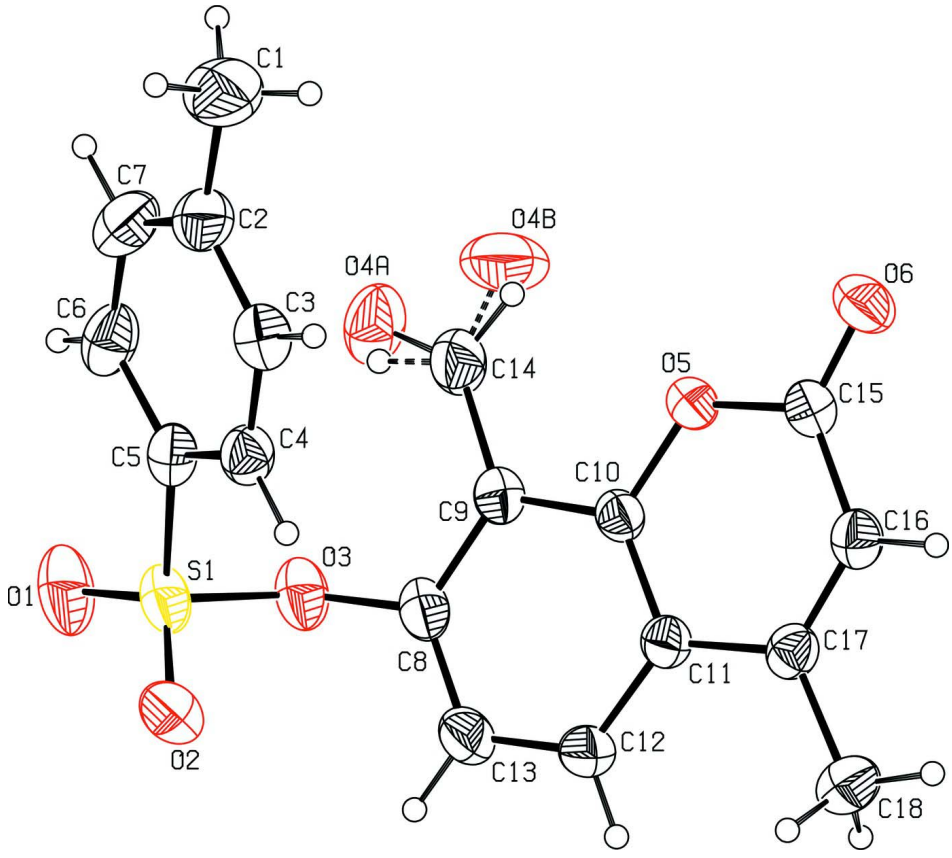


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

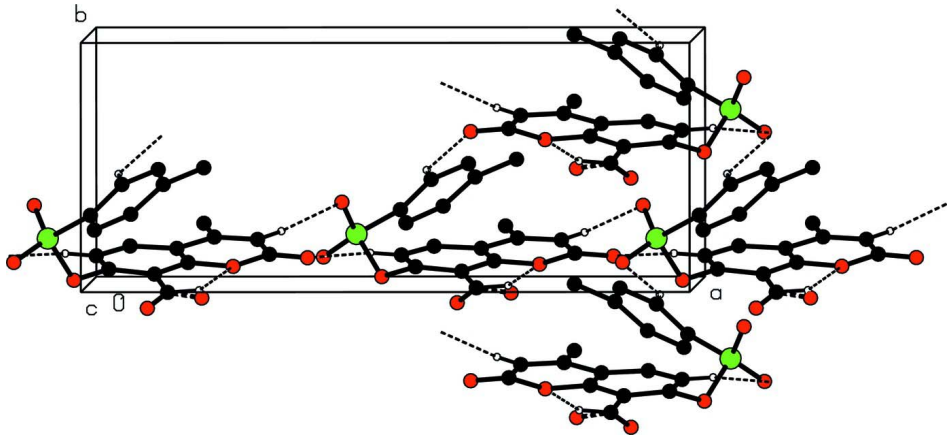


Figure 2

The molecular packing of the title compound, showing the C—H···O interactions (dashed lines). For clarity, hydrogen atoms which are not involved in hydrogen bonding are omitted.

8-Formyl-4-methyl-2-oxo-2*H*-chromen-7-yl 4-methylbenzenesulfonate

Crystal data

$C_{18}H_{14}O_6S$
$M_r = 358.35$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 17.6174$ (7) Å
$b = 7.2025$ (3) Å
$c = 25.7706$ (10) Å
$V = 3270.0$ (2) Å^3
$Z = 8$
$F(000) = 1488$
$D_x = 1.456$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6552 reflections
$\theta = 2.3$–$26.6°$
$\mu = 0.23$ mm^{-1}
$T = 293$ K
Plate, colorless
0.14 × 0.13 × 0.13 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
48911 measured reflections
4234 independent reflections
3095 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 28.7°$, $\theta_{min} = 1.6°$
$h = -23 \rightarrow 23$
$k = -9 \rightarrow 9$
$l = -34 \rightarrow 34$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.135$
$S = 1.02$
4234 reflections
238 parameters
14 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
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 0.8242P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-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 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
C1	0.70245 (18)	0.5004 (5)	0.48070 (11)	0.1076 (9)	
H1A	0.7160	0.4100	0.4550	0.161*	
H1B	0.7446	0.5202	0.5037	0.161*	
H1C	0.6895	0.6152	0.4639	0.161*	
C2	0.63513 (13)	0.4313 (3)	0.51137 (8)	0.0712 (5)	
C3	0.62555 (11)	0.4882 (3)	0.56260 (8)	0.0652 (5)	

H3	0.6605	0.5692	0.5773	0.078*	
C4	0.56508 (10)	0.4264 (3)	0.59184 (7)	0.0585 (4)	
H4	0.5587	0.4663	0.6259	0.070*	
C5	0.51398 (10)	0.3038 (2)	0.56962 (7)	0.0563 (4)	
C6	0.52174 (14)	0.2479 (3)	0.51834 (8)	0.0708 (5)	
H6	0.4866	0.1677	0.5034	0.085*	
C7	0.58218 (16)	0.3130 (3)	0.49004 (8)	0.0791 (6)	
H7	0.5875	0.2763	0.4556	0.095*	
C8	0.54138 (10)	0.0811 (3)	0.67455 (7)	0.0578 (4)	
C9	0.61696 (10)	0.0624 (2)	0.65996 (6)	0.0525 (4)	
C10	0.67090 (9)	0.1065 (2)	0.69784 (6)	0.0472 (3)	
C11	0.65136 (9)	0.1600 (2)	0.74813 (6)	0.0495 (4)	
C12	0.57417 (11)	0.1691 (3)	0.76024 (7)	0.0631 (5)	
H12	0.5595	0.2012	0.7937	0.076*	
C13	0.51960 (10)	0.1319 (3)	0.72389 (8)	0.0680 (5)	
H13	0.4684	0.1408	0.7324	0.082*	
C14	0.63965 (14)	−0.0075 (4)	0.60842 (8)	0.0772 (6)	
H14A	0.6916	0.0009	0.6025	0.093*	0.548 (5)
H14B	0.5992	−0.0394	0.5871	0.093*	0.452 (5)
C15	0.80427 (9)	0.1381 (2)	0.71607 (7)	0.0534 (4)	
C16	0.78344 (10)	0.1945 (2)	0.76774 (7)	0.0550 (4)	
H16	0.8220	0.2264	0.7907	0.066*	
C17	0.71185 (10)	0.2035 (2)	0.78441 (6)	0.0513 (4)	
C18	0.69355 (13)	0.2552 (3)	0.83935 (7)	0.0720 (5)	
H18A	0.7398	0.2772	0.8581	0.108*	
H18B	0.6660	0.1558	0.8555	0.108*	
H18C	0.6631	0.3658	0.8396	0.108*	
O1	0.38782 (9)	0.1146 (3)	0.57769 (7)	0.0957 (6)	
O2	0.41980 (9)	0.3388 (2)	0.64607 (6)	0.0814 (4)	
O3	0.48511 (7)	0.03917 (19)	0.63759 (6)	0.0685 (4)	
O4A	0.60724 (19)	−0.0694 (4)	0.57442 (11)	0.0912 (13)	0.548 (5)
O4B	0.6962 (2)	−0.0293 (10)	0.59052 (17)	0.136 (2)	0.452 (5)
O5	0.74534 (6)	0.09179 (18)	0.68306 (4)	0.0539 (3)	
O6	0.86731 (7)	0.1254 (2)	0.69874 (6)	0.0738 (4)	
S1	0.44287 (3)	0.20842 (8)	0.60799 (2)	0.06651 (18)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.113 (2)	0.114 (2)	0.0953 (18)	0.0111 (18)	0.0263 (16)	0.0339 (16)
C2	0.0815 (14)	0.0662 (12)	0.0660 (11)	0.0140 (10)	0.0039 (10)	0.0138 (10)
C3	0.0622 (11)	0.0601 (10)	0.0735 (12)	0.0003 (9)	−0.0090 (9)	0.0002 (9)
C4	0.0580 (10)	0.0607 (10)	0.0569 (9)	0.0028 (8)	−0.0095 (8)	−0.0079 (8)
C5	0.0581 (9)	0.0538 (9)	0.0570 (9)	0.0043 (8)	−0.0142 (8)	−0.0006 (7)
C6	0.0929 (15)	0.0587 (10)	0.0607 (10)	0.0035 (10)	−0.0224 (10)	−0.0065 (9)
C7	0.1139 (18)	0.0721 (13)	0.0513 (10)	0.0132 (13)	−0.0026 (11)	−0.0005 (9)
C8	0.0468 (8)	0.0596 (10)	0.0671 (10)	−0.0013 (7)	−0.0085 (7)	0.0120 (8)
C9	0.0506 (9)	0.0523 (9)	0.0546 (9)	0.0037 (7)	−0.0045 (7)	0.0034 (7)

C10	0.0425 (8)	0.0477 (8)	0.0513 (8)	0.0046 (6)	−0.0005 (6)	0.0047 (6)
C11	0.0489 (8)	0.0501 (8)	0.0496 (8)	0.0055 (7)	0.0010 (7)	0.0078 (7)
C12	0.0554 (10)	0.0788 (12)	0.0549 (9)	0.0106 (9)	0.0095 (8)	0.0116 (9)
C13	0.0442 (9)	0.0882 (14)	0.0715 (11)	0.0044 (9)	0.0055 (8)	0.0176 (10)
C14	0.0680 (13)	0.0969 (16)	0.0667 (12)	0.0167 (12)	−0.0161 (11)	−0.0185 (11)
C15	0.0473 (8)	0.0543 (9)	0.0588 (9)	0.0035 (7)	−0.0040 (7)	0.0000 (7)
C16	0.0550 (9)	0.0540 (9)	0.0559 (9)	0.0008 (7)	−0.0089 (7)	−0.0021 (7)
C17	0.0589 (9)	0.0468 (8)	0.0483 (8)	0.0035 (7)	−0.0022 (7)	0.0030 (7)
C18	0.0799 (13)	0.0841 (13)	0.0519 (9)	0.0003 (11)	0.0025 (9)	−0.0045 (9)
O1	0.0631 (9)	0.1010 (12)	0.1230 (14)	−0.0170 (8)	−0.0409 (9)	0.0130 (10)
O2	0.0605 (8)	0.0953 (11)	0.0884 (10)	0.0165 (8)	0.0070 (7)	0.0052 (9)
O3	0.0530 (7)	0.0674 (8)	0.0850 (9)	−0.0080 (6)	−0.0181 (6)	0.0112 (7)
O4A	0.111 (3)	0.084 (2)	0.0780 (19)	0.0174 (17)	−0.0341 (17)	−0.0248 (15)
O4B	0.078 (3)	0.241 (6)	0.089 (3)	−0.013 (3)	0.016 (2)	−0.065 (3)
O5	0.0435 (6)	0.0660 (7)	0.0522 (6)	0.0061 (5)	−0.0009 (5)	−0.0045 (5)
O6	0.0454 (7)	0.0988 (11)	0.0773 (9)	0.0045 (7)	0.0020 (6)	−0.0126 (8)
S1	0.0460 (2)	0.0741 (3)	0.0795 (3)	−0.0003 (2)	−0.0156 (2)	0.0070 (2)

Geometric parameters (Å, º)

C1—C2	1.510 (3)	C11—C12	1.397 (2)
C1—H1A	0.9600	C11—C17	1.452 (2)
C1—H1B	0.9600	C12—C13	1.369 (3)
C1—H1C	0.9600	C12—H12	0.9300
C2—C7	1.378 (3)	C13—H13	0.9300
C2—C3	1.393 (3)	C14—O4B	1.109 (4)
C3—C4	1.379 (3)	C14—O4A	1.137 (3)
C3—H3	0.9300	C14—H14A	0.9300
C4—C5	1.385 (2)	C14—H14B	0.9300
C4—H4	0.9300	C15—O6	1.200 (2)
C5—C6	1.388 (3)	C15—O5	1.383 (2)
C5—S1	1.737 (2)	C15—C16	1.440 (2)
C6—C7	1.373 (3)	C16—C17	1.334 (2)
C6—H6	0.9300	C16—H16	0.9300
C7—H7	0.9300	C17—C18	1.499 (2)
C8—C13	1.378 (3)	C18—H18A	0.9600
C8—C9	1.390 (2)	C18—H18B	0.9600
C8—O3	1.407 (2)	C18—H18C	0.9600
C9—C10	1.399 (2)	O1—S1	1.4165 (16)
C9—C14	1.476 (3)	O2—S1	1.4179 (17)
C10—O5	1.3696 (19)	O3—S1	1.6191 (14)
C10—C11	1.395 (2)		
C2—C1—H1A	109.5	C12—C11—C17	124.09 (16)
C2—C1—H1B	109.5	C13—C12—C11	121.44 (17)
H1A—C1—H1B	109.5	C13—C12—H12	119.3
C2—C1—H1C	109.5	C11—C12—H12	119.3
H1A—C1—H1C	109.5	C12—C13—C8	119.21 (17)

H1B—C1—H1C	109.5	C12—C13—H13	120.4
C7—C2—C3	118.6 (2)	C8—C13—H13	120.4
C7—C2—C1	121.8 (2)	O4B—C14—C9	131.8 (3)
C3—C2—C1	119.6 (2)	O4A—C14—C9	133.7 (3)
C4—C3—C2	121.12 (19)	C9—C14—H14A	113.1
C4—C3—H3	119.4	C9—C14—H14B	114.2
C2—C3—H3	119.4	O6—C15—O5	116.59 (16)
C3—C4—C5	118.82 (17)	O6—C15—C16	126.95 (16)
C3—C4—H4	120.6	O5—C15—C16	116.45 (15)
C5—C4—H4	120.6	C17—C16—C15	123.55 (16)
C4—C5—C6	120.96 (19)	C17—C16—H16	118.2
C4—C5—S1	119.03 (14)	C15—C16—H16	118.2
C6—C5—S1	119.89 (16)	C16—C17—C11	118.42 (15)
C7—C6—C5	118.9 (2)	C16—C17—C18	121.31 (17)
C7—C6—H6	120.6	C11—C17—C18	120.27 (16)
C5—C6—H6	120.6	C17—C18—H18A	109.5
C6—C7—C2	121.63 (19)	C17—C18—H18B	109.5
C6—C7—H7	119.2	H18A—C18—H18B	109.5
C2—C7—H7	119.2	C17—C18—H18C	109.5
C13—C8—C9	122.83 (17)	H18A—C18—H18C	109.5
C13—C8—O3	119.04 (16)	H18B—C18—H18C	109.5
C9—C8—O3	118.08 (17)	C8—O3—S1	118.74 (12)
C8—C9—C10	116.10 (16)	C10—O5—C15	121.95 (13)
C8—C9—C14	122.41 (17)	O1—S1—O2	120.07 (11)
C10—C9—C14	121.43 (16)	O1—S1—O3	102.44 (9)
O5—C10—C11	121.05 (14)	O2—S1—O3	107.72 (9)
O5—C10—C9	116.03 (14)	O1—S1—C5	111.62 (10)
C11—C10—C9	122.91 (15)	O2—S1—C5	109.80 (10)
C10—C11—C12	117.44 (16)	O3—S1—C5	103.55 (8)
C10—C11—C17	118.47 (15)		

C7—C2—C3—C4	0.8 (3)	C8—C9—C14—O4B	179.2 (6)
C1—C2—C3—C4	−179.4 (2)	C10—C9—C14—O4B	−3.5 (7)
C2—C3—C4—C5	0.9 (3)	C8—C9—C14—O4A	−7.1 (5)
C3—C4—C5—C6	−2.0 (3)	C10—C9—C14—O4A	170.2 (3)
C3—C4—C5—S1	173.98 (14)	O6—C15—C16—C17	−179.34 (19)
C4—C5—C6—C7	1.5 (3)	O5—C15—C16—C17	0.0 (3)
S1—C5—C6—C7	−174.49 (16)	C15—C16—C17—C11	−2.1 (3)
C5—C6—C7—C2	0.3 (3)	C15—C16—C17—C18	177.28 (18)
C3—C2—C7—C6	−1.4 (3)	C10—C11—C17—C16	1.5 (2)
C1—C2—C7—C6	178.9 (2)	C12—C11—C17—C16	−178.16 (18)
C13—C8—C9—C10	−2.8 (3)	C10—C11—C17—C18	−177.90 (17)
O3—C8—C9—C10	179.68 (15)	C12—C11—C17—C18	2.5 (3)
C13—C8—C9—C14	174.6 (2)	C13—C8—O3—S1	80.5 (2)
O3—C8—C9—C14	−2.9 (3)	C9—C8—O3—S1	−101.90 (18)
C8—C9—C10—O5	−178.68 (15)	C11—C10—O5—C15	−3.4 (2)
C14—C9—C10—O5	3.9 (3)	C9—C10—O5—C15	177.47 (15)
C8—C9—C10—C11	2.2 (2)	O6—C15—O5—C10	−177.79 (16)

C14—C9—C10—C11	−175.20 (18)	C16—C15—O5—C10	2.8 (2)
O5—C10—C11—C12	−179.13 (16)	C8—O3—S1—O1	−175.87 (15)
C9—C10—C11—C12	−0.1 (3)	C8—O3—S1—O2	−48.35 (16)
O5—C10—C11—C17	1.2 (2)	C8—O3—S1—C5	67.94 (15)
C9—C10—C11—C17	−179.74 (15)	C4—C5—S1—O1	169.10 (15)
C10—C11—C12—C13	−1.7 (3)	C6—C5—S1—O1	−14.87 (19)
C17—C11—C12—C13	177.95 (18)	C4—C5—S1—O2	33.42 (17)
C11—C12—C13—C8	1.2 (3)	C6—C5—S1—O2	−150.56 (16)
C9—C8—C13—C12	1.2 (3)	C4—C5—S1—O3	−81.39 (16)
O3—C8—C13—C12	178.67 (18)	C6—C5—S1—O3	94.64 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···O6^{i}	0.93	2.56	3.326 (2)	140
C13—H13···O6^{ii}	0.93	2.52	3.343 (2)	148
C16—H16···O2^{iii}	0.93	2.51	3.433 (2)	175

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