organic compounds

N-[2-(3,4-Dimethoxyphenyl)ethyl]-N-methylnaphthalene-1-sulfonamide

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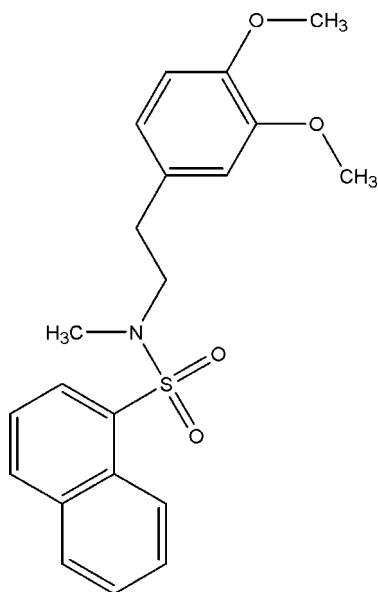
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In the title compound, $C_{21}H_{23}NO_4S$, the dihedral angle between the naphthalene residue and the benzene ring is 7.66 (3)°. In the molecule, there are some short C—H⋯O interactions. In the crystal, the structure is stabilized by weak intramolecular C—H⋯O hydrogen bonds and the crystal structure is stabilized by weak C—H⋯O, C—H⋯π and π–π [centroid–centroid distance = 3.710 (2) Å] interactions.

Related literature

For biological activities of sulfonamide derivatives, see: Schultz et al. (2001); Sheppard (2006); Xiong et al. (2007). For related structures, see: Vennila, Thilagavathi et al. (2008); Vennila, Kavitha et al. (2008).

Experimental

Crystal data

$C_{21}H_{23}NO_4S$	$V = 3872$ (2) Å³
$M_r = 385.46$	$Z = 8$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
$a = 10.070$ (5) Å	$\mu = 0.19$ mm⁻¹
$b = 14.120$ (4) Å	$T = 295$ K
$c = 27.229$ (5) Å	$0.34 \times 0.30 \times 0.28$ mm

Data collection

Bruker Kappa APEXII diffractometer	9215 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	5239 independent reflections
	3248 reflections with $I > 2\sigma(I)$
$T_{min} = 0.937$, $T_{max} = 0.948$	$R_{int} = 0.041$
	Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$	247 parameters
$wR(F^2) = 0.120$	H-atom parameters constrained
$S = 1.01$	$\Delta\rho_{max} = 0.21$ e Å⁻³
5239 reflections	$\Delta\rho_{min} = -0.38$ e Å⁻³

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

$Cg2$ and $Cg3$ are the centroids of the C2–C7 and C14–C19 rings, respectively.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C3—H3⋯O2	0.93	2.53	3.132 (3)	122
C10—H10⋯O1	0.93	2.37	2.804 (3)	109
C11—H11B⋯O2	0.96	2.34	2.821 (3)	110
C4—H4⋯O3ⁱ	0.93	2.46	3.310 (3)	152
C8—H8⋯$Cg3$ⁱⁱ	0.93	2.59	3.488 (3)	163
C20—H20C⋯$Cg2$ⁱⁱⁱ	0.96	2.92	3.740 (3)	144

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

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: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5826).

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supporting information

N-[2-(3,4-Dimethoxyphenyl)ethyl]-*N*-methylnaphthalene-1-sulfonamide

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S1. Comment

In view of the biological activities of sulfonamide derivatives such as insecticidal, antimicrobial and anticancer (Schultz *et al.*, 2001; Sheppard *et al.*, 2006; Xiong *et al.*, 2007), we herewith report the crystal structure of the title compound (I), (Fig. 1). The geometric parameters of the title compound (I) are comparable with the similar reported compounds (Vennila, Thilagavathi *et al.*, 2008; Vennila, Kavitha *et al.*, 2008).

The naphthalene and benzene rings are oriented at an angle of 7.66 (3)°. The molecular structure is stabilized by weak intramolecular C-H···O hydrogen bonds (Table 1) and the crystal structure is formed by weak intermolecular C-H···O (Fig. 2), C-H.*π* (Table 1) and *π*–*π* [Cg1···Cg3 (x,1/2-y,1/2+z) distance 3.710 (2)Å; Cg1 and Cg3 are the centroids of the rings (C1/C2/C7/C8/C9/C10) and (C14-C19), respectively] interactions.

S2. Experimental

About 5.0 g (25 mmol) of [2-(3, 4-dimethoxy-phenyl)-ethyl]-methyl-amine and 6.8 g (30 mmol) of naphthalene-1-sulfonyl chloride were dissolved in 40mL of methylene dichloride. To this mixture, 5.1 g (51 mmol) of triethylamine was added at 298 K. The reaction mixture was warmed to 313 K and maintained at that temperature for 4 to 6 hrs. The completion of the reaction was checked by TLC. The reaction mixture was cooled to 288 K and added 50 mL of water. The organic layer was separated, washed to neutral pH with 5 % aqueous sodium bicarbonate solution, dried over anhydrous sodium sulphate and concentrated. The crude compound was column purified by using petroleum ether and ethyl acetate. Recrystallisation of the compound with the mixture of ethyl acetate and n-heptane mixture yielded colourless crystals of diffraction quality.

S3. Refinement

All H atoms were positioned geometrically with C—H = 0.93–0.97 Å and allowed to ride on their parent atoms with $U_{iso}(H) = 1.2Ueq(C)$ or $1.5Ueq(C_{methyl})$.
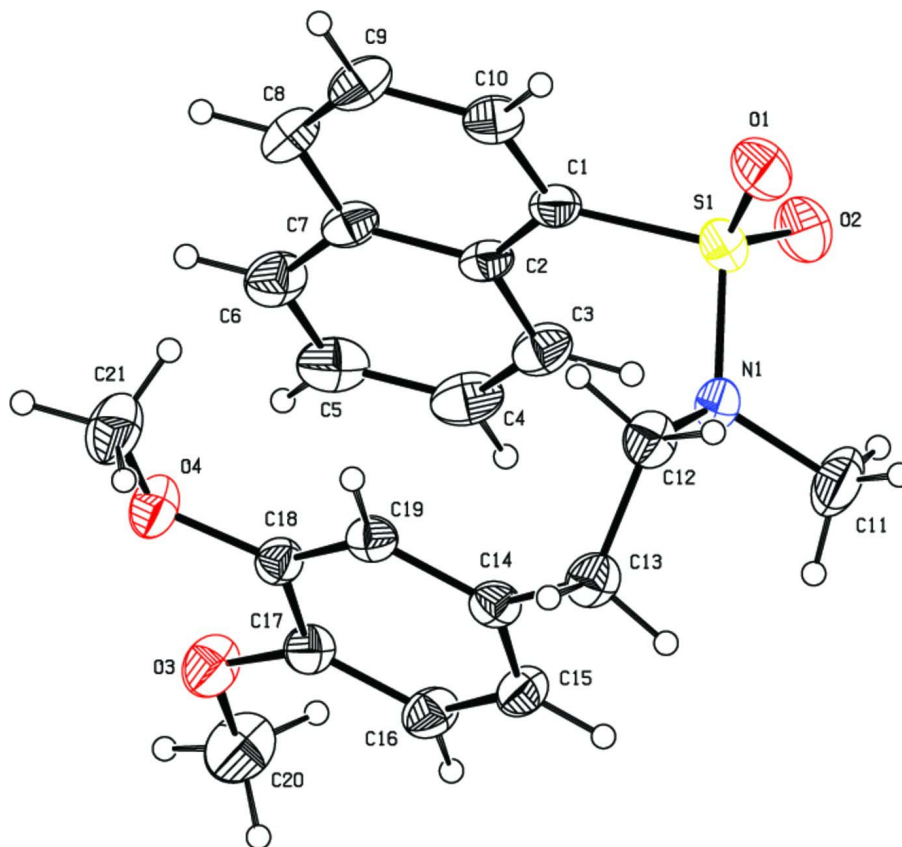
Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.
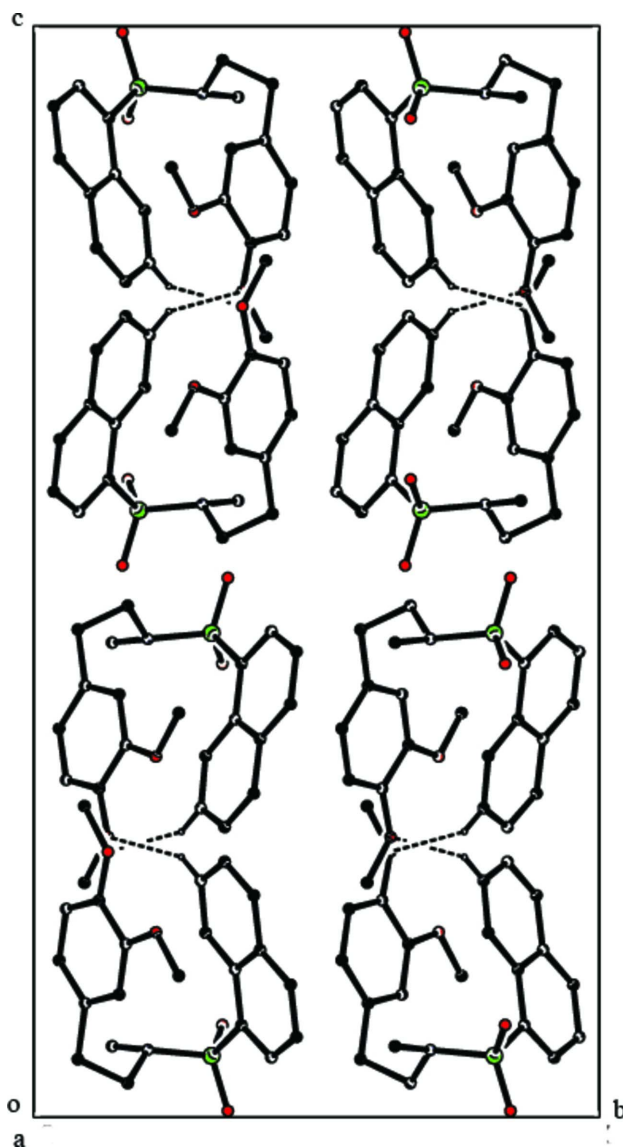
Figure 2

The packing of (I), viewed down the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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$C_{21}H_{23}NO_4S$	$F(000) = 1632$
$M_r = 385.46$	$D_x = 1.323$ Mg m^{-3}
Orthorhombic, *Pbca*	Mo *Kα* radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2ab	Cell parameters from 26403 reflections
$a = 10.070$ (5) Å	$\theta = 2.5–29.3°$
$b = 14.120$ (4) Å	$\mu = 0.19$ mm^{-1}
$c = 27.229$ (5) Å	$T = 295$ K
$V = 3872$ (2) Å^3	Block, colourless
$Z = 8$	$0.34 \times 0.30 \times 0.28$ mm

Data collection

Bruker Kappa APEXII diffractometer	9215 measured reflections
Radiation source: fine-focus sealed tube	5239 independent reflections
Graphite monochromator	3248 reflections with $I > 2\sigma(I)$
ω and φ scans	$R_{int} = 0.041$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 29.3°$, $\theta_{min} = 2.5°$
	$h = -13 \rightarrow 13$
	$k = -10 \rightarrow 19$
$T_{min} = 0.937$, $T_{max} = 0.948$	$l = -36 \rightarrow 37$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.045$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.120$	
$S = 1.01$	H-atom parameters constrained
5239 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2 + 1.1352P]$ where $P = (F_o^2 + 2F_c^2)/3$
247 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.21$ e Å^{-3}
	$\Delta\rho_{min} = -0.38$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
C1	0.92055 (17)	0.36733 (11)	0.08433 (6)	0.0419 (4)
C2	0.94855 (17)	0.35623 (11)	0.13542 (6)	0.0404 (4)
C3	0.8706 (2)	0.30395 (13)	0.16901 (7)	0.0524 (5)
H3	0.7930	0.2749	0.1583	0.063*
C4	0.9080 (2)	0.29561 (14)	0.21685 (7)	0.0623 (6)
H4	0.8551	0.2612	0.2384	0.075*
C5	1.0239 (2)	0.33759 (14)	0.23403 (7)	0.0640 (6)
H5	1.0485	0.3303	0.2667	0.077*
C6	1.1009 (2)	0.38904 (14)	0.20327 (7)	0.0583 (5)
H6	1.1779	0.4173	0.2151	0.070*
C7	1.06558 (19)	0.40032 (12)	0.15342 (6)	0.0463 (4)
C8	1.1458 (2)	0.45408 (13)	0.12135 (8)	0.0586 (5)
H8	1.2222	0.4829	0.1334	0.070*
C9	1.1141 (2)	0.46457 (14)	0.07347 (8)	0.0614 (5)
H9	1.1674	0.5012	0.0531	0.074*
C10	1.0010 (2)	0.42025 (12)	0.05468 (7)	0.0521 (5)
H10	0.9803	0.4268	0.0216	0.063*
C11	0.6973 (2)	0.13869 (18)	0.06506 (9)	0.0765 (7)
H11A	0.6656	0.1242	0.0327	0.115*
H11B	0.6282	0.1695	0.0834	0.115*
H11C	0.7224	0.0812	0.0814	0.115*
C12	0.92293 (19)	0.16608 (13)	0.03129 (6)	0.0498 (4)
H12A	0.9896	0.2153	0.0282	0.060*
H12B	0.8901	0.1516	−0.0014	0.060*
C13	0.98652 (19)	0.07800 (12)	0.05306 (6)	0.0493 (4)

H13A	0.9214	0.0274	0.0533	0.059*
H13B	1.0591	0.0583	0.0320	0.059*
C14	1.03892 (17)	0.09117 (11)	0.10439 (6)	0.0408 (4)
C15	0.98454 (18)	0.04479 (12)	0.14386 (6)	0.0481 (4)
H15	0.9130	0.0042	0.1390	0.058*
C16	1.03471 (19)	0.05758 (12)	0.19086 (6)	0.0496 (4)
H16	0.9955	0.0264	0.2172	0.059*
C17	1.14125 (18)	0.11561 (12)	0.19879 (6)	0.0432 (4)
C18	1.19942 (16)	0.16272 (12)	0.15871 (6)	0.0400 (4)
C19	1.14727 (16)	0.15094 (12)	0.11246 (6)	0.0396 (4)
H19	1.1847	0.1833	0.0861	0.048*
C20	1.1405 (3)	0.08946 (18)	0.28507 (7)	0.0775 (7)
H20A	1.0503	0.1109	0.2878	0.116*
H20B	1.1889	0.1075	0.3140	0.116*
H20C	1.1417	0.0218	0.2818	0.116*
C21	1.3788 (2)	0.25648 (17)	0.12955 (8)	0.0718 (6)
H21A	1.4030	0.2076	0.1068	0.108*
H21B	1.4575	0.2871	0.1415	0.108*
H21C	1.3233	0.3021	0.1133	0.108*
N1	0.81255 (14)	0.20151 (10)	0.06160 (5)	0.0460 (4)
O1	0.78111 (16)	0.34316 (12)	0.00575 (6)	0.0787 (5)
O2	0.66402 (14)	0.33351 (11)	0.08444 (7)	0.0782 (5)
O3	1.20031 (14)	0.13109 (10)	0.24318 (4)	0.0611 (4)
O4	1.30859 (13)	0.21602 (10)	0.16952 (5)	0.0563 (3)
S1	0.78111 (5)	0.31428 (4)	0.056242 (19)	0.05377 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0431 (9)	0.0320 (8)	0.0507 (10)	0.0023 (7)	0.0041 (8)	0.0032 (7)
C2	0.0467 (9)	0.0276 (8)	0.0469 (9)	0.0013 (7)	0.0096 (8)	−0.0001 (7)
C3	0.0557 (11)	0.0467 (11)	0.0549 (11)	−0.0065 (9)	0.0141 (9)	0.0008 (8)
C4	0.0846 (15)	0.0499 (12)	0.0524 (12)	−0.0034 (11)	0.0223 (11)	0.0054 (9)
C5	0.0966 (17)	0.0504 (12)	0.0449 (10)	0.0050 (12)	0.0016 (11)	−0.0040 (9)
C6	0.0765 (14)	0.0458 (11)	0.0526 (11)	−0.0035 (10)	−0.0043 (10)	−0.0114 (9)
C7	0.0569 (11)	0.0311 (9)	0.0510 (10)	−0.0020 (8)	0.0051 (8)	−0.0066 (7)
C8	0.0617 (12)	0.0451 (11)	0.0689 (13)	−0.0199 (9)	0.0048 (10)	−0.0040 (9)
C9	0.0691 (13)	0.0511 (12)	0.0640 (12)	−0.0204 (10)	0.0132 (11)	0.0092 (10)
C10	0.0632 (12)	0.0449 (10)	0.0484 (10)	−0.0020 (9)	0.0045 (9)	0.0100 (8)
C11	0.0538 (13)	0.0750 (16)	0.1008 (18)	−0.0260 (11)	−0.0027 (12)	−0.0060 (13)
C12	0.0542 (11)	0.0564 (11)	0.0389 (9)	−0.0039 (9)	−0.0016 (8)	−0.0026 (8)
C13	0.0562 (11)	0.0451 (10)	0.0467 (10)	−0.0019 (9)	−0.0007 (8)	−0.0122 (8)
C14	0.0465 (9)	0.0346 (8)	0.0413 (9)	0.0060 (7)	0.0008 (7)	−0.0070 (7)
C15	0.0513 (10)	0.0409 (9)	0.0521 (10)	−0.0090 (8)	−0.0017 (9)	−0.0022 (8)
C16	0.0579 (11)	0.0460 (10)	0.0447 (10)	−0.0100 (9)	0.0034 (8)	0.0051 (8)
C17	0.0489 (10)	0.0420 (9)	0.0388 (9)	−0.0004 (8)	−0.0017 (8)	−0.0016 (7)
C18	0.0384 (9)	0.0369 (9)	0.0447 (9)	0.0000 (7)	0.0020 (7)	−0.0030 (7)
C19	0.0416 (9)	0.0367 (9)	0.0405 (9)	0.0037 (7)	0.0068 (7)	−0.0008 (7)

C20	0.1034 (19)	0.0884 (16)	0.0407 (11)	−0.0257 (15)	−0.0018 (12)	0.0064 (11)
C21	0.0554 (12)	0.0881 (17)	0.0717 (14)	−0.0249 (12)	0.0095 (11)	0.0059 (12)
N1	0.0383 (7)	0.0474 (9)	0.0524 (9)	−0.0076 (6)	−0.0042 (6)	0.0007 (7)
O1	0.0816 (11)	0.0849 (11)	0.0697 (10)	−0.0032 (9)	−0.0314 (8)	0.0276 (8)
O2	0.0397 (8)	0.0758 (11)	0.1191 (14)	0.0113 (7)	0.0055 (8)	0.0047 (9)
O3	0.0721 (9)	0.0705 (9)	0.0408 (7)	−0.0192 (7)	−0.0081 (6)	0.0050 (6)
O4	0.0484 (7)	0.0687 (9)	0.0518 (7)	−0.0179 (6)	−0.0003 (6)	0.0008 (6)
S1	0.0413 (2)	0.0552 (3)	0.0648 (3)	0.0029 (2)	−0.0096 (2)	0.0108 (2)

Geometric parameters (Å, °)

C1—C10	1.366 (2)	C12—H12B	0.9700
C1—C2	1.428 (2)	C13—C14	1.506 (2)
C1—S1	1.7656 (19)	C13—H13A	0.9700
C2—C3	1.413 (2)	C13—H13B	0.9700
C2—C7	1.420 (2)	C14—C15	1.372 (2)
C3—C4	1.361 (3)	C14—C19	1.397 (2)
C3—H3	0.9300	C15—C16	1.388 (2)
C4—C5	1.390 (3)	C15—H15	0.9300
C4—H4	0.9300	C16—C17	1.367 (2)
C5—C6	1.353 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—O3	1.365 (2)
C6—C7	1.412 (3)	C17—C18	1.406 (2)
C6—H6	0.9300	C18—O4	1.364 (2)
C7—C8	1.411 (3)	C18—C19	1.375 (2)
C8—C9	1.350 (3)	C19—H19	0.9300
C8—H8	0.9300	C20—O3	1.418 (2)
C9—C10	1.396 (3)	C20—H20A	0.9600
C9—H9	0.9300	C20—H20B	0.9600
C10—H10	0.9300	C20—H20C	0.9600
C11—N1	1.464 (2)	C21—O4	1.418 (2)
C11—H11A	0.9600	C21—H21A	0.9600
C11—H11B	0.9600	C21—H21B	0.9600
C11—H11C	0.9600	C21—H21C	0.9600
C12—N1	1.472 (2)	N1—S1	1.6300 (16)
C12—C13	1.519 (2)	O1—S1	1.4341 (15)
C12—H12A	0.9700	O2—S1	1.4330 (16)
C10—C1—C2	121.23 (16)	C14—C13—H13B	108.7
C10—C1—S1	116.60 (14)	C12—C13—H13B	108.7
C2—C1—S1	122.17 (12)	H13A—C13—H13B	107.6
C3—C2—C7	117.79 (17)	C15—C14—C19	118.48 (16)
C3—C2—C1	125.33 (17)	C15—C14—C13	121.88 (16)
C7—C2—C1	116.87 (15)	C19—C14—C13	119.63 (15)
C4—C3—C2	120.74 (19)	C14—C15—C16	120.98 (17)
C4—C3—H3	119.6	C14—C15—H15	119.5
C2—C3—H3	119.6	C16—C15—H15	119.5
C3—C4—C5	121.16 (19)	C17—C16—C15	120.63 (16)

C3—C4—H4	119.4	C17—C16—H16	119.7
C5—C4—H4	119.4	C15—C16—H16	119.7
C6—C5—C4	120.11 (19)	O3—C17—C16	125.31 (16)
C6—C5—H5	119.9	O3—C17—C18	115.48 (16)
C4—C5—H5	119.9	C16—C17—C18	119.20 (16)
C5—C6—C7	120.8 (2)	O4—C18—C19	124.91 (15)
C5—C6—H6	119.6	O4—C18—C17	115.41 (15)
C7—C6—H6	119.6	C19—C18—C17	119.66 (16)
C8—C7—C6	120.76 (18)	C18—C19—C14	121.04 (15)
C8—C7—C2	119.83 (17)	C18—C19—H19	119.5
C6—C7—C2	119.41 (17)	C14—C19—H19	119.5
C9—C8—C7	121.38 (19)	O3—C20—H20A	109.5
C9—C8—H8	119.3	O3—C20—H20B	109.5
C7—C8—H8	119.3	H20A—C20—H20B	109.5
C8—C9—C10	119.84 (18)	O3—C20—H20C	109.5
C8—C9—H9	120.1	H20A—C20—H20C	109.5
C10—C9—H9	120.1	H20B—C20—H20C	109.5
C1—C10—C9	120.81 (18)	O4—C21—H21A	109.5
C1—C10—H10	119.6	O4—C21—H21B	109.5
C9—C10—H10	119.6	H21A—C21—H21B	109.5
N1—C11—H11A	109.5	O4—C21—H21C	109.5
N1—C11—H11B	109.5	H21A—C21—H21C	109.5
H11A—C11—H11B	109.5	H21B—C21—H21C	109.5
N1—C11—H11C	109.5	C11—N1—C12	115.39 (16)
H11A—C11—H11C	109.5	C11—N1—S1	116.34 (14)
H11B—C11—H11C	109.5	C12—N1—S1	115.37 (12)
N1—C12—C13	112.19 (14)	C17—O3—C20	117.45 (16)
N1—C12—H12A	109.2	C18—O4—C21	117.28 (15)
C13—C12—H12A	109.2	O2—S1—O1	117.38 (10)
N1—C12—H12B	109.2	O2—S1—N1	107.27 (9)
C13—C12—H12B	109.2	O1—S1—N1	111.32 (9)
H12A—C12—H12B	107.9	O2—S1—C1	109.99 (10)
C14—C13—C12	114.14 (14)	O1—S1—C1	107.14 (9)
C14—C13—H13A	108.7	N1—S1—C1	102.78 (8)
C12—C13—H13A	108.7		
C10—C1—C2—C3	179.26 (17)	C15—C16—C17—C18	0.3 (3)
S1—C1—C2—C3	−0.5 (2)	O3—C17—C18—O4	1.2 (2)
C10—C1—C2—C7	−1.8 (2)	C16—C17—C18—O4	−177.34 (16)
S1—C1—C2—C7	178.39 (12)	O3—C17—C18—C19	179.58 (15)
C7—C2—C3—C4	−0.7 (3)	C16—C17—C18—C19	1.0 (3)
C1—C2—C3—C4	178.20 (17)	O4—C18—C19—C14	176.77 (15)
C2—C3—C4—C5	−0.4 (3)	C17—C18—C19—C14	−1.4 (2)
C3—C4—C5—C6	1.0 (3)	C15—C14—C19—C18	0.5 (2)
C4—C5—C6—C7	−0.5 (3)	C13—C14—C19—C18	−178.45 (15)
C5—C6—C7—C8	179.94 (19)	C13—C12—N1—C11	−65.3 (2)
C5—C6—C7—C2	−0.6 (3)	C13—C12—N1—S1	154.41 (12)
C3—C2—C7—C8	−179.36 (17)	C16—C17—O3—C20	−5.1 (3)

C1—C2—C7—C8	1.6 (2)	C18—C17—O3—C20	176.43 (18)
C3—C2—C7—C6	1.2 (2)	C19—C18—O4—C21	−4.9 (3)
C1—C2—C7—C6	−177.81 (16)	C17—C18—O4—C21	173.40 (17)
C6—C7—C8—C9	179.26 (19)	C11—N1—S1—O2	34.67 (17)
C2—C7—C8—C9	−0.2 (3)	C12—N1—S1—O2	174.52 (13)
C7—C8—C9—C10	−1.2 (3)	C11—N1—S1—O1	−95.00 (16)
C2—C1—C10—C9	0.5 (3)	C12—N1—S1—O1	44.86 (15)
S1—C1—C10—C9	−179.67 (15)	C11—N1—S1—C1	150.62 (15)
C8—C9—C10—C1	1.0 (3)	C12—N1—S1—C1	−69.52 (14)
N1—C12—C13—C14	−57.6 (2)	C10—C1—S1—O2	−130.70 (15)
C12—C13—C14—C15	113.75 (19)	C2—C1—S1—O2	49.10 (16)
C12—C13—C14—C19	−67.3 (2)	C10—C1—S1—O1	−2.07 (17)
C19—C14—C15—C16	0.7 (3)	C2—C1—S1—O1	177.73 (14)
C13—C14—C15—C16	179.70 (16)	C10—C1—S1—N1	115.32 (14)
C14—C15—C16—C17	−1.1 (3)	C2—C1—S1—N1	−64.88 (15)
C15—C16—C17—O3	−178.17 (17)		

Hydrogen-bond geometry (Å, º)

*Cg*2 and *Cg*3 are the centroids of the C2–C7 and C14–C19 rings, respectively.

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C3—H3⋯O2	0.93	2.53	3.132 (3)	122
C10—H10⋯O1	0.93	2.37	2.804 (3)	109
C11—H11*B*⋯O2	0.96	2.34	2.821 (3)	110
C4—H4⋯O3[i]	0.93	2.46	3.310 (3)	152
C8—H8⋯*Cg*3[ii]	0.93	2.59	3.488 (3)	163
C20—H20*C*⋯*Cg*2[iii]	0.96	2.92	3.740 (3)	144

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