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Phenyl(1-phenylsulfonyl-1*H*-indol-2-yl)-methanone

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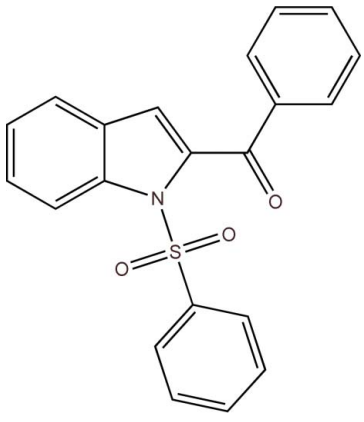
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.138; data-to-parameter ratio = 18.6.

The asymmetric unit of the title compound, $C_{21}H_{15}NO_3S$, contains two crystallographically independent molecules. As a result of the electron-withdrawing character of the phenylsulfonyl groups, the N—Csp^2 bond lengths are slightly longer than the anticipated value of approximately 1.35 Å for N atoms with planar configurations. Both unique S atoms have a distorted tetrahedral configuration. In each molecule, the indole ring system is essentially planar (r.m.s. deviations for all non-H atoms of 0.020 and 0.023 Å). In one molecule, the indole ring system makes dihedral angles of 65.7 (8) and 73.4 (8)°, respectively, with the benzene and phenyl rings [62.2 (7) and 72.1 (7)°, respectively, in the other molecule].

Related literature

For the biological activity of compounds containing an indole ring system, see: Ma *et al.* (2001); Zhou *et al.* (2006); Zhao *et al.* (2002); Williams *et al.* (1993). For related structures, see: Chakkaravarthi *et al.* (2010); Kavitha *et al.* (2010). For a discussion of the geometry at the N atom, see: Beddoes *et al.* (1986). For standard bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{21}H_{15}NO_3S$
M_r = 361.40
Triclinic, $P\overline{1}$
a = 9.3291 (6) Å
b = 11.1498 (7) Å
c = 17.8134 (10) Å
α = 89.433 (3)°
β = 81.623 (2)°
γ = 71.993 (3)°
V = 1742.13 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 293 K
0.25 × 0.22 × 0.19 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.985
30464 measured reflections
8730 independent reflections
6363 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.138
S = 0.99
8730 reflections
470 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2081).

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supporting information

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S1. Comment

The indole ring system is present in a number of natural products, many of which are found to possess anticancer, antimalarial and antihypertensive activities (Ma *et al.*, 2001; Zhou *et al.*, 2006; Zhao *et al.*, 2002). In addition, phenylsulfonyl indole compounds inhibit the HIV-1 RT enzyme *in vitro* and HTLVIIIb viral spread in MT-4 human T-lymphoid cells (Williams *et al.*, 1993). Sulfonamide derivates are well known drugs and are used to control diseases caused by bacterial infections. Against this background and in order to obtain detailed information on molecular conformations in the solid state, an X-ray study of the title compound was carried out.

X-Ray analysis confirms the molecular structure and atom connectivity as illustrated in Fig. 1. The bond lengths and angles in (Fig. 1) agree with those observed in other phenylsulfonylindoles (Chakkaravarthi *et al.*, 2010). In both the molecules, the indole ring systems are essentially planar, with r.m.s. deviation of 0.028 and 0.034Å for atoms C6 and C6′. In both the molecules, the sum of bond angles around N1[359.1 (11)°] of the pyrrole ring is in accordance with sp^3 hybridization (Beddoes *et al.*, 1986). In molecule A, indole ring system make the dihedral angles of 65.7 (8) and 73.4 (8)°, respectively, with the benzene and phenyl rings and also in molecule B, indole ring system make the dihedral angles of 62.2 (7) and 72.1 (7)°, respectively, with the benzene and phenyl rings.

The S–O, S–C, and S–N distances are 1.421 (1), 1.755 (2) and 1.673 (1) Å, respectively and these values are comparable as observed in similar structures (Chakkaravarthi *et al.*, 2010). As a result of the electron-withdrawing character of the phenylsulfonyl groups, the N–Csp^2 bond lengths, *viz*. N1–C1 [1.414 (2) Å], N1′–C1′ [1.415 (2) Å], N1–C8 [1.416 (2) Å] and N1′–C8′ [1.417 (2) Å], are longer than the mean value of 1.355 (1)Å reported for N atoms with planar configurations (Allen *et al.*, 1987). In both the molecules,the S atom exhibits significant deviation from that of a regular tetrahedron, with the largest deviations being seen for the O–S–O [O1–S1–O2 119.5 (9)° & O1′–S1′–O2′ 119.7 (8)°] and O–S–N angles [O1–S1–N1 105.1 (7)° & O1′–S1′–N1′ 104.8 (7)°]. The widening of the angles may be due to repulsive interactions between the two short S=O bonds, similar to what is observed in related structures (Kavitha *et al.*, 2010).

S2. Experimental

To a solution of *N*-(2-Formylphenyl)benzenesulfonamide (0.5 g, 1.91 mmol) in dry CH_3CN (20 ml), K_2CO_3 (0.8 g, 5.79 mmol), phenacylbromides (0.45 g, 2.26 mmol) were added. The reaction mixture was stirred at room temperature for 6 h under N_2 atmosphere. The solvent was removed and the residue was quenched with ice-water (50 ml), extracted with chloroform (3 *x* 10 ml) and dried (Na_2SO_4). Removal of solvent followed by the residue was dissolved in CH_3CN (20 ml), Conc.HCl (3 ml) was added. The reaction mixture was then refluxed for 2 h. It was then poured over ice-water (50 ml), extracted with $CHCl_3$ (3 *x* 10 ml) and dried (Na_2SO_4). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a solution of the title compound in methanol at room temperature.

S3. Refinement

All H atoms were fixed geometrically and allowed to ride on their parent C atoms, with C—H distances fixed in the range 0.93–0.97 Å with U_{iso}(H) = 1.5U_{eq}(C) for methyl H 1.2U_{eq}(C) for other H atoms.

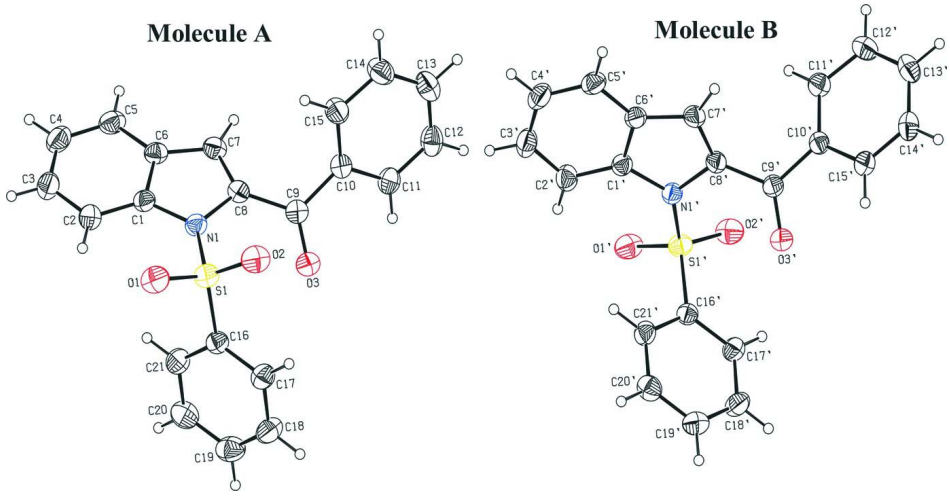

Figure 1

The two crystallographically unique molecules. Displacement ellipsoids are drawn at the 30% probability level.

Phenyl(1-phenylsulfonyl-1*H*-indol-2-yl)methanone

Crystal data

$C_{21}H_{15}NO_3S$
M_r = 361.40
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 9.3291 (6) Å
b = 11.1498 (7) Å
c = 17.8134 (10) Å
α = 89.433 (3)°
β = 81.623 (2)°
γ = 71.993 (3)°
V = 1742.13 (18) Å^3

Z = 4
F(000) = 752
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8730 reflections
θ = 1.2–28.7°
μ = 0.21 mm^{-1}
T = 293 K
Block, white
0.25 × 0.22 × 0.19 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, 1996)
T_{min} = 0.981, T_{max} = 0.985

30464 measured reflections
8730 independent reflections
6363 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 28.7°, θ_{min} = 1.2°
h = −12→12
k = −14→14
l = −23→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.138
S = 0.99

8730 reflections
470 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
$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 0.1847P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.085 (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}
C1	1.12210 (18)	0.80297 (15)	0.33999 (9)	0.0466 (4)
C1′	1.04606 (17)	0.31674 (14)	0.15061 (8)	0.0427 (3)
C2′	1.1137 (2)	0.19223 (16)	0.16963 (10)	0.0549 (4)
H2′	1.0634	0.1321	0.1694	0.066*
C2	1.1947 (2)	0.67756 (17)	0.31637 (11)	0.0593 (4)
H2	1.1406	0.6201	0.3160	0.071*
C3	1.3500 (2)	0.6420 (2)	0.29356 (11)	0.0679 (5)
H3	1.4015	0.5585	0.2779	0.082*
C3′	1.2583 (2)	0.16248 (19)	0.18871 (10)	0.0620 (5)
H3′	1.3061	0.0802	0.2016	0.074*
C4′	1.3354 (2)	0.25122 (19)	0.18944 (10)	0.0630 (5)
H4′	1.4333	0.2271	0.2022	0.076*
C4	1.4318 (2)	0.7265 (2)	0.29317 (12)	0.0701 (6)
H4	1.5367	0.6987	0.2777	0.084*
C5	1.3603 (2)	0.8508 (2)	0.31527 (11)	0.0621 (5)
H5	1.4157	0.9074	0.3146	0.074*
C5′	1.26861 (18)	0.37364 (18)	0.17157 (10)	0.0559 (4)
H5′	1.3200	0.4330	0.1720	0.067*
C6	1.20280 (18)	0.89080 (16)	0.33877 (9)	0.0486 (4)
C6′	1.12073 (17)	0.40739 (15)	0.15260 (9)	0.0454 (3)
C7	1.09697 (19)	1.00924 (16)	0.36680 (10)	0.0514 (4)
H7	1.1201	1.0840	0.3712	0.062*
C7′	1.02433 (17)	0.52315 (15)	0.12936 (9)	0.0475 (4)
H7′	1.0458	0.5993	0.1265	0.057*
C8′	0.89647 (17)	0.50409 (14)	0.11210 (9)	0.0429 (3)
C8	0.95772 (18)	0.99525 (15)	0.38603 (9)	0.0461 (3)
C9′	0.78298 (17)	0.58882 (14)	0.06981 (9)	0.0439 (3)
C9	0.82428 (18)	1.08384 (16)	0.43345 (9)	0.0493 (4)
C10′	0.74687 (16)	0.72726 (14)	0.08203 (9)	0.0415 (3)

C10	0.79218 (18)	1.22132 (15)	0.42177 (9)	0.0468 (4)
C11	0.72410 (19)	1.30446 (17)	0.48355 (10)	0.0537 (4)
H11	0.7030	1.2735	0.5312	0.064*
C11′	0.74584 (19)	0.78266 (15)	0.15170 (9)	0.0493 (4)
H11′	0.7738	0.7326	0.1925	0.059*
C12′	0.7028 (2)	0.91320 (17)	0.16001 (11)	0.0586 (4)
H12′	0.6983	0.9508	0.2070	0.070*
C12	0.6877 (2)	1.43246 (18)	0.47447 (12)	0.0635 (5)
H12	0.6452	1.4878	0.5163	0.076*
C13	0.7142 (2)	1.47895 (18)	0.40350 (14)	0.0707 (5)
H13	0.6873	1.5656	0.3974	0.085*
C13′	0.6669 (2)	0.98698 (16)	0.09905 (12)	0.0595 (5)
H13′	0.6400	1.0743	0.1047	0.071*
C14′	0.67055 (19)	0.93190 (16)	0.02912 (11)	0.0556 (4)
H14′	0.6486	0.9820	−0.0124	0.067*
C14	0.7801 (3)	1.39750 (19)	0.34158 (13)	0.0721 (6)
H14	0.7972	1.4293	0.2938	0.087*
C15	0.8211 (2)	1.26808 (17)	0.35029 (10)	0.0593 (4)
H15	0.8676	1.2130	0.3087	0.071*
C15′	0.70660 (17)	0.80322 (15)	0.02128 (9)	0.0480 (4)
H15′	0.7041	0.7666	−0.0250	0.058*
C16	0.78168 (17)	0.77029 (15)	0.46542 (9)	0.0460 (3)
C16′	0.76892 (17)	0.26929 (14)	0.03053 (9)	0.0425 (3)
C17′	0.64230 (19)	0.31640 (17)	−0.00556 (10)	0.0525 (4)
H17′	0.5545	0.3754	0.0191	0.063*
C17	0.6358 (2)	0.81398 (18)	0.50410 (11)	0.0604 (4)
H17	0.5582	0.8697	0.4820	0.073*
C18′	0.6491 (2)	0.27381 (19)	−0.07907 (11)	0.0615 (5)
H18′	0.5651	0.3047	−0.1042	0.074*
C18	0.6068 (3)	0.7732 (2)	0.57678 (12)	0.0728 (6)
H18	0.5088	0.8018	0.6039	0.087*
C19	0.7221 (3)	0.6908 (2)	0.60898 (11)	0.0720 (6)
H19	0.7017	0.6646	0.6580	0.086*
C19′	0.7790 (2)	0.18625 (18)	−0.11532 (10)	0.0595 (4)
H19′	0.7826	0.1588	−0.1649	0.071*
C20	0.8674 (2)	0.64670 (19)	0.56934 (12)	0.0674 (5)
H20	0.9447	0.5904	0.5913	0.081*
C20′	0.9040 (2)	0.13900 (17)	−0.07847 (11)	0.0572 (4)
H20′	0.9913	0.0793	−0.1031	0.069*
C21′	0.89966 (18)	0.18017 (15)	−0.00517 (10)	0.0500 (4)
H21′	0.9835	0.1485	0.0200	0.060*
C21	0.8978 (2)	0.68629 (17)	0.49705 (10)	0.0559 (4)
H21	0.9955	0.6568	0.4697	0.067*
N1	0.96883 (15)	0.86837 (12)	0.36984 (7)	0.0467 (3)
N1′	0.90578 (14)	0.37628 (11)	0.12457 (7)	0.0426 (3)
O1′	0.80070 (16)	0.20614 (12)	0.16827 (7)	0.0645 (4)
O1	0.87435 (16)	0.70347 (13)	0.32343 (7)	0.0672 (4)
O2′	0.62388 (13)	0.41561 (13)	0.14936 (7)	0.0630 (3)

O2	0.69510 (15)	0.91680 (14)	0.35443 (8)	0.0673 (4)
O3	0.74722 (15)	1.04506 (12)	0.48283 (7)	0.0645 (3)
O3′	0.72679 (15)	0.54592 (11)	0.02333 (7)	0.0602 (3)
S1′	0.76114 (4)	0.31681 (4)	0.12514 (2)	0.04706 (13)
S1	0.81966 (5)	0.81457 (4)	0.37162 (2)	0.05089 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0480 (8)	0.0498 (8)	0.0411 (8)	−0.0155 (7)	−0.0035 (6)	0.0043 (7)
C1′	0.0429 (8)	0.0457 (8)	0.0392 (7)	−0.0125 (6)	−0.0073 (6)	0.0004 (6)
C2′	0.0607 (10)	0.0490 (9)	0.0533 (10)	−0.0134 (8)	−0.0115 (8)	0.0090 (7)
C2	0.0634 (11)	0.0521 (10)	0.0576 (10)	−0.0154 (8)	0.0006 (8)	−0.0032 (8)
C3	0.0633 (11)	0.0638 (11)	0.0618 (12)	−0.0044 (9)	0.0048 (9)	0.0003 (9)
C3′	0.0611 (11)	0.0620 (11)	0.0512 (10)	−0.0002 (9)	−0.0134 (8)	0.0085 (8)
C4′	0.0468 (9)	0.0795 (13)	0.0536 (10)	−0.0025 (9)	−0.0160 (8)	−0.0050 (9)
C4	0.0478 (10)	0.0844 (14)	0.0652 (12)	−0.0069 (10)	0.0018 (9)	0.0135 (11)
C5	0.0480 (9)	0.0751 (12)	0.0648 (11)	−0.0225 (9)	−0.0077 (8)	0.0190 (10)
C5′	0.0421 (8)	0.0696 (11)	0.0554 (10)	−0.0145 (8)	−0.0109 (7)	−0.0107 (8)
C6	0.0480 (8)	0.0543 (9)	0.0459 (8)	−0.0189 (7)	−0.0093 (7)	0.0106 (7)
C6′	0.0422 (8)	0.0493 (8)	0.0449 (8)	−0.0135 (7)	−0.0085 (6)	−0.0040 (7)
C7	0.0527 (9)	0.0491 (9)	0.0562 (10)	−0.0207 (7)	−0.0100 (7)	0.0083 (7)
C7′	0.0453 (8)	0.0435 (8)	0.0574 (9)	−0.0176 (7)	−0.0105 (7)	−0.0017 (7)
C8′	0.0432 (8)	0.0393 (7)	0.0479 (8)	−0.0146 (6)	−0.0084 (6)	0.0016 (6)
C8	0.0489 (8)	0.0442 (8)	0.0464 (8)	−0.0151 (7)	−0.0093 (7)	0.0042 (7)
C9′	0.0413 (8)	0.0439 (8)	0.0480 (8)	−0.0145 (6)	−0.0082 (6)	0.0016 (6)
C9	0.0495 (9)	0.0514 (9)	0.0483 (9)	−0.0169 (7)	−0.0092 (7)	0.0025 (7)
C10′	0.0366 (7)	0.0411 (7)	0.0469 (8)	−0.0125 (6)	−0.0054 (6)	0.0020 (6)
C10	0.0469 (8)	0.0469 (8)	0.0472 (9)	−0.0137 (7)	−0.0110 (7)	−0.0008 (7)
C11	0.0499 (9)	0.0575 (10)	0.0520 (9)	−0.0134 (8)	−0.0085 (7)	−0.0041 (8)
C11′	0.0521 (9)	0.0501 (9)	0.0459 (9)	−0.0169 (7)	−0.0061 (7)	0.0022 (7)
C12′	0.0617 (10)	0.0544 (10)	0.0585 (10)	−0.0194 (8)	−0.0012 (8)	−0.0122 (8)
C12	0.0565 (10)	0.0572 (11)	0.0749 (13)	−0.0128 (9)	−0.0129 (9)	−0.0175 (9)
C13	0.0742 (13)	0.0469 (10)	0.0918 (16)	−0.0160 (9)	−0.0213 (11)	0.0011 (10)
C13′	0.0523 (10)	0.0404 (8)	0.0825 (13)	−0.0135 (7)	−0.0015 (9)	0.0004 (9)
C14′	0.0475 (9)	0.0502 (9)	0.0667 (11)	−0.0122 (7)	−0.0084 (8)	0.0154 (8)
C14	0.0906 (15)	0.0569 (11)	0.0682 (12)	−0.0203 (10)	−0.0163 (11)	0.0143 (10)
C15	0.0727 (12)	0.0522 (10)	0.0505 (10)	−0.0154 (9)	−0.0103 (9)	0.0018 (8)
C15′	0.0441 (8)	0.0505 (9)	0.0480 (9)	−0.0125 (7)	−0.0075 (7)	0.0042 (7)
C16	0.0454 (8)	0.0494 (8)	0.0485 (9)	−0.0218 (7)	−0.0079 (7)	−0.0002 (7)
C16′	0.0414 (7)	0.0425 (8)	0.0492 (8)	−0.0202 (6)	−0.0090 (6)	0.0036 (6)
C17′	0.0431 (8)	0.0557 (9)	0.0591 (10)	−0.0130 (7)	−0.0135 (7)	−0.0017 (8)
C17	0.0479 (9)	0.0646 (11)	0.0661 (11)	−0.0161 (8)	−0.0030 (8)	0.0049 (9)
C18′	0.0569 (10)	0.0734 (12)	0.0590 (11)	−0.0206 (9)	−0.0234 (8)	0.0028 (9)
C18	0.0672 (12)	0.0823 (14)	0.0642 (12)	−0.0260 (11)	0.0116 (10)	−0.0008 (11)
C19	0.0952 (16)	0.0792 (14)	0.0492 (10)	−0.0406 (12)	−0.0055 (10)	0.0034 (10)
C19′	0.0677 (11)	0.0671 (11)	0.0502 (10)	−0.0294 (9)	−0.0108 (8)	−0.0017 (8)
C20	0.0764 (13)	0.0684 (12)	0.0638 (12)	−0.0252 (10)	−0.0255 (10)	0.0125 (10)

C20′	0.0509 (9)	0.0571 (10)	0.0606 (11)	−0.0166 (8)	0.0010 (8)	−0.0061 (8)
C21′	0.0417 (8)	0.0506 (9)	0.0590 (10)	−0.0143 (7)	−0.0116 (7)	0.0040 (7)
C21	0.0479 (9)	0.0632 (10)	0.0577 (10)	−0.0182 (8)	−0.0090 (8)	0.0008 (8)
N1	0.0466 (7)	0.0470 (7)	0.0483 (7)	−0.0194 (6)	−0.0016 (6)	−0.0014 (6)
N1′	0.0433 (7)	0.0406 (6)	0.0490 (7)	−0.0177 (5)	−0.0130 (5)	0.0048 (5)
O1′	0.0880 (9)	0.0694 (8)	0.0565 (7)	−0.0497 (7)	−0.0219 (7)	0.0190 (6)
O1	0.0812 (9)	0.0753 (9)	0.0569 (7)	−0.0428 (7)	−0.0059 (6)	−0.0125 (6)
O2′	0.0451 (6)	0.0798 (9)	0.0639 (8)	−0.0232 (6)	0.0018 (6)	−0.0145 (7)
O2	0.0564 (7)	0.0859 (9)	0.0659 (8)	−0.0249 (7)	−0.0245 (6)	0.0188 (7)
O3	0.0687 (8)	0.0578 (7)	0.0618 (8)	−0.0197 (6)	0.0071 (6)	0.0036 (6)
O3′	0.0687 (8)	0.0488 (7)	0.0688 (8)	−0.0171 (6)	−0.0303 (6)	−0.0006 (6)
S1′	0.0479 (2)	0.0545 (2)	0.0467 (2)	−0.02702 (18)	−0.00772 (17)	0.00296 (17)
S1	0.0513 (2)	0.0616 (3)	0.0474 (2)	−0.0268 (2)	−0.01145 (18)	0.00232 (19)

Geometric parameters (Å, º)

C1—C2	1.391 (2)	C12′—C13′	1.373 (3)
C1—C6	1.406 (2)	C12′—H12′	0.9300
C1—N1	1.414 (2)	C12—C13	1.379 (3)
C1′—C6′	1.397 (2)	C12—H12	0.9300
C1′—C2′	1.397 (2)	C13—C14	1.377 (3)
C1′—N1′	1.4150 (18)	C13—H13	0.9300
C2′—C3′	1.378 (3)	C13′—C14′	1.386 (3)
C2′—H2′	0.9300	C13′—H13′	0.9300
C2—C3	1.378 (3)	C14′—C15′	1.372 (2)
C2—H2	0.9300	C14′—H14′	0.9300
C3—C4	1.383 (3)	C14—C15	1.387 (3)
C3—H3	0.9300	C14—H14	0.9300
C3′—C4′	1.393 (3)	C15—H15	0.9300
C3′—H3′	0.9300	C15′—H15′	0.9300
C4′—C5′	1.370 (3)	C16—C17	1.374 (2)
C4′—H4′	0.9300	C16—C21	1.381 (2)
C4—C5	1.372 (3)	C16—S1	1.7551 (16)
C4—H4	0.9300	C16′—C17′	1.384 (2)
C5—C6	1.398 (2)	C16′—C21′	1.384 (2)
C5—H5	0.9300	C16′—S1′	1.7563 (16)
C5′—C6′	1.404 (2)	C17′—C18′	1.383 (3)
C5′—H5′	0.9300	C17′—H17′	0.9300
C6—C7	1.425 (2)	C17—C18	1.385 (3)
C6′—C7′	1.423 (2)	C17—H17	0.9300
C7—C8	1.350 (2)	C18′—C19′	1.375 (3)
C7—H7	0.9300	C18′—H18′	0.9300
C7′—C8′	1.352 (2)	C18—C19	1.374 (3)
C7′—H7′	0.9300	C18—H18	0.9300
C8′—N1′	1.4179 (18)	C19—C20	1.376 (3)
C8′—C9′	1.477 (2)	C19—H19	0.9300
C8—N1	1.416 (2)	C19′—C20′	1.380 (3)
C8—C9	1.479 (2)	C19′—H19′	0.9300

C9′—O3′	1.2158 (19)	C20—C21	1.376 (3)
C9′—C10′	1.486 (2)	C20—H20	0.9300
C9—O3	1.216 (2)	C20′—C21′	1.379 (3)
C9—C10	1.487 (2)	C20′—H20′	0.9300
C10′—C11′	1.389 (2)	C21′—H21′	0.9300
C10′—C15′	1.390 (2)	C21—H21	0.9300
C10—C11	1.388 (2)	N1—S1	1.6734 (13)
C10—C15	1.393 (2)	N1′—S1′	1.6761 (12)
C11—C12	1.375 (2)	O1′—S1′	1.4254 (12)
C11—H11	0.9300	O1—S1	1.4264 (14)
C11′—C12′	1.388 (2)	O2′—S1′	1.4197 (13)
C11′—H11′	0.9300	O2—S1	1.4217 (13)
C2—C1—C6	121.55 (16)	C14—C13—C12	120.26 (18)
C2—C1—N1	131.80 (16)	C14—C13—H13	119.9
C6—C1—N1	106.64 (14)	C12—C13—H13	119.9
C6′—C1′—C2′	121.26 (14)	C12′—C13′—C14′	120.30 (16)
C6′—C1′—N1′	107.10 (13)	C12′—C13′—H13′	119.8
C2′—C1′—N1′	131.59 (14)	C14′—C13′—H13′	119.8
C3′—C2′—C1′	117.05 (17)	C15′—C14′—C13′	119.78 (16)
C3′—C2′—H2′	121.5	C15′—C14′—H14′	120.1
C1′—C2′—H2′	121.5	C13′—C14′—H14′	120.1
C3—C2—C1	117.18 (19)	C13—C14—C15	120.16 (19)
C3—C2—H2	121.4	C13—C14—H14	119.9
C1—C2—H2	121.4	C15—C14—H14	119.9
C2—C3—C4	122.13 (19)	C14—C15—C10	119.49 (18)
C2—C3—H3	118.9	C14—C15—H15	120.3
C4—C3—H3	118.9	C10—C15—H15	120.3
C2′—C3′—C4′	122.34 (17)	C14′—C15′—C10′	120.45 (16)
C2′—C3′—H3′	118.8	C14′—C15′—H15′	119.8
C4′—C3′—H3′	118.8	C10′—C15′—H15′	119.8
C5′—C4′—C3′	120.69 (16)	C17—C16—C21	121.50 (16)
C5′—C4′—H4′	119.7	C17—C16—S1	119.44 (13)
C3′—C4′—H4′	119.7	C21—C16—S1	118.96 (13)
C5—C4—C3	120.89 (18)	C17′—C16′—C21′	121.27 (15)
C5—C4—H4	119.6	C17′—C16′—S1′	119.65 (13)
C3—C4—H4	119.6	C21′—C16′—S1′	118.99 (12)
C4—C5—C6	118.82 (18)	C18′—C17′—C16′	118.61 (16)
C4—C5—H5	120.6	C18′—C17′—H17′	120.7
C6—C5—H5	120.6	C16′—C17′—H17′	120.7
C4′—C5′—C6′	118.42 (17)	C16—C17—C18	118.52 (18)
C4′—C5′—H5′	120.8	C16—C17—H17	120.7
C6′—C5′—H5′	120.8	C18—C17—H17	120.7
C5—C6—C1	119.41 (16)	C19′—C18′—C17′	120.57 (17)
C5—C6—C7	132.82 (17)	C19′—C18′—H18′	119.7
C1—C6—C7	107.72 (14)	C17′—C18′—H18′	119.7
C1′—C6′—C5′	120.22 (15)	C19—C18—C17	120.33 (19)
C1′—C6′—C7′	107.86 (13)	C19—C18—H18	119.8

C5′—C6′—C7′	131.83 (16)	C17—C18—H18	119.8
C8—C7—C6	108.95 (15)	C18—C19—C20	120.59 (18)
C8—C7—H7	125.5	C18—C19—H19	119.7
C6—C7—H7	125.5	C20—C19—H19	119.7
C8′—C7′—C6′	108.73 (14)	C18′—C19′—C20′	120.29 (17)
C8′—C7′—H7′	125.6	C18′—C19′—H19′	119.9
C6′—C7′—H7′	125.6	C20′—C19′—H19′	119.9
C7′—C8′—N1′	108.63 (13)	C21—C20—C19	119.68 (18)
C7′—C8′—C9′	126.66 (14)	C21—C20—H20	120.2
N1′—C8′—C9′	123.14 (13)	C19—C20—H20	120.2
C7—C8—N1	108.47 (14)	C21′—C20′—C19′	120.09 (17)
C7—C8—C9	126.76 (15)	C21′—C20′—H20′	120.0
N1—C8—C9	123.09 (14)	C19′—C20′—H20′	120.0
O3′—C9′—C8′	120.50 (14)	C20′—C21′—C16′	119.15 (15)
O3′—C9′—C10′	121.06 (14)	C20′—C21′—H21′	120.4
C8′—C9′—C10′	118.33 (13)	C16′—C21′—H21′	120.4
O3—C9—C8	120.57 (15)	C20—C21—C16	119.37 (17)
O3—C9—C10	121.10 (15)	C20—C21—H21	120.3
C8—C9—C10	118.26 (14)	C16—C21—H21	120.3
C11′—C10′—C15′	119.57 (14)	C1—N1—C8	108.21 (13)
C11′—C10′—C9′	122.77 (14)	C1—N1—S1	126.37 (11)
C15′—C10′—C9′	117.61 (14)	C8—N1—S1	124.59 (11)
C11—C10—C15	119.75 (16)	C1′—N1′—C8′	107.66 (12)
C11—C10—C9	118.40 (15)	C1′—N1′—S1′	126.32 (10)
C15—C10—C9	121.76 (15)	C8′—N1′—S1′	124.95 (10)
C12—C11—C10	120.12 (17)	O2′—S1′—O1′	119.73 (8)
C12—C11—H11	119.9	O2′—S1′—N1′	107.50 (7)
C10—C11—H11	119.9	O1′—S1′—N1′	104.83 (7)
C12′—C11′—C10′	119.56 (16)	O2′—S1′—C16′	110.44 (8)
C12′—C11′—H11′	120.2	O1′—S1′—C16′	107.87 (8)
C10′—C11′—H11′	120.2	N1′—S1′—C16′	105.46 (7)
C13′—C12′—C11′	120.25 (18)	O2—S1—O1	119.56 (9)
C13′—C12′—H12′	119.9	O2—S1—N1	107.30 (7)
C11′—C12′—H12′	119.9	O1—S1—N1	105.18 (7)
C11—C12—C13	120.17 (18)	O2—S1—C16	110.09 (8)
C11—C12—H12	119.9	O1—S1—C16	108.48 (8)
C13—C12—H12	119.9	N1—S1—C16	105.20 (7)

C6′—C1′—C2′—C3′	−1.4 (2)	C13′—C14′—C15′—C10′	−3.2 (2)
N1′—C1′—C2′—C3′	175.84 (16)	C11′—C10′—C15′—C14′	2.0 (2)
C6—C1—C2—C3	1.7 (3)	C9′—C10′—C15′—C14′	179.39 (14)
N1—C1—C2—C3	−176.50 (17)	C21′—C16′—C17′—C18′	−0.8 (2)
C1—C2—C3—C4	−0.6 (3)	S1′—C16′—C17′—C18′	−177.48 (14)
C1′—C2′—C3′—C4′	0.1 (3)	C21—C16—C17—C18	0.8 (3)
C2′—C3′—C4′—C5′	0.6 (3)	S1—C16—C17—C18	177.02 (16)
C2—C3—C4—C5	−0.5 (3)	C16′—C17′—C18′—C19′	0.2 (3)
C3—C4—C5—C6	0.4 (3)	C16—C17—C18—C19	−0.1 (3)
C3′—C4′—C5′—C6′	0.1 (3)	C17—C18—C19—C20	−0.6 (3)

C4—C5—C6—C1	0.7 (3)	C17′—C18′—C19′—C20′	0.5 (3)
C4—C5—C6—C7	177.74 (18)	C18—C19—C20—C21	0.5 (3)
C2—C1—C6—C5	−1.8 (2)	C18′—C19′—C20′—C21′	−0.5 (3)
N1—C1—C6—C5	176.81 (15)	C19′—C20′—C21′—C16′	−0.2 (3)
C2—C1—C6—C7	−179.50 (16)	C17′—C16′—C21′—C20′	0.8 (2)
N1—C1—C6—C7	−0.91 (17)	S1′—C16′—C21′—C20′	177.51 (13)
C2′—C1′—C6′—C5′	2.1 (2)	C19—C20—C21—C16	0.2 (3)
N1′—C1′—C6′—C5′	−175.76 (14)	C17—C16—C21—C20	−0.9 (3)
C2′—C1′—C6′—C7′	179.13 (15)	S1—C16—C21—C20	−177.14 (14)
N1′—C1′—C6′—C7′	1.29 (17)	C2—C1—N1—C8	178.72 (17)
C4′—C5′—C6′—C1′	−1.4 (2)	C6—C1—N1—C8	0.33 (17)
C4′—C5′—C6′—C7′	−177.59 (17)	C2—C1—N1—S1	−11.4 (3)
C5—C6—C7—C8	−176.10 (18)	C6—C1—N1—S1	170.23 (11)
C1—C6—C7—C8	1.19 (19)	C7—C8—N1—C1	0.41 (18)
C1′—C6′—C7′—C8′	−1.27 (18)	C9—C8—N1—C1	−165.74 (14)
C5′—C6′—C7′—C8′	175.31 (17)	C7—C8—N1—S1	−169.71 (12)
C6′—C7′—C8′—N1′	0.73 (18)	C9—C8—N1—S1	24.1 (2)
C6′—C7′—C8′—C9′	−165.23 (15)	C6′—C1′—N1′—C8′	−0.86 (16)
C6—C7—C8—N1	−0.98 (18)	C2′—C1′—N1′—C8′	−178.39 (16)
C6—C7—C8—C9	164.52 (15)	C6′—C1′—N1′—S1′	−169.40 (11)
C7′—C8′—C9′—O3′	139.58 (18)	C2′—C1′—N1′—S1′	13.1 (2)
N1′—C8′—C9′—O3′	−24.5 (2)	C7′—C8′—N1′—C1′	0.08 (17)
C7′—C8′—C9′—C10′	−36.7 (2)	C9′—C8′—N1′—C1′	166.64 (14)
N1′—C8′—C9′—C10′	159.25 (14)	C7′—C8′—N1′—S1′	168.82 (12)
C7—C8—C9—O3	−135.37 (19)	C9′—C8′—N1′—S1′	−24.6 (2)
N1—C8—C9—O3	28.2 (2)	C1′—N1′—S1′—O2′	137.76 (13)
C7—C8—C9—C10	41.5 (2)	C8′—N1′—S1′—O2′	−28.89 (15)
N1—C8—C9—C10	−154.98 (15)	C1′—N1′—S1′—O1′	9.35 (15)
O3′—C9′—C10′—C11′	149.60 (16)	C8′—N1′—S1′—O1′	−157.30 (13)
C8′—C9′—C10′—C11′	−34.2 (2)	C1′—N1′—S1′—C16′	−104.39 (13)
O3′—C9′—C10′—C15′	−27.7 (2)	C8′—N1′—S1′—C16′	88.95 (14)
C8′—C9′—C10′—C15′	148.56 (14)	C17′—C16′—S1′—O2′	−8.10 (15)
O3—C9—C10—C11	27.8 (2)	C21′—C16′—S1′—O2′	175.18 (12)
C8—C9—C10—C11	−148.99 (15)	C17′—C16′—S1′—O1′	124.45 (13)
O3—C9—C10—C15	−148.71 (18)	C21′—C16′—S1′—O1′	−52.28 (14)
C8—C9—C10—C15	34.5 (2)	C17′—C16′—S1′—N1′	−123.95 (13)
C15—C10—C11—C12	−1.1 (3)	C21′—C16′—S1′—N1′	59.33 (13)
C9—C10—C11—C12	−177.72 (16)	C1—N1—S1—O2	−140.16 (13)
C15′—C10′—C11′—C12′	0.8 (2)	C8—N1—S1—O2	28.17 (15)
C9′—C10′—C11′—C12′	−176.44 (15)	C1—N1—S1—O1	−11.85 (15)
C10′—C11′—C12′—C13′	−2.4 (3)	C8—N1—S1—O1	156.48 (13)
C10—C11—C12—C13	2.1 (3)	C1—N1—S1—C16	102.62 (14)
C11—C12—C13—C14	−1.4 (3)	C8—N1—S1—C16	−89.06 (14)
C11′—C12′—C13′—C14′	1.2 (3)	C17—C16—S1—O2	13.85 (17)
C12′—C13′—C14′—C15′	1.6 (3)	C21—C16—S1—O2	−169.87 (14)
C12—C13—C14—C15	−0.4 (3)	C17—C16—S1—O1	−118.69 (15)
C13—C14—C15—C10	1.4 (3)	C21—C16—S1—O1	57.58 (15)
C11—C10—C15—C14	−0.6 (3)	C17—C16—S1—N1	129.16 (15)

C9—C10—C15—C14	175.87 (18)	C21—C16—S1—N1	−54.56 (15)