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(*E*)-Methyl 3-(2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)but-2-enoate

T. Kavitha,[a] M. Thenmozhi,[a] G. Gobi Rajeshwaran,[b] A. K. Mohanakrishnan[b] and M. N. Ponnuswamy[a]*

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, and [b]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: mnpsy2004@yahoo.com

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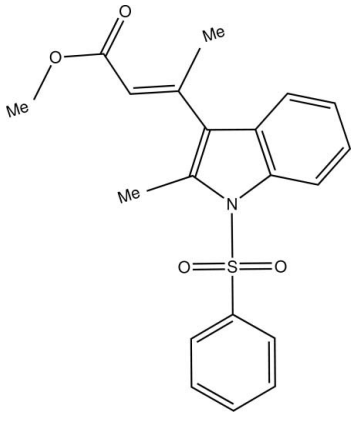
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.137; data-to-parameter ratio = 23.7.

In the title compound, $C_{20}H_{19}NO_4S$, the indole ring system is planar [r.m.s. deviation = 0.023 (2) Å]. The sulfonyl-bound phenyl ring is almost perpendicular to the indole ring system [dihedral angle = 86.75 (7)°]. The ester group is almost planar (r.m.s. deviation = 0.030 Å) and is oriented at an angle of 62.53 (5)° with respect to the indole ring system. Molecules are linked into a two-dimensional network parallel to the *ab* plane by intermolecular C—H···O hydrogen bonds.

Related literature

For the biological activities of indole and its derivatives, see: Chandrakantha *et al.* (1992); Rodriguez *et al.* (1985). For related literature For the configuration at the S atom, see: Bassindale (1984). For the N atom hybridization, see: Beddoes *et al.* (1986).



Experimental

Crystal data

$C_{20}H_{19}NO_4S$
M_r = 369.42
Monoclinic, $P2_1/c$
a = 8.9498 (3) Å
b = 8.8427 (2) Å
c = 23.2836 (7) Å
β = 97.085 (1)°
V = 1828.60 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.957, T_{max} = 0.968
23203 measured reflections
5673 independent reflections
3833 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.137
S = 1.01
5673 reflections
239 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O2^{i}	0.93	2.58	3.391 (2)	146
C13—H13···O3^{ii}	0.93	2.50	3.277 (2)	141

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

TK thanks Dr Babu Varghese, SAIF, IIT-Madras, Chennai, India, for his help with the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2752).

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S1. Comment

Indole and its derivatives have long been known for their chemical and biological activities (Chandrakantha *et al.*, 1992). The indole ring system is present in a number of natural products, many of which are found to possess pharmacological properties like anti-microbial, anti-inflammatory and anti-implantation activities (Rodriguez *et al.*, 1985).

Due to Thorpe–Ignold effect (Bassindale, 1984), bond angles around atom S1 show significant deviation from ideal tetrahedral value, with significant deviations in angles O1—S1—O2 [120.37 (9)°] and N1—S1—C10 [104.96 (6)°]. The indole ring system is essentially planar. The sum of the bond angles around atom N1 (355.9°) indicates sp^2 hybridization (Beddoes *et al.*, 1986). The sulfonyl bound phenyl ring is oriented almost perpendicular to the indole ring system as can be seen from the dihedral angle of 86.75 (7)°. The ester group attached to the indole ring system adopts an extended conformation which is confirmed by the torsion angles C3—C17—C19—C20 = -177.59 (14)°, C17—C19—C20—O4 = -176.02 (15)° and C19—C20—O4—C21 = -178.62 (15)°.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into a two-dimensional network parallel to the *ab* plane (Fig. 2).

S2. Experimental

To a stirred suspension of NaH (29 mg, 1.20 mmol, hexane washed) in THF (5 ml), a solution of vinyl indole (0.23 g, 1 mmol) in THF (5 ml) was added and stirred for 30 min at room temperature. To the reaction mixture, a solution of $PhSO_2Cl$ (0.21 g, 1.20 mmol) was added and stirring was continued for further 6 h. After the indole was consumed (monitored by TLC), the reaction mixture was quenched with cold diluted HCl (25 ml), extracted with ethyl acetate (2 × 10 ml) and dried (Na_2SO_4). Removal of solvent followed by recrystallization (MeOH) afforded yellow crystals of the title compound.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(C) for other H atoms.

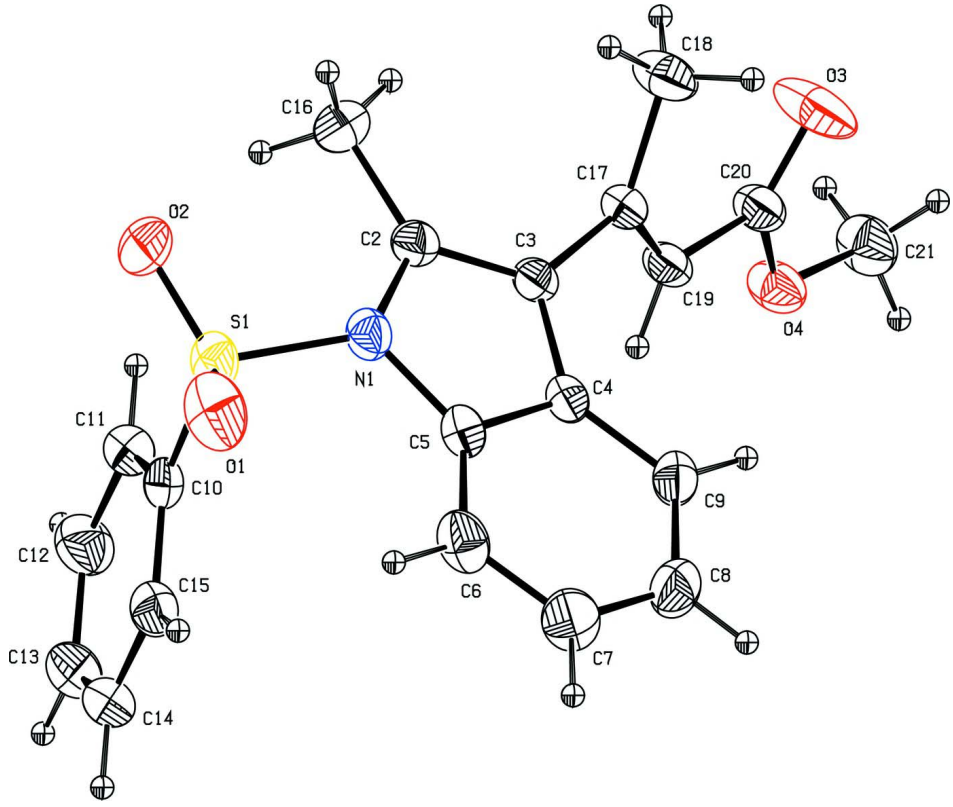

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 20% probability level.

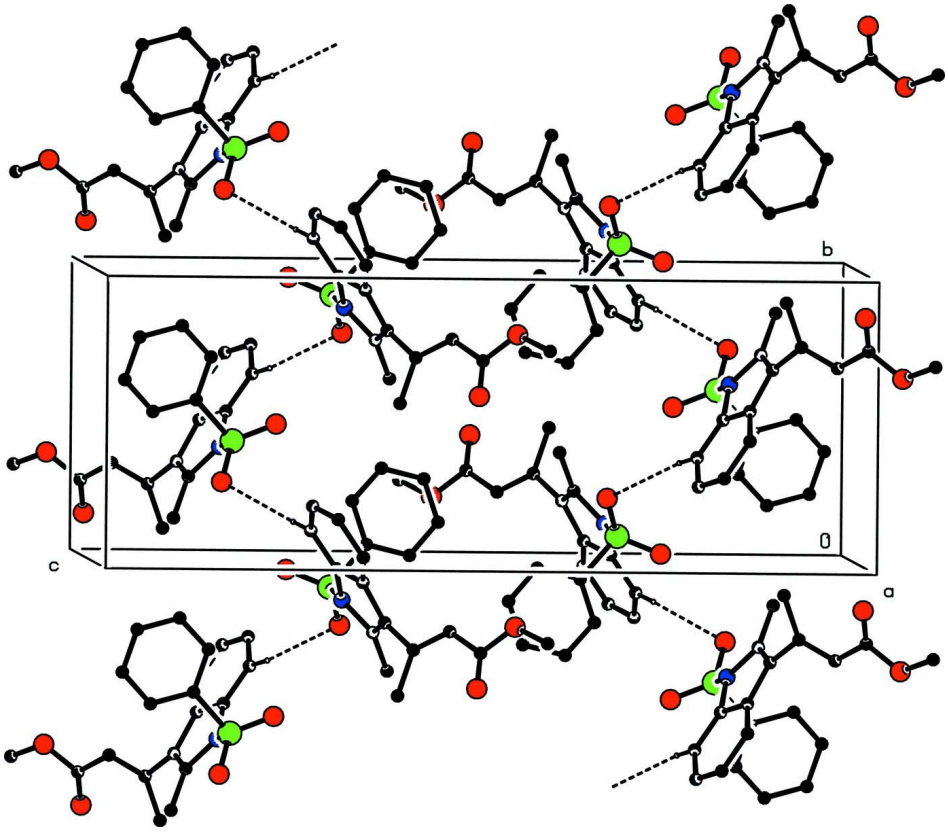

Figure 2

Crystal packing of the title compound, viewed down the *a* axis. H atoms not involved in hydrogen bonding have been omitted for clarity.

(*E*)-Methyl 3-(2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)but-2-enoate

Crystal data

$C_{20}H_{19}NO_4S$
$M_r = 369.42$
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$c = 23.2836\ (7)$ Å
$\beta = 97.085\ (1)°$
$V = 1828.60\ (9)$ Å^3
$Z = 4$
$F(000) = 776$
$D_x = 1.342$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5673 reflections
$\theta = 2.3–31.0°$
$\mu = 0.20$ mm^{-1}
$T = 293$ K
Block, yellow
0.25 × 0.20 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
$T_{min} = 0.957$, $T_{max} = 0.968$
23203 measured reflections
5673 independent reflections
3833 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 31.0°$, $\theta_{min} = 2.3°$
$h = -12\rightarrow11$
$k = -7\rightarrow12$
$l = -32\rightarrow33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.137$
$S = 1.01$
5673 reflections
239 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
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.402P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.016$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0057 (11)

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}
C2	0.71830 (17)	0.73053 (17)	0.13969 (7)	0.0461 (3)
C3	0.85936 (15)	0.68775 (16)	0.13101 (6)	0.0406 (3)
C4	0.89541 (15)	0.54808 (16)	0.16149 (6)	0.0408 (3)
C5	0.77241 (15)	0.50989 (17)	0.19043 (6)	0.0430 (3)
C6	0.77105 (19)	0.3804 (2)	0.22371 (7)	0.0587 (4)
H6	0.6889	0.3562	0.2428	0.070*
C7	0.8966 (2)	0.2887 (2)	0.22744 (8)	0.0703 (5)
H7	0.8983	0.2001	0.2490	0.084*
C8	1.0202 (2)	0.3256 (2)	0.19985 (9)	0.0682 (5)
H8	1.1036	0.2621	0.2036	0.082*
C9	1.02144 (17)	0.45440 (19)	0.16699 (7)	0.0546 (4)
H9	1.1050	0.4786	0.1487	0.065*
C10	0.42383 (15)	0.44900 (18)	0.13523 (7)	0.0462 (3)
C11	0.38591 (18)	0.4876 (2)	0.07757 (7)	0.0550 (4)
H11	0.3946	0.5871	0.0655	0.066*
C12	0.3352 (2)	0.3766 (2)	0.03848 (9)	0.0702 (5)
H12	0.3097	0.4009	−0.0003	0.084*
C13	0.3223 (2)	0.2295 (2)	0.05676 (10)	0.0739 (6)
H13	0.2870	0.1553	0.0302	0.089*
C14	0.3607 (2)	0.1917 (2)	0.11349 (11)	0.0720 (5)
H14	0.3524	0.0919	0.1253	0.086*
C15	0.41202 (19)	0.3013 (2)	0.15350 (9)	0.0598 (4)
H15	0.4382	0.2760	0.1922	0.072*

C16	0.6333 (2)	0.8675 (2)	0.11697 (10)	0.0724 (5)
H16A	0.6151	0.9315	0.1487	0.109*
H16B	0.5389	0.8374	0.0960	0.109*
H16C	0.6911	0.9218	0.0916	0.109*
C17	0.96483 (16)	0.77322 (16)	0.09861 (6)	0.0430 (3)
C18	1.0118 (2)	0.92731 (19)	0.12070 (8)	0.0648 (5)
H18A	1.1128	0.9231	0.1400	0.097*
H18B	0.9452	0.9609	0.1474	0.097*
H18C	1.0074	0.9967	0.0888	0.097*
C19	1.01726 (16)	0.70573 (17)	0.05409 (7)	0.0466 (3)
H19	0.9820	0.6090	0.0444	0.056*
C20	1.12631 (18)	0.77169 (18)	0.01894 (7)	0.0497 (4)
C21	1.2556 (2)	0.7283 (2)	−0.06194 (8)	0.0670 (5)
H21A	1.2073	0.7956	−0.0909	0.101*
H21B	1.2938	0.6419	−0.0804	0.101*
H21C	1.3373	0.7801	−0.0395	0.101*
N1	0.66229 (13)	0.62376 (15)	0.17753 (5)	0.0465 (3)
O1	0.48023 (16)	0.53321 (19)	0.24184 (5)	0.0801 (4)
O2	0.40094 (14)	0.72716 (15)	0.16816 (7)	0.0756 (4)
O3	1.1914 (2)	0.88897 (17)	0.02638 (7)	0.0984 (6)
O4	1.14823 (13)	0.67953 (13)	−0.02447 (5)	0.0583 (3)
S1	0.48136 (4)	0.59233 (5)	0.185184 (18)	0.05532 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0440 (7)	0.0399 (7)	0.0552 (8)	−0.0028 (6)	0.0092 (6)	−0.0070 (6)
C3	0.0391 (7)	0.0365 (7)	0.0464 (7)	−0.0050 (6)	0.0066 (5)	−0.0042 (6)
C4	0.0347 (6)	0.0432 (7)	0.0444 (7)	−0.0066 (6)	0.0039 (5)	−0.0023 (6)
C5	0.0372 (7)	0.0527 (8)	0.0390 (7)	−0.0063 (6)	0.0038 (5)	−0.0022 (6)
C6	0.0520 (9)	0.0750 (12)	0.0489 (8)	−0.0117 (8)	0.0058 (7)	0.0168 (8)
C7	0.0648 (11)	0.0738 (13)	0.0695 (11)	−0.0025 (10)	−0.0021 (9)	0.0318 (10)
C8	0.0492 (9)	0.0664 (12)	0.0872 (13)	0.0085 (9)	0.0006 (9)	0.0222 (10)
C9	0.0373 (7)	0.0568 (10)	0.0698 (10)	0.0002 (7)	0.0074 (7)	0.0080 (8)
C10	0.0295 (6)	0.0496 (8)	0.0607 (9)	0.0002 (6)	0.0104 (6)	−0.0014 (7)
C11	0.0497 (9)	0.0484 (9)	0.0661 (10)	−0.0034 (7)	0.0034 (7)	0.0018 (7)
C12	0.0663 (12)	0.0699 (12)	0.0706 (12)	−0.0108 (10)	−0.0063 (9)	−0.0070 (9)
C13	0.0593 (11)	0.0595 (12)	0.0994 (15)	−0.0112 (9)	−0.0042 (10)	−0.0160 (11)
C14	0.0521 (10)	0.0459 (10)	0.1173 (17)	−0.0077 (8)	0.0082 (10)	0.0056 (10)
C15	0.0433 (8)	0.0582 (10)	0.0782 (11)	−0.0038 (7)	0.0079 (8)	0.0114 (9)
C16	0.0593 (11)	0.0506 (10)	0.1084 (16)	0.0094 (8)	0.0149 (10)	0.0063 (10)
C17	0.0406 (7)	0.0369 (7)	0.0511 (8)	−0.0059 (6)	0.0045 (6)	0.0012 (6)
C18	0.0794 (12)	0.0473 (9)	0.0714 (11)	−0.0209 (9)	0.0234 (9)	−0.0137 (8)
C19	0.0461 (8)	0.0376 (7)	0.0576 (8)	−0.0109 (6)	0.0119 (6)	−0.0019 (6)
C20	0.0513 (8)	0.0421 (8)	0.0574 (9)	−0.0096 (7)	0.0139 (7)	−0.0024 (7)
C21	0.0692 (11)	0.0700 (12)	0.0673 (11)	−0.0114 (9)	0.0306 (9)	−0.0010 (9)
N1	0.0389 (6)	0.0512 (7)	0.0510 (7)	−0.0031 (5)	0.0118 (5)	−0.0068 (5)
O1	0.0728 (8)	0.1164 (12)	0.0584 (7)	−0.0149 (8)	0.0369 (6)	−0.0148 (7)

O2	0.0534 (7)	0.0642 (8)	0.1135 (11)	0.0126 (6)	0.0278 (7)	−0.0269 (8)
O3	0.1299 (14)	0.0687 (9)	0.1106 (12)	−0.0562 (9)	0.0702 (10)	−0.0333 (8)
O4	0.0646 (7)	0.0522 (7)	0.0626 (7)	−0.0135 (6)	0.0255 (5)	−0.0074 (5)
S1	0.0418 (2)	0.0660 (3)	0.0624 (3)	−0.00185 (18)	0.02337 (17)	−0.01782 (19)

Geometric parameters (Å, º)

C2—C3	1.357 (2)	C13—H13	0.93
C2—N1	1.4241 (19)	C14—C15	1.383 (3)
C2—C16	1.493 (2)	C14—H14	0.93
C3—C4	1.441 (2)	C15—H15	0.93
C3—C17	1.4857 (19)	C16—H16A	0.96
C4—C9	1.393 (2)	C16—H16B	0.96
C4—C5	1.4012 (19)	C16—H16C	0.96
C5—C6	1.383 (2)	C17—C19	1.331 (2)
C5—N1	1.415 (2)	C17—C18	1.498 (2)
C6—C7	1.380 (3)	C18—H18A	0.96
C6—H6	0.93	C18—H18B	0.96
C7—C8	1.385 (3)	C18—H18C	0.96
C7—H7	0.93	C19—C20	1.470 (2)
C8—C9	1.373 (2)	C19—H19	0.93
C8—H8	0.93	C20—O3	1.1915 (19)
C9—H9	0.93	C20—O4	1.3315 (19)
C10—C15	1.381 (2)	C21—O4	1.4415 (19)
C10—C11	1.386 (2)	C21—H21A	0.96
C10—S1	1.7540 (16)	C21—H21B	0.96
C11—C12	1.377 (3)	C21—H21C	0.96
C11—H11	0.93	N1—S1	1.6740 (12)
C12—C13	1.378 (3)	O1—S1	1.4202 (14)
C12—H12	0.93	O2—S1	1.4234 (14)
C13—C14	1.365 (3)		
C3—C2—N1	108.20 (13)	C10—C15—H15	120.4
C3—C2—C16	128.09 (15)	C14—C15—H15	120.4
N1—C2—C16	123.67 (14)	C2—C16—H16A	109.5
C2—C3—C4	108.77 (12)	C2—C16—H16B	109.5
C2—C3—C17	126.51 (13)	H16A—C16—H16B	109.5
C4—C3—C17	124.64 (12)	C2—C16—H16C	109.5
C9—C4—C5	119.20 (14)	H16A—C16—H16C	109.5
C9—C4—C3	133.22 (14)	H16B—C16—H16C	109.5
C5—C4—C3	107.57 (13)	C19—C17—C3	118.34 (13)
C6—C5—C4	122.05 (14)	C19—C17—C18	124.36 (14)
C6—C5—N1	130.83 (13)	C3—C17—C18	117.20 (13)
C4—C5—N1	107.12 (13)	C17—C18—H18A	109.5
C7—C6—C5	117.28 (15)	C17—C18—H18B	109.5
C7—C6—H6	121.4	H18A—C18—H18B	109.5
C5—C6—H6	121.4	C17—C18—H18C	109.5
C6—C7—C8	121.55 (17)	H18A—C18—H18C	109.5

C6—C7—H7	119.2	H18B—C18—H18C	109.5
C8—C7—H7	119.2	C17—C19—C20	125.32 (14)
C9—C8—C7	121.06 (17)	C17—C19—H19	117.3
C9—C8—H8	119.5	C20—C19—H19	117.3
C7—C8—H8	119.5	O3—C20—O4	121.87 (14)
C8—C9—C4	118.85 (15)	O3—C20—C19	127.63 (15)
C8—C9—H9	120.6	O4—C20—C19	110.48 (13)
C4—C9—H9	120.6	O4—C21—H21A	109.5
C15—C10—C11	120.80 (16)	O4—C21—H21B	109.5
C15—C10—S1	120.41 (13)	H21A—C21—H21B	109.5
C11—C10—S1	118.76 (12)	O4—C21—H21C	109.5
C12—C11—C10	119.07 (17)	H21A—C21—H21C	109.5
C12—C11—H11	120.5	H21B—C21—H21C	109.5
C10—C11—H11	120.5	C5—N1—C2	108.30 (11)
C11—C12—C13	120.15 (19)	C5—N1—S1	121.12 (10)
C11—C12—H12	119.9	C2—N1—S1	126.50 (11)
C13—C12—H12	119.9	C20—O4—C21	116.60 (13)
C14—C13—C12	120.61 (19)	O1—S1—O2	120.37 (9)
C14—C13—H13	119.7	O1—S1—N1	106.13 (7)
C12—C13—H13	119.7	O2—S1—N1	107.09 (8)
C13—C14—C15	120.24 (18)	O1—S1—C10	108.35 (9)
C13—C14—H14	119.9	O2—S1—C10	108.88 (8)
C15—C14—H14	119.9	N1—S1—C10	104.96 (6)
C10—C15—C14	119.12 (18)		

N1—C2—C3—C4	2.26 (16)	C2—C3—C17—C18	60.7 (2)
C16—C2—C3—C4	179.74 (16)	C4—C3—C17—C18	−115.44 (17)
N1—C2—C3—C17	−174.38 (13)	C3—C17—C19—C20	−177.59 (14)
C16—C2—C3—C17	3.1 (3)	C18—C17—C19—C20	−1.3 (3)
C2—C3—C4—C9	179.15 (16)	C17—C19—C20—O3	5.1 (3)
C17—C3—C4—C9	−4.1 (3)	C17—C19—C20—O4	−176.02 (15)
C2—C3—C4—C5	−1.70 (16)	C6—C5—N1—C2	−178.24 (16)
C17—C3—C4—C5	175.01 (13)	C4—C5—N1—C2	0.92 (15)
C9—C4—C5—C6	−1.0 (2)	C6—C5—N1—S1	−19.6 (2)
C3—C4—C5—C6	179.68 (14)	C4—C5—N1—S1	159.59 (10)
C9—C4—C5—N1	179.72 (13)	C3—C2—N1—C5	−2.00 (16)
C3—C4—C5—N1	0.44 (15)	C16—C2—N1—C5	−179.62 (15)
C4—C5—C6—C7	−0.1 (2)	C3—C2—N1—S1	−159.21 (11)
N1—C5—C6—C7	178.98 (16)	C16—C2—N1—S1	23.2 (2)
C5—C6—C7—C8	1.0 (3)	O3—C20—O4—C21	0.4 (3)
C6—C7—C8—C9	−0.9 (3)	C19—C20—O4—C21	−178.62 (15)
C7—C8—C9—C4	−0.3 (3)	C5—N1—S1—O1	50.95 (13)
C5—C4—C9—C8	1.2 (2)	C2—N1—S1—O1	−154.49 (13)
C3—C4—C9—C8	−179.75 (17)	C5—N1—S1—O2	−179.29 (11)
C15—C10—C11—C12	0.4 (2)	C2—N1—S1—O2	−24.73 (14)
S1—C10—C11—C12	−177.57 (14)	C5—N1—S1—C10	−63.66 (12)
C10—C11—C12—C13	0.2 (3)	C2—N1—S1—C10	90.89 (13)
C11—C12—C13—C14	−0.6 (3)	C15—C10—S1—O1	−11.22 (15)

C12—C13—C14—C15	0.6 (3)	C11—C10—S1—O1	166.71 (12)
C11—C10—C15—C14	−0.4 (2)	C15—C10—S1—O2	−143.79 (13)
S1—C10—C15—C14	177.49 (13)	C11—C10—S1—O2	34.14 (14)
C13—C14—C15—C10	−0.1 (3)	C15—C10—S1—N1	101.83 (13)
C2—C3—C17—C19	−122.74 (17)	C11—C10—S1—N1	−80.24 (13)
C4—C3—C17—C19	61.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O2^{i}	0.93	2.58	3.391 (2)	146
C13—H13···O3^{ii}	0.93	2.50	3.277 (2)	141

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