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# Crystal structure of (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)(phenyl)methanone

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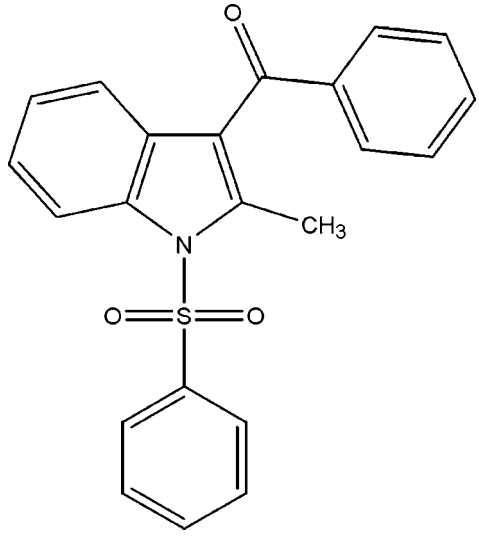
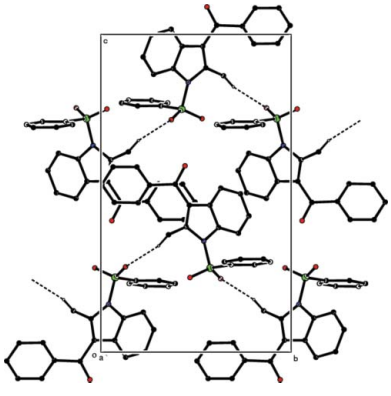
In the title compound, $C_{22}H_{17}NO_3S$, the sulfonyl-bound phenyl ring is almost orthogonal to the indole ring system, making a dihedral angle of 84.89 (7)°. The carbonyl-bound phenyl ring forms a dihedral angle of 57.32 (5)° with the indole ring system. The two phenyl rings are inclined at 52.68 (7)°. The S atom has a distorted tetrahedral configuration. In the crystal, weak C—H···O interactions link the molecules, forming a helical chain along the *b*-axis direction.

## 1. Chemical context

In a continuation of our studies on indole derivatives, which possess various biological activities such as antihepatitis B virus (Chai *et al.*, 2006) and antibacterial (Nieto *et al.*, 2005) *etc*, we herein report the synthesis and the crystal structure of the title compound, (I).



## 2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The sulfonyl-bound phenyl ring (C1–C6) is almost orthogonal to the indole ring system (N1/C7–C14), making a dihedral angle of 84.89 (7)°. The carbonyl-bound phenyl ring (C17–C22) forms a dihedral angle of 57.32 (5)° with the indole ring system. The two phenyl rings are inclined at an angle of 52.68 (7)°. Atom S1 has a distorted tetrahedral configuration

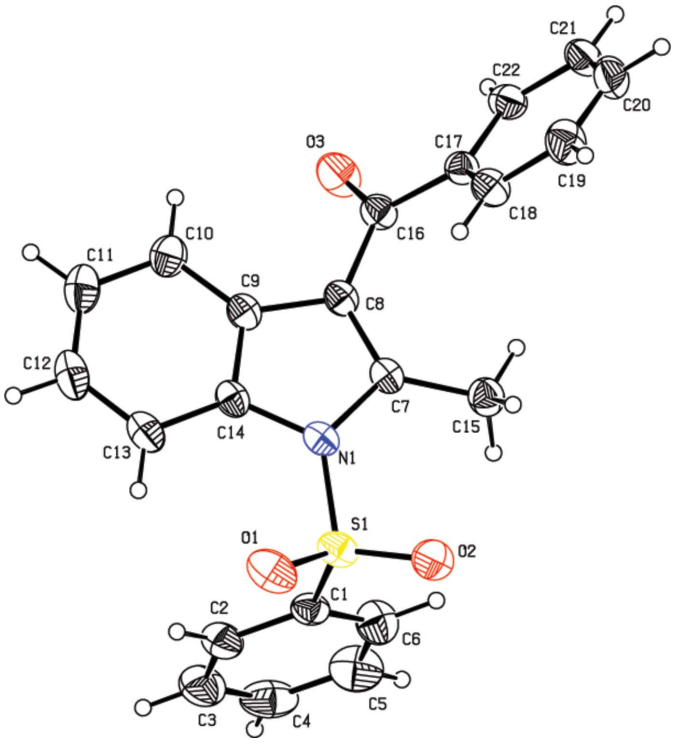



**Figure 1**
The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

with angles O1—S1—O2 [119.97 (10)°] and N1—S1—C1 [104.99 (8)°] differing from the ideal tetrahedral value. As a result of the electron-withdrawing character of the phenylsulfonyl group, the bond lengths N1—C7 [1.420 (2) Å] and N1—C14 [1.419 (2) Å] are longer than the mean value of 1.355 (14) Å (Allen *et al.*, 1987). The geometric parameters of (I) agree well with those in similar reported structures (Chakkaravarthi *et al.*, 2008, 2009).

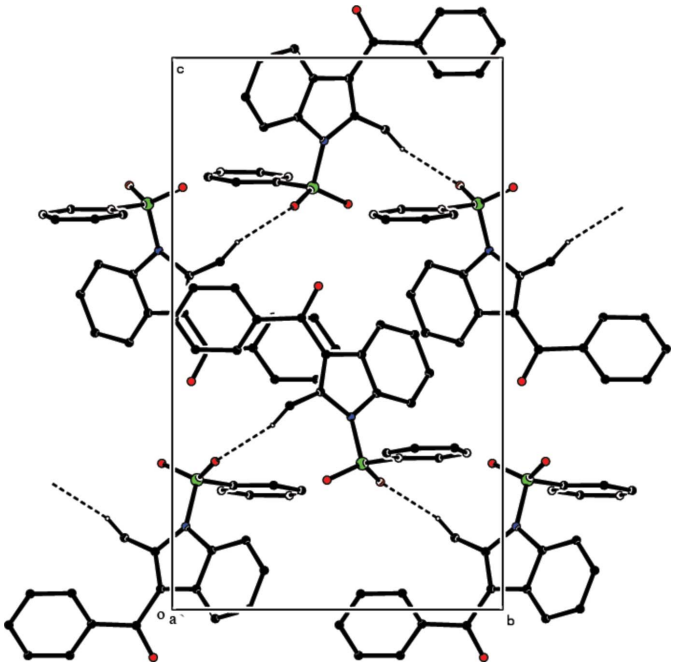



**Figure 2**
The packing diagram of the title compound, viewed down the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C15—H15$C$···O1$^{i}$ | 0.96 | 2.59 | 3.525 (3) | 165 |

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

## 3. Supramolecular features

In the crystal, weak C—H···O interactions link the molecules, forming a helical chain along the *b*-axis direction (Table 1 and Fig. 2). No significant $\pi$–$\pi$ or C—H···$\pi$ interactions are observed.

## 4. Database survey

A search of the Cambridge Structural Database (Version 5.35, last update May 2014; Groom & Allen, 2014). indicated 123 compounds having a phenylsulfonyl-1*H*-indole moiety. Of these compounds, several similar structures have been

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{22}H_{17}NO_3S$ |
| $M_r$ | 375.43 |
| Crystal system, space group | Orthorhombic, $P2_12_12_1$ |
| Temperature (K) | 295 |
| $a, b, c$ (Å) | 8.9989 (7), 11.0036 (9), 18.4209 (16) |
| $V$ (Å$^3$) | 1824.0 (3) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.20 |
| Crystal size (mm) | 0.28 × 0.24 × 0.20 |
| | |
| Data collection | |
| Diffractometer | Bruker APEXII CCD |
| Absorption correction | Multi-scan (*SADABS*; Sheldrick, 1996) |
| $T_{min}$, $T_{max}$ | 0.946, 0.961 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 26244, 5020, 3493 |
| $R_{int}$ | 0.034 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.708 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.036, 0.091, 1.02 |
| No. of reflections | 5020 |
| No. of parameters | 246 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.17, −0.25 |
| Absolute structure | Flack (1983), 2109 Friedel pairs |
| Absolute structure parameter | −0.01 (7) |

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

reported earlier, *i.e.* ethyl 2-acetoxymethyl-1-phenylsulfonyl-1*H*-indole-3-carboxylate (Gunasekaran *et al.*, 2009), 3-iodo-2-methyl-1-phenylsulfonyl-1*H*-indole (Ramathilagam *et al.*, 2011) and 1-(2-bromomethyl-1-phenylsulfonyl-1*H*-indol-3-yl)propan-1-one (Umadevi *et al.*, 2013). In these structures, the sulfonyl-bound phenyl ring is almost orthogonal to the indole ring system, the dihedral angles of 83.35 (5), 82.84 (9) and 89.91 (11)°, respectively, being are comparable with that in the title compound.

## 5. Synthesis and crystallization

To a solution of benzoyl chloride (1.55 g, 11.07 mmol) in dry DCM (25 ml), $SnCl_4$ (2.88 g, 10.10 mmol) at 273 K was added dropwise. To this, phenylsulfonyl-1*H*-indole (2 g, 7.38 mmol) in dry DCM (10 ml) was added dropwise (5 min) and stirred for 30 min at the same temperature. After completion of the reaction (monitored by TLC), it was poured over ice–water (50 ml) and extracted with saturated aqueous $NaHCO_3$ (2 × 30 ml) and brine (2 × 30 ml), dried ($Na_2SO_4$) and concentrated under reduced pressure. Then, the crude product was crystallized from methanol to afford single crystals of the title compound suitable for X-ray diffraction.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms for $C_{aromatic}$ and $C_{methyl}$ were positioned geometrically and refined using a riding model, with C—H = 0.93 and 0.97 Å, respectively with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H atoms and 1.2$U_{eq}$(C) for other H atoms.

## Acknowledgements

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# supporting information

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# Crystal structure of (2-methyl-1-phenylsulfonyl-1*H*-indol-3-yl)(phenyl)-methanone

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## Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); 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* (Sheldrick, 2008).

### (2-Methyl-1-phenylsulfonyl-1*H*-indol-3-yl)(phenyl)methanone

*Crystal data*

$C_{22}H_{17}NO_3S$
$M_r$ = 375.43
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a$ = 8.9989 (7) Å
$b$ = 11.0036 (9) Å
$c$ = 18.4209 (16) Å
$V$ = 1824.0 (3) Å$^3$
$Z$ = 4
$F(000)$ = 784
$D_x$ = 1.367 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 812 reflections
$\theta$ = 2.2–30.2°
$\mu$ = 0.20 mm$^{-1}$
$T$ = 295 K
Block, colourless
0.28 × 0.24 × 0.20 mm

*Data collection*

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.946, $T_{max}$ = 0.961
26244 measured reflections
5020 independent reflections
3493 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.034
$\theta_{max}$ = 30.2°, $\theta_{min}$ = 2.2°
$h$ = −12→12
$k$ = −14→14
$l$ = −25→24

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.091
$S$ = 1.02
5020 reflections
246 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
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.2764P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.25 e Å$^{-3}$

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0039 (8)

Absolute structure: Flack (1983), 2109 Friedel pairs
Absolute structure parameter: −0.01 (7)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.2369 (2) | 0.81475 (17) | 0.72517 (9) | 0.0469 (4) |
| C2 | 0.2009 (3) | 0.69315 (19) | 0.72539 (12) | 0.0623 (6) |
| H2 | 0.1029 | 0.6684 | 0.7318 | 0.075* |
| C3 | 0.3119 (4) | 0.6089 (2) | 0.71605 (14) | 0.0779 (8) |
| H3 | 0.2891 | 0.5265 | 0.7160 | 0.093* |
| C4 | 0.4552 (4) | 0.6457 (3) | 0.70682 (13) | 0.0797 (8) |
| H4 | 0.5295 | 0.5881 | 0.6999 | 0.096* |
| C5 | 0.4904 (3) | 0.7661 (3) | 0.70759 (15) | 0.0815 (8) |
| H5 | 0.5889 | 0.7903 | 0.7025 | 0.098* |
| C6 | 0.3812 (3) | 0.8512 (2) | 0.71586 (13) | 0.0658 (6) |
| H6 | 0.4047 | 0.9335 | 0.7152 | 0.079* |
| C7 | 0.1037 (2) | 1.05176 (15) | 0.60528 (9) | 0.0405 (4) |
| C8 | 0.0471 (2) | 1.03514 (16) | 0.53755 (10) | 0.0417 (4) |
| C9 | −0.0431 (2) | 0.92698 (17) | 0.53745 (10) | 0.0421 (4) |
| C10 | −0.1247 (2) | 0.86956 (18) | 0.48385 (12) | 0.0566 (5) |
| H10 | −0.1258 | 0.8998 | 0.4367 | 0.068* |
| C11 | −0.2046 (3) | 0.7663 (2) | 0.50152 (15) | 0.0667 (6) |
| H11 | −0.2593 | 0.7266 | 0.4659 | 0.080* |
| C12 | −0.2040 (3) | 0.72186 (19) | 0.57128 (15) | 0.0651 (6) |
| H12 | −0.2588 | 0.6524 | 0.5819 | 0.078* |
| C13 | −0.1248 (2) | 0.77715 (17) | 0.62583 (13) | 0.0549 (5) |
| H13 | −0.1251 | 0.7466 | 0.6729 | 0.066* |
| C14 | −0.0439 (2) | 0.88084 (16) | 0.60774 (11) | 0.0429 (4) |
| C15 | 0.2119 (2) | 1.14443 (19) | 0.63034 (11) | 0.0521 (5) |
| H15A | 0.2445 | 1.1921 | 0.5897 | 0.078* |
| H15B | 0.2959 | 1.1047 | 0.6520 | 0.078* |
| H15C | 0.1654 | 1.1964 | 0.6655 | 0.078* |
| C16 | 0.0714 (2) | 1.10898 (16) | 0.47141 (10) | 0.0462 (4) |
| C17 | 0.0621 (2) | 1.24405 (16) | 0.47428 (10) | 0.0425 (4) |
| C18 | −0.0098 (2) | 1.30428 (18) | 0.52995 (12) | 0.0513 (5) |
| H18 | −0.0503 | 1.2605 | 0.5683 | 0.062* |
| C19 | −0.0215 (3) | 1.4297 (2) | 0.52874 (14) | 0.0667 (6) |

| | | | | |
|---|---|---|---|---|
| H19 | −0.0699 | 1.4700 | 0.5663 | 0.080* |
| C20 | 0.0380 (3) | 1.4945 (2) | 0.47233 (15) | 0.0684 (7) |
| H20 | 0.0296 | 1.5787 | 0.4716 | 0.082* |
| C21 | 0.1096 (3) | 1.4360 (2) | 0.41704 (13) | 0.0633 (6) |
| H21 | 0.1511 | 1.4805 | 0.3792 | 0.076* |
| C22 | 0.1204 (2) | 1.31043 (19) | 0.41723 (11) | 0.0512 (5) |
| H22 | 0.1671 | 1.2707 | 0.3789 | 0.061* |
| N1 | 0.04557 (17) | 0.95902 (13) | 0.65071 (8) | 0.0436 (4) |
| O1 | −0.02677 (18) | 0.87038 (14) | 0.76860 (8) | 0.0700 (4) |
| O2 | 0.16072 (19) | 1.03169 (12) | 0.76515 (8) | 0.0632 (4) |
| O3 | 0.0922 (2) | 1.05764 (13) | 0.41366 (7) | 0.0699 (4) |
| S1 | 0.09803 (6) | 0.92484 (4) | 0.73525 (3) | 0.04934 (14) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0585 (12) | 0.0484 (10) | 0.0339 (9) | 0.0054 (9) | 0.0015 (9) | 0.0024 (9) |
| C2 | 0.0712 (14) | 0.0513 (12) | 0.0644 (14) | 0.0075 (11) | −0.0075 (12) | 0.0094 (11) |
| C3 | 0.103 (2) | 0.0516 (14) | 0.0789 (17) | 0.0201 (14) | −0.0139 (16) | −0.0001 (12) |
| C4 | 0.098 (2) | 0.0856 (19) | 0.0556 (14) | 0.0464 (17) | −0.0027 (14) | −0.0015 (13) |
| C5 | 0.0655 (17) | 0.095 (2) | 0.0836 (19) | 0.0196 (15) | 0.0100 (14) | 0.0062 (16) |
| C6 | 0.0626 (14) | 0.0606 (13) | 0.0743 (15) | 0.0054 (12) | 0.0048 (12) | −0.0017 (11) |
| C7 | 0.0405 (9) | 0.0364 (9) | 0.0448 (9) | 0.0027 (8) | 0.0077 (8) | 0.0009 (7) |
| C8 | 0.0453 (10) | 0.0362 (9) | 0.0436 (10) | 0.0040 (8) | 0.0065 (8) | −0.0015 (8) |
| C9 | 0.0441 (9) | 0.0346 (9) | 0.0476 (10) | 0.0067 (8) | 0.0068 (8) | −0.0029 (8) |
| C10 | 0.0608 (13) | 0.0529 (11) | 0.0560 (12) | −0.0004 (11) | 0.0006 (11) | −0.0103 (10) |
| C11 | 0.0660 (15) | 0.0526 (13) | 0.0813 (16) | −0.0068 (11) | 0.0007 (13) | −0.0177 (12) |
| C12 | 0.0555 (14) | 0.0402 (11) | 0.0995 (19) | −0.0051 (10) | 0.0087 (13) | −0.0040 (12) |
| C13 | 0.0497 (12) | 0.0417 (10) | 0.0732 (13) | 0.0019 (10) | 0.0084 (11) | 0.0106 (10) |
| C14 | 0.0395 (9) | 0.0350 (9) | 0.0541 (11) | 0.0043 (8) | 0.0071 (8) | 0.0014 (8) |
| C15 | 0.0556 (12) | 0.0503 (11) | 0.0505 (11) | −0.0049 (10) | 0.0045 (10) | 0.0007 (9) |
| C16 | 0.0526 (12) | 0.0440 (10) | 0.0422 (10) | 0.0019 (9) | 0.0055 (9) | 0.0012 (8) |
| C17 | 0.0403 (10) | 0.0430 (10) | 0.0443 (10) | −0.0004 (8) | −0.0011 (8) | 0.0036 (8) |
| C18 | 0.0530 (12) | 0.0469 (11) | 0.0539 (12) | 0.0055 (9) | 0.0062 (10) | 0.0011 (10) |
| C19 | 0.0682 (14) | 0.0498 (12) | 0.0821 (16) | 0.0095 (12) | −0.0013 (13) | −0.0096 (13) |
| C20 | 0.0693 (15) | 0.0408 (11) | 0.095 (2) | −0.0042 (11) | −0.0175 (15) | 0.0054 (13) |
| C21 | 0.0614 (13) | 0.0547 (12) | 0.0736 (14) | −0.0124 (12) | −0.0097 (12) | 0.0233 (12) |
| C22 | 0.0468 (11) | 0.0554 (12) | 0.0512 (11) | −0.0008 (10) | −0.0007 (9) | 0.0098 (9) |
| N1 | 0.0454 (9) | 0.0403 (8) | 0.0452 (8) | 0.0020 (7) | 0.0056 (7) | 0.0064 (7) |
| O1 | 0.0734 (10) | 0.0768 (10) | 0.0599 (9) | 0.0050 (8) | 0.0309 (8) | 0.0169 (8) |
| O2 | 0.0924 (11) | 0.0505 (8) | 0.0466 (8) | 0.0073 (7) | 0.0019 (8) | −0.0101 (7) |
| O3 | 0.1119 (13) | 0.0526 (8) | 0.0453 (8) | 0.0015 (10) | 0.0186 (9) | −0.0054 (7) |
| S1 | 0.0614 (3) | 0.0477 (3) | 0.0389 (2) | 0.0074 (2) | 0.0117 (2) | 0.0022 (2) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.369 (3) | C12—H12 | 0.9300 |
| C1—C2 | 1.377 (3) | C13—C14 | 1.394 (3) |

| | | | |
|---|---|---|---|
| C1—S1 | 1.750 (2) | C13—H13 | 0.9300 |
| C2—C3 | 1.373 (3) | C14—N1 | 1.419 (2) |
| C2—H2 | 0.9300 | C15—H15A | 0.9600 |
| C3—C4 | 1.362 (4) | C15—H15B | 0.9600 |
| C3—H3 | 0.9300 | C15—H15C | 0.9600 |
| C4—C5 | 1.363 (4) | C16—O3 | 1.219 (2) |
| C4—H4 | 0.9300 | C16—C17 | 1.490 (3) |
| C5—C6 | 1.366 (3) | C17—C18 | 1.382 (3) |
| C5—H5 | 0.9300 | C17—C22 | 1.383 (3) |
| C6—H6 | 0.9300 | C18—C19 | 1.384 (3) |
| C7—C8 | 1.360 (2) | C18—H18 | 0.9300 |
| C7—N1 | 1.420 (2) | C19—C20 | 1.369 (3) |
| C7—C15 | 1.483 (3) | C19—H19 | 0.9300 |
| C8—C9 | 1.441 (3) | C20—C21 | 1.366 (3) |
| C8—C16 | 1.481 (2) | C20—H20 | 0.9300 |
| C9—C10 | 1.383 (3) | C21—C22 | 1.385 (3) |
| C9—C14 | 1.391 (3) | C21—H21 | 0.9300 |
| C10—C11 | 1.384 (3) | C22—H22 | 0.9300 |
| C10—H10 | 0.9300 | N1—S1 | 1.6701 (16) |
| C11—C12 | 1.375 (4) | O1—S1 | 1.4134 (15) |
| C11—H11 | 0.9300 | O2—S1 | 1.4156 (15) |
| C12—C13 | 1.374 (3) | | |

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| C6—C1—C2 | 120.5 (2) | C9—C14—C13 | 121.60 (19) |
| C6—C1—S1 | 119.18 (17) | C9—C14—N1 | 107.17 (16) |
| C2—C1—S1 | 120.28 (17) | C13—C14—N1 | 131.22 (19) |
| C3—C2—C1 | 119.0 (2) | C7—C15—H15A | 109.5 |
| C3—C2—H2 | 120.5 | C7—C15—H15B | 109.5 |
| C1—C2—H2 | 120.5 | H15A—C15—H15B | 109.5 |
| C4—C3—C2 | 120.3 (2) | C7—C15—H15C | 109.5 |
| C4—C3—H3 | 119.9 | H15A—C15—H15C | 109.5 |
| C2—C3—H3 | 119.9 | H15B—C15—H15C | 109.5 |
| C3—C4—C5 | 120.5 (3) | O3—C16—C8 | 119.11 (16) |
| C3—C4—H4 | 119.7 | O3—C16—C17 | 120.13 (17) |
| C5—C4—H4 | 119.7 | C8—C16—C17 | 120.66 (16) |
| C4—C5—C6 | 120.0 (3) | C18—C17—C22 | 119.23 (18) |
| C4—C5—H5 | 120.0 | C18—C17—C16 | 122.10 (17) |
| C6—C5—H5 | 120.0 | C22—C17—C16 | 118.58 (17) |
| C5—C6—C1 | 119.7 (2) | C17—C18—C19 | 120.1 (2) |
| C5—C6—H6 | 120.1 | C17—C18—H18 | 119.9 |
| C1—C6—H6 | 120.1 | C19—C18—H18 | 119.9 |
| C8—C7—N1 | 107.82 (15) | C20—C19—C18 | 120.1 (2) |
| C8—C7—C15 | 128.60 (16) | C20—C19—H19 | 120.0 |
| N1—C7—C15 | 123.54 (16) | C18—C19—H19 | 120.0 |
| C7—C8—C9 | 108.87 (16) | C21—C20—C19 | 120.3 (2) |
| C7—C8—C16 | 128.73 (17) | C21—C20—H20 | 119.8 |
| C9—C8—C16 | 122.38 (17) | C19—C20—H20 | 119.8 |
| C10—C9—C14 | 119.69 (18) | C20—C21—C22 | 120.1 (2) |

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| C10—C9—C8 | 132.63 (18) | C20—C21—H21 | 120.0 |
| C14—C9—C8 | 107.64 (17) | C22—C21—H21 | 120.0 |
| C9—C10—C11 | 118.9 (2) | C17—C22—C21 | 120.1 (2) |
| C9—C10—H10 | 120.6 | C17—C22—H22 | 119.9 |
| C11—C10—H10 | 120.6 | C21—C22—H22 | 119.9 |
| C12—C11—C10 | 120.6 (2) | C14—N1—C7 | 108.41 (14) |
| C12—C11—H11 | 119.7 | C14—N1—S1 | 122.94 (12) |
| C10—C11—H11 | 119.7 | C7—N1—S1 | 127.40 (13) |
| C13—C12—C11 | 121.9 (2) | O1—S1—O2 | 119.97 (10) |
| C13—C12—H12 | 119.1 | O1—S1—N1 | 106.03 (10) |
| C11—C12—H12 | 119.1 | O2—S1—N1 | 106.76 (8) |
| C12—C13—C14 | 117.3 (2) | O1—S1—C1 | 108.67 (10) |
| C12—C13—H13 | 121.4 | O2—S1—C1 | 109.36 (10) |
| C14—C13—H13 | 121.4 | N1—S1—C1 | 104.99 (8) |

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| C6—C1—C2—C3 | −0.1 (3) | C8—C16—C17—C18 | −19.3 (3) |
| S1—C1—C2—C3 | 178.83 (18) | O3—C16—C17—C22 | −19.3 (3) |
| C1—C2—C3—C4 | 0.1 (4) | C8—C16—C17—C22 | 164.22 (18) |
| C2—C3—C4—C5 | 0.8 (4) | C22—C17—C18—C19 | −0.6 (3) |
| C3—C4—C5—C6 | −1.6 (4) | C16—C17—C18—C19 | −177.1 (2) |
| C4—C5—C6—C1 | 1.6 (4) | C17—C18—C19—C20 | 0.0 (3) |
| C2—C1—C6—C5 | −0.8 (3) | C18—C19—C20—C21 | −0.2 (4) |
| S1—C1—C6—C5 | −179.70 (19) | C19—C20—C21—C22 | 1.0 (4) |
| N1—C7—C8—C9 | −2.92 (19) | C18—C17—C22—C21 | 1.4 (3) |
| C15—C7—C8—C9 | 174.62 (18) | C16—C17—C22—C21 | 178.01 (19) |
| N1—C7—C8—C16 | 178.71 (17) | C20—C21—C22—C17 | −1.6 (3) |
| C15—C7—C8—C16 | −3.8 (3) | C9—C14—N1—C7 | −1.39 (19) |
| C7—C8—C9—C10 | −179.9 (2) | C13—C14—N1—C7 | 179.84 (19) |
| C16—C8—C9—C10 | −1.4 (3) | C9—C14—N1—S1 | −169.49 (12) |
| C7—C8—C9—C14 | 2.1 (2) | C13—C14—N1—S1 | 11.7 (3) |
| C16—C8—C9—C14 | −179.42 (16) | C8—C7—N1—C14 | 2.70 (19) |
| C14—C9—C10—C11 | −0.5 (3) | C15—C7—N1—C14 | −174.99 (17) |
| C8—C9—C10—C11 | −178.31 (19) | C8—C7—N1—S1 | 170.12 (13) |
| C9—C10—C11—C12 | 0.5 (3) | C15—C7—N1—S1 | −7.6 (2) |
| C10—C11—C12—C13 | −0.1 (4) | C14—N1—S1—O1 | −40.28 (16) |
| C11—C12—C13—C14 | −0.1 (3) | C7—N1—S1—O1 | 153.97 (15) |
| C10—C9—C14—C13 | 0.2 (3) | C14—N1—S1—O2 | −169.29 (14) |
| C8—C9—C14—C13 | 178.55 (17) | C7—N1—S1—O2 | 24.96 (17) |
| C10—C9—C14—N1 | −178.67 (16) | C14—N1—S1—C1 | 74.67 (16) |
| C8—C9—C14—N1 | −0.37 (19) | C7—N1—S1—C1 | −91.08 (16) |
| C12—C13—C14—C9 | 0.1 (3) | C6—C1—S1—O1 | −159.68 (17) |
| C12—C13—C14—N1 | 178.71 (19) | C2—C1—S1—O1 | 21.40 (19) |
| C7—C8—C16—O3 | 137.3 (2) | C6—C1—S1—O2 | −27.02 (19) |
| C9—C8—C16—O3 | −40.9 (3) | C2—C1—S1—O2 | 154.07 (17) |
| C7—C8—C16—C17 | −46.2 (3) | C6—C1—S1—N1 | 87.22 (18) |
| C9—C8—C16—C17 | 135.63 (18) | C2—C1—S1—N1 | −91.69 (17) |
| O3—C16—C17—C18 | 157.2 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C15—H15*C*···O1$^{i}$ | 0.96 | 2.59 | 3.525 (3) | 165 |

Symmetry code: (i) −*x*, *y*+1/2, −*z*+3/2.