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8-[(Hydrazinylidene)methyl]-4-methyl-2-oxo-2*H*-chromen-7-yl 4-methylbenzenesulfonate

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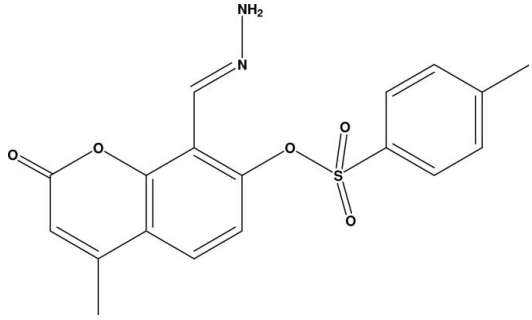
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.116; data-to-parameter ratio = 18.0.

In the title compound, $C_{18}H_{16}N_2O_5S$, the coumarin ring system is nearly planar, with a maximum out-of-plane deviation of 0.078 (1) Å (r.m.s. deviation = 0.046 Å). The dihedral angle between the coumarin ring system and the toluene ring (r.m.s. deviation = 0.004 Å) is 2.77 (1)°. The crystal packing is stabilized by C—H···O and N—H···O intermolecular hydrogen bonds generating $C(8)$, $C(9)$ and $C(11)$ chains and $R_2^2(14)$, $R_2^2(23)$ and $R_4^3(13)$ ring graph sets.

Related literature

For the biological activity of coumarins, see: Kulkarni *et al.* (2006); Kalkhambkar *et al.* (2008); Laakso *et al.* (1994); Nofal *et al.* (2000). For related structures, see: Kokila *et al.* (1995); Vasudevan *et al.* (1990). For graph-set analysis of hydrogen-bond patterns, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{16}N_2O_5S$ M_r = 372.39
Monoclinic, $P2_1/n$
a = 9.1947 (3) Å
b = 16.1867 (4) Å
c = 11.6538 (3) Å
β = 99.670 (1)°
V = 1709.81 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 K
0.2 × 0.19 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
26334 measured reflections
4260 independent reflections
3285 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.116
S = 1.04
4260 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O5^{i}	0.86	2.59	3.303 (2)	141
N2—H2B···O1^{ii}	0.86	2.27	3.045 (2)	150
C10—H10···O4^{iii}	0.93	2.55	3.469 (2)	169
C16—H16A···O4^{ii}	0.96	2.55	3.405 (3)	149
C18—H18···O1^{iv}	0.93	2.53	3.166 (2)	126

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

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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2319).

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8-[(Hydrazinylidene)methyl]-4-methyl-2-oxo-2*H*-chromen-7-yl 4-methylbenzenesulfonate

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

S1. Comment

Coumarins represent a group of naturally occurring lactones, whose potential as anti-inflammatory, anti-microbial, anticancer and protease inhibiting agents has recently been reviewed (Kulkarni *et al.*, 2006). Coumarin derivatives with various substituents at the C-4 position with their biological activities have been reported from our laboratory (Kalkhambkar *et al.*, 2008). Many natural coumarins are reported for their wide range of biological and antitumor properties (Nofal *et al.*, 2000). Solid-state conformations of 4-aryloxymethyl and 4-aryl aminomethyl coumarins have been found to be significantly different. The former exhibits a centro-symmetric nature (Vasudevan *et al.*, 1990) in the solid state, whereas the latter have been found to exhibit a layer like structure stabilized by inter molecular hydrogen bonds (Kokila *et al.*, 1995). In view of biological importance of coumarin we synthesized the title compound and report here its structure.

The molecular structure of the title compound is shown in Fig.1. The coumarin ring system is nearly planar with a maximum out-of-plane deviation of 0.078 (1) Å (r.m.s. deviation = 0.046 Å). The dihedral angle between the coumarin ring system and the toluene ring (r.m.s. deviation = 0.004 Å) is 2.77 (1)°. Atoms O1 and C4 lie 0.066 (2) and 0.005 (2) Å, respectively, below the least-squares plane of the atoms (C1/C2/C3/C5/C6/O2). Atom C16 lies -0.008 (2) Å from the least-squares plane of the ring to which it is attached. Torsion angle C8—C7—C11—N1 (-15.2 (2)°) indicates slight deviation of hydrazonomethyl group from the plane of benzo-ring in coumarin moeity.

The crystal packing is stabilized by N—H···O and C—H···O intermolecular hydrogen bonds. N2—H2A···O5^{i}, C18—H18···O1^{iv}; N2—H2B···O1^{ii}, C16—H16A···O4^{ii} generate chains of C(9), C(11) {along [010]}; C(9), C(8) {along [100]}, respectively. These intermolecular hydrogen bonds, in turn, generate $R_2^2(14)$, $R_2^2(23)$ and $R_4^3(13)$ graph sets (Bernstein *et al.*, 1995) (Table 1, Fig. 2). The crystal packing is further stabilized by C10—H10···O4^{iii} intermolecular hydrogen bond generating C(8) chain along *ac* plane. The glide plane symmetry operation and translation along the *a* axis link the molecules into a three-dimensional network *via* intermolecular hydrogen bonds (Fig. 3).

S2. Experimental

A mixture of toluene-4-sulfonicacid-8-formyl-4-methyl-2-oxo-2*H*-chromen- 7-ylester (6 mmol), and hydrazine hydrate (6 mmol) in 20 ml of ethanol- acetic acid mixture (2:1) was refluxed on water bath for 6 h. Once the reaction was over, the excess of solvent was removed under reduced pressure and filtered the separated solids. The solids were then washed with excess of cold water, dried and crystallized from ethanol and dioxan mixture. Yield: 78%; Colorless crystalline solid (ethanol); mp 160–162 °C; R_f 0.66 (benzene); IR (KBr) cm^{-1} 3405, 1724, 1627, 1341; ^{1}H NMR ($CDCl_3$ + TFA) δ 2.37 (3*H*, s), 2.54 (3*H*, s), 6.47 (1*H*, s), 7.34 (2*H*, s), 7.47 (6*H*, m), 8.68 (1*H*, s); Anal.Calc.for $C_{18}H_{16}N_2O_5S$: C, 58.05; H, 4.33; N, 7.52; Found: C, 57.91; H, 4.20; N, 7.27.

S3. Refinement

All H-atoms were refined using a riding model with d(C—H) = 0.93 Å, U_{iso} = 1.2U_{eq} (C) for aromatic CH, 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3 and 0.86 Å, U_{iso} = 1.2U_{eq} (N) for NH_2 atom.

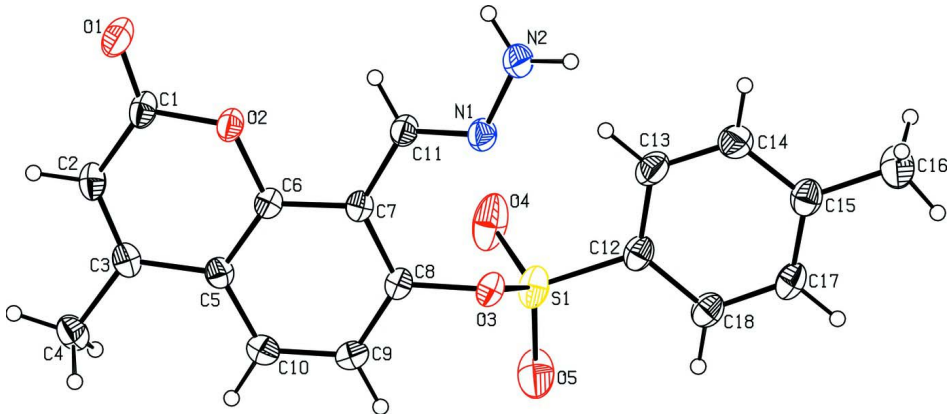

Figure 1

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

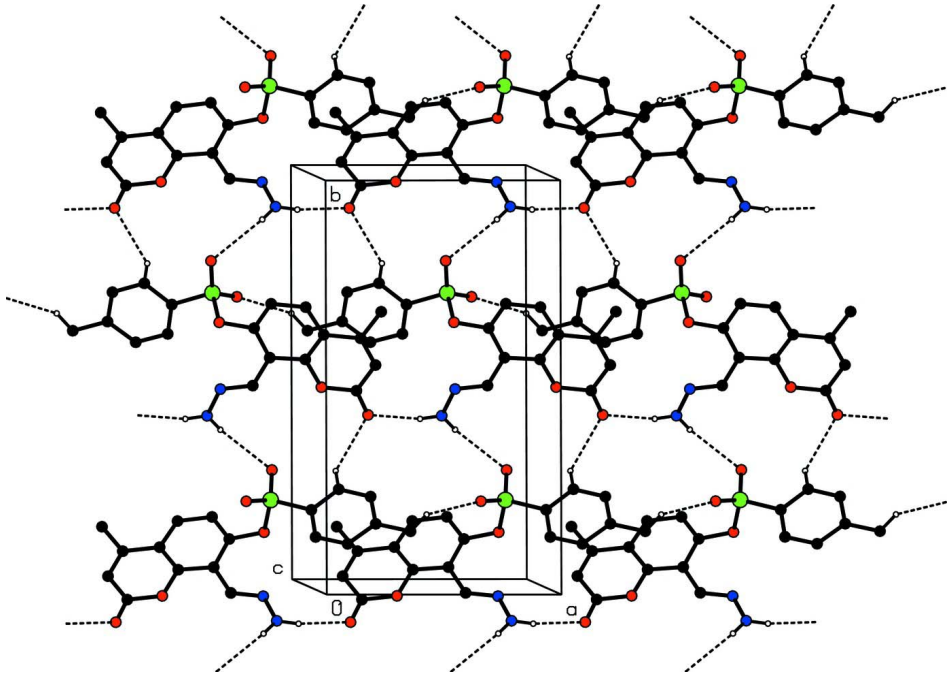

Figure 2

The molecular packing of (I) showing the ring graph sets generated by N—H···O and C—H···O intermolecular interactions. For clarity, hydrogen atoms which are not involved in hydrogen bonding are omitted.

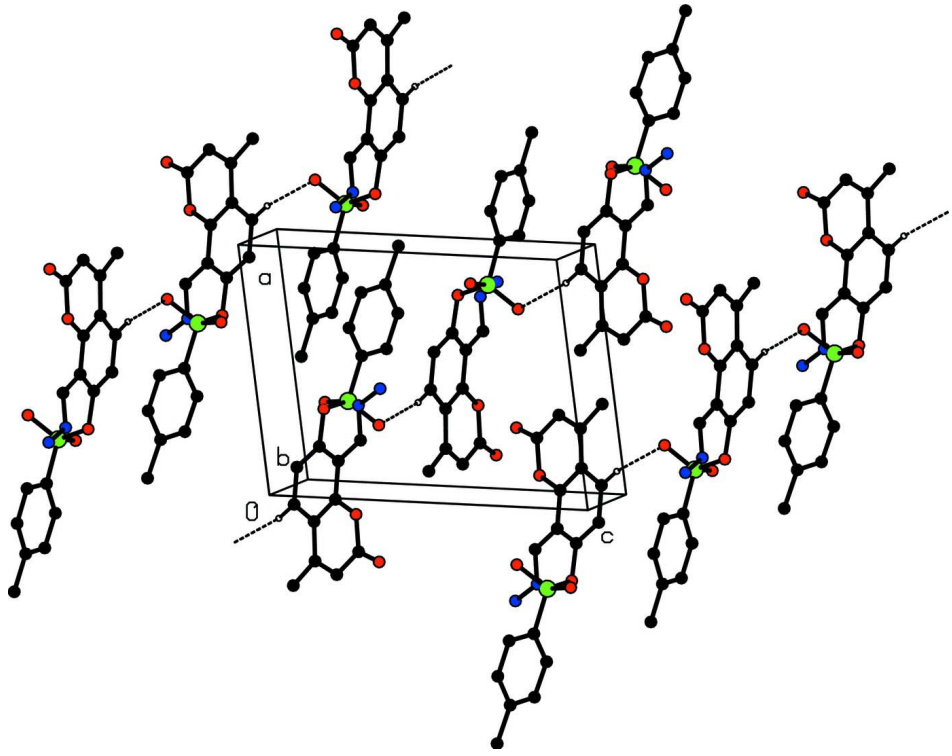

Figure 3

The molecular packing of (I) showing C10—H10···O4 intermolecular interaction. For clarity, hydrogen atoms which are not involved in hydrogen bonding are omitted.

8-[(Hydrazinylidene)methyl]-4-methyl-2-oxo-2*H*-chromen-7-yl 4-methylbenzenesulfonate

Crystal data

$C_{18}H_{16}N_2O_5S$
$M_r = 372.39$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 9.1947\ (3)$ Å
$b = 16.1867\ (4)$ Å
$c = 11.6538\ (3)$ Å
$\beta = 99.670\ (1)°$
$V = 1709.81\ (8)$ Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.447$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7131 reflections
$\theta = 2.2–27.3°$
$\mu = 0.22$ mm^{-1}
$T = 293$ K
Plate, colorless
0.2 × 0.19 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
26334 measured reflections
4260 independent reflections
3285 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.2°$
$h = -12\rightarrow12$
$k = -21\rightarrow21$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.116$
$S = 1.04$
4260 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.5733P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.87241 (5)	0.20073 (3)	0.74789 (4)	0.04805 (14)
O2	0.40215 (11)	−0.02903 (6)	0.69872 (10)	0.0400 (3)
O3	0.83056 (11)	0.12613 (6)	0.65832 (10)	0.0381 (3)
O1	0.21065 (13)	−0.09419 (7)	0.74469 (14)	0.0591 (4)
O4	0.78108 (16)	0.19431 (11)	0.83435 (14)	0.0793 (5)
O5	0.86864 (16)	0.27548 (8)	0.68331 (17)	0.0777 (5)
C11	0.70098 (16)	−0.02353 (9)	0.74255 (14)	0.0371 (3)
H11	0.6508	−0.0599	0.7837	0.045*
C7	0.61790 (16)	0.04122 (9)	0.67270 (13)	0.0330 (3)
C8	0.67779 (16)	0.11089 (9)	0.62748 (13)	0.0357 (3)
C5	0.37380 (16)	0.09308 (9)	0.57881 (13)	0.0355 (3)
C6	0.46285 (16)	0.03608 (9)	0.64762 (13)	0.0331 (3)
C12	1.05418 (18)	0.17468 (10)	0.80513 (14)	0.0409 (4)
C17	1.3108 (2)	0.20553 (11)	0.83220 (17)	0.0488 (4)
H17	1.3876	0.2392	0.8175	0.059*
C2	0.15966 (17)	0.02146 (10)	0.62033 (15)	0.0416 (4)
H2	0.0578	0.0161	0.6127	0.050*
C9	0.59404 (19)	0.16704 (11)	0.55527 (15)	0.0457 (4)
H9	0.6394	0.2107	0.5234	0.055*
C1	0.25173 (17)	−0.03775 (10)	0.69100 (16)	0.0417 (4)
C4	0.11620 (19)	0.14562 (12)	0.49470 (15)	0.0484 (4)
H4A	0.0150	0.1316	0.4958	0.073*
H4B	0.1342	0.1451	0.4159	0.073*
H4C	0.1363	0.1997	0.5272	0.073*
C3	0.21464 (17)	0.08395 (10)	0.56514 (14)	0.0377 (3)

C10	0.44325 (19)	0.15798 (11)	0.53077 (15)	0.0460 (4)
H10	0.3870	0.1955	0.4817	0.055*
C18	1.16766 (19)	0.22511 (11)	0.78238 (16)	0.0453 (4)
H18	1.1480	0.2712	0.7346	0.054*
C14	1.2259 (2)	0.08804 (12)	0.92495 (17)	0.0524 (4)
H14	1.2454	0.0419	0.9725	0.063*
C13	1.0825 (2)	0.10645 (12)	0.87741 (16)	0.0500 (4)
H13	1.0054	0.0736	0.8935	0.060*
C15	1.34283 (19)	0.13723 (11)	0.90328 (16)	0.0468 (4)
C16	1.4988 (2)	0.11716 (14)	0.9572 (2)	0.0643 (5)
H16A	1.5640	0.1583	0.9351	0.096*
H16B	1.5251	0.0640	0.9306	0.096*
H16C	1.5070	0.1164	1.0404	0.096*
N1	0.83982 (14)	−0.03170 (8)	0.74886 (13)	0.0411 (3)
N2	0.90695 (16)	−0.09370 (10)	0.81607 (14)	0.0519 (4)
H2A	0.8559	−0.1258	0.8526	0.062*
H2B	1.0006	−0.1009	0.8222	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0384 (2)	0.0402 (2)	0.0663 (3)	−0.00432 (16)	0.01104 (19)	−0.01826 (19)
O2	0.0273 (5)	0.0324 (5)	0.0604 (7)	0.0000 (4)	0.0079 (5)	0.0048 (5)
O3	0.0329 (5)	0.0358 (6)	0.0473 (6)	−0.0059 (4)	0.0112 (4)	−0.0073 (5)
O1	0.0357 (6)	0.0406 (7)	0.1039 (11)	−0.0001 (5)	0.0202 (7)	0.0154 (7)
O4	0.0507 (8)	0.1124 (13)	0.0803 (10)	−0.0143 (8)	0.0272 (8)	−0.0508 (10)
O5	0.0566 (9)	0.0329 (7)	0.1361 (15)	−0.0016 (6)	−0.0055 (9)	0.0022 (8)
C11	0.0309 (7)	0.0354 (8)	0.0459 (8)	−0.0009 (6)	0.0084 (6)	0.0008 (6)
C7	0.0311 (7)	0.0332 (7)	0.0355 (7)	−0.0003 (5)	0.0076 (6)	−0.0050 (6)
C8	0.0311 (7)	0.0372 (7)	0.0397 (8)	−0.0035 (6)	0.0084 (6)	−0.0034 (6)
C5	0.0339 (7)	0.0374 (8)	0.0352 (7)	0.0020 (6)	0.0052 (6)	−0.0027 (6)
C6	0.0322 (7)	0.0306 (7)	0.0374 (7)	−0.0006 (5)	0.0085 (6)	−0.0039 (6)
C12	0.0398 (8)	0.0394 (8)	0.0445 (8)	−0.0087 (6)	0.0099 (7)	−0.0108 (7)
C17	0.0415 (9)	0.0480 (9)	0.0580 (10)	−0.0150 (7)	0.0116 (8)	−0.0064 (8)
C2	0.0280 (7)	0.0410 (8)	0.0547 (10)	0.0021 (6)	0.0036 (7)	−0.0080 (7)
C9	0.0455 (9)	0.0460 (9)	0.0467 (9)	−0.0046 (7)	0.0107 (7)	0.0116 (7)
C1	0.0297 (7)	0.0334 (8)	0.0632 (10)	−0.0006 (6)	0.0113 (7)	−0.0047 (7)
C4	0.0412 (9)	0.0561 (10)	0.0459 (9)	0.0102 (8)	0.0012 (7)	0.0019 (8)
C3	0.0340 (7)	0.0396 (8)	0.0381 (8)	0.0050 (6)	0.0024 (6)	−0.0083 (6)
C10	0.0442 (9)	0.0485 (10)	0.0442 (9)	0.0033 (7)	0.0040 (7)	0.0109 (7)
C18	0.0466 (9)	0.0379 (8)	0.0518 (10)	−0.0106 (7)	0.0093 (7)	−0.0047 (7)
C14	0.0549 (11)	0.0502 (10)	0.0505 (10)	−0.0092 (8)	0.0040 (8)	0.0042 (8)
C13	0.0498 (10)	0.0508 (10)	0.0505 (10)	−0.0173 (8)	0.0116 (8)	−0.0010 (8)
C15	0.0433 (9)	0.0492 (10)	0.0481 (9)	−0.0063 (7)	0.0079 (7)	−0.0097 (7)
C16	0.0479 (11)	0.0686 (13)	0.0739 (14)	−0.0012 (9)	0.0030 (10)	−0.0027 (11)
N1	0.0321 (6)	0.0398 (7)	0.0513 (8)	0.0020 (5)	0.0070 (6)	0.0035 (6)
N2	0.0338 (7)	0.0548 (9)	0.0668 (10)	0.0064 (6)	0.0074 (7)	0.0177 (7)

Geometric parameters (Å, º)

S1—O4	1.4197 (15)	C2—C3	1.342 (2)
S1—O5	1.4222 (16)	C2—C1	1.442 (2)
S1—O3	1.6003 (11)	C2—H2	0.9300
S1—C12	1.7441 (17)	C9—C10	1.376 (2)
O2—C6	1.3742 (18)	C9—H9	0.9300
O2—C1	1.3781 (18)	C4—C3	1.497 (2)
O3—C8	1.4119 (18)	C4—H4A	0.9600
O1—C1	1.203 (2)	C4—H4B	0.9600
C11—N1	1.2732 (19)	C4—H4C	0.9600
C11—C7	1.461 (2)	C10—H10	0.9300
C11—H11	0.9300	C18—H18	0.9300
C7—C8	1.397 (2)	C14—C13	1.374 (3)
C7—C6	1.409 (2)	C14—C15	1.395 (2)
C8—C9	1.382 (2)	C14—H14	0.9300
C5—C6	1.394 (2)	C13—H13	0.9300
C5—C10	1.395 (2)	C15—C16	1.501 (3)
C5—C3	1.453 (2)	C16—H16A	0.9600
C12—C18	1.385 (2)	C16—H16B	0.9600
C12—C13	1.387 (2)	C16—H16C	0.9600
C17—C15	1.383 (3)	N1—N2	1.3561 (19)
C17—C18	1.384 (3)	N2—H2A	0.8600
C17—H17	0.9300	N2—H2B	0.8600
O4—S1—O5	118.24 (11)	O1—C1—C2	126.59 (15)
O4—S1—O3	107.55 (8)	O2—C1—C2	117.10 (14)
O5—S1—O3	108.36 (9)	C3—C4—H4A	109.5
O4—S1—C12	110.73 (10)	C3—C4—H4B	109.5
O5—S1—C12	110.17 (9)	H4A—C4—H4B	109.5
O3—S1—C12	100.20 (7)	C3—C4—H4C	109.5
C6—O2—C1	121.77 (12)	H4A—C4—H4C	109.5
C8—O3—S1	114.70 (9)	H4B—C4—H4C	109.5
N1—C11—C7	122.14 (14)	C2—C3—C5	118.53 (14)
N1—C11—H11	118.9	C2—C3—C4	121.58 (15)
C7—C11—H11	118.9	C5—C3—C4	119.84 (15)
C8—C7—C6	114.76 (13)	C9—C10—C5	120.70 (15)
C8—C7—C11	125.94 (13)	C9—C10—H10	119.7
C6—C7—C11	119.30 (13)	C5—C10—H10	119.7
C9—C8—C7	123.11 (14)	C17—C18—C12	118.61 (17)
C9—C8—O3	117.97 (13)	C17—C18—H18	120.7
C7—C8—O3	118.91 (13)	C12—C18—H18	120.7
C6—C5—C10	117.71 (14)	C13—C14—C15	121.31 (18)
C6—C5—C3	118.63 (14)	C13—C14—H14	119.3
C10—C5—C3	123.60 (14)	C15—C14—H14	119.3
O2—C6—C5	120.98 (13)	C14—C13—C12	119.15 (16)
O2—C6—C7	115.20 (13)	C14—C13—H13	120.4
C5—C6—C7	123.80 (14)	C12—C13—H13	120.4

C18—C12—C13	121.00 (16)	C17—C15—C14	118.17 (17)
C18—C12—S1	119.25 (14)	C17—C15—C16	121.05 (17)
C13—C12—S1	119.67 (13)	C14—C15—C16	120.78 (18)
C15—C17—C18	121.75 (16)	C15—C16—H16A	109.5
C15—C17—H17	119.1	C15—C16—H16B	109.5
C18—C17—H17	119.1	H16A—C16—H16B	109.5
C3—C2—C1	122.85 (14)	C15—C16—H16C	109.5
C3—C2—H2	118.6	H16A—C16—H16C	109.5
C1—C2—H2	118.6	H16B—C16—H16C	109.5
C10—C9—C8	119.70 (15)	C11—N1—N2	117.71 (14)
C10—C9—H9	120.2	N1—N2—H2A	120.0
C8—C9—H9	120.2	N1—N2—H2B	120.0
O1—C1—O2	116.30 (15)	H2A—N2—H2B	120.0
O4—S1—O3—C8	42.38 (14)	C7—C8—C9—C10	3.9 (3)
O5—S1—O3—C8	−86.51 (12)	O3—C8—C9—C10	−174.80 (15)
C12—S1—O3—C8	158.10 (11)	C6—O2—C1—O1	−175.70 (15)
N1—C11—C7—C8	−15.2 (2)	C6—O2—C1—C2	4.0 (2)
N1—C11—C7—C6	165.64 (15)	C3—C2—C1—O1	178.45 (18)
C6—C7—C8—C9	−5.4 (2)	C3—C2—C1—O2	−1.2 (2)
C11—C7—C8—C9	175.39 (15)	C1—C2—C3—C5	−1.0 (2)
C6—C7—C8—O3	173.29 (13)	C1—C2—C3—C4	−178.52 (15)
C11—C7—C8—O3	−5.9 (2)	C6—C5—C3—C2	0.7 (2)
S1—O3—C8—C9	72.10 (16)	C10—C5—C3—C2	−176.51 (16)
S1—O3—C8—C7	−106.67 (13)	C6—C5—C3—C4	178.20 (14)
C1—O2—C6—C5	−4.5 (2)	C10—C5—C3—C4	1.0 (2)
C1—O2—C6—C7	173.91 (13)	C8—C9—C10—C5	0.5 (3)
C10—C5—C6—O2	179.38 (14)	C6—C5—C10—C9	−2.9 (2)
C3—C5—C6—O2	2.0 (2)	C3—C5—C10—C9	174.32 (16)
C10—C5—C6—C7	1.1 (2)	C15—C17—C18—C12	0.2 (3)
C3—C5—C6—C7	−176.24 (14)	C13—C12—C18—C17	0.8 (3)
C8—C7—C6—O2	−175.49 (13)	S1—C12—C18—C17	177.42 (13)
C11—C7—C6—O2	3.8 (2)	C15—C14—C13—C12	1.0 (3)
C8—C7—C6—C5	2.9 (2)	C18—C12—C13—C14	−1.3 (3)
C11—C7—C6—C5	−177.88 (14)	S1—C12—C13—C14	−177.96 (14)
O4—S1—C12—C18	−133.39 (14)	C18—C17—C15—C14	−0.5 (3)
O5—S1—C12—C18	−0.71 (17)	C18—C17—C15—C16	−179.64 (18)
O3—S1—C12—C18	113.30 (14)	C13—C14—C15—C17	0.0 (3)
O4—S1—C12—C13	43.30 (17)	C13—C14—C15—C16	179.07 (19)
O5—S1—C12—C13	175.97 (14)	C7—C11—N1—N2	179.96 (14)
O3—S1—C12—C13	−70.01 (14)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O5^{i}	0.86	2.59	3.303 (2)	141
N2—H2*B*···O1^{ii}	0.86	2.27	3.045 (2)	150
C10—H10···O4^{iii}	0.93	2.55	3.469 (2)	169

C16—H16*A*···O4^{ii}	0.96	2.55	3.405 (3)	149
C18—H18···O1^{iv}	0.93	2.53	3.166 (2)	126

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